

The **Weyl representation** expresses an operator $A(R, P)$ as a superposition of **displacement operators**

9 Apr 14
CINA

$$A(R, P) = \int \frac{d\sigma d\tau}{(2\pi\hbar)^{3N}} e^{i(\sigma \cdot R + \tau \cdot P)/\hbar} \alpha(\sigma, \tau) ;$$

I've defined this expansion in such a way that α has the same units as A .

To find the "expansion coefficients" α , we evaluate

$$\text{Tr} [e^{-i(\bar{\sigma} \cdot R + \bar{\tau} \cdot P)/\hbar} A] = \int \frac{d\sigma d\tau}{(2\pi\hbar)^{3N}} \alpha(\sigma, \tau)$$

$$\times \text{Tr} [e^{i(\sigma \cdot R + \tau \cdot P)/\hbar} e^{-i(\bar{\sigma} \cdot R + \bar{\tau} \cdot P)/\hbar}]$$

$$\int d\tau e^{i(\sigma - \bar{\sigma}) \cdot \tau / \hbar} \langle r | e^{i\tau \cdot P / \hbar} e^{-i\bar{\tau} \cdot P / \hbar} | r \rangle e^{\frac{i}{2\hbar} (\sigma \cdot \tau - \bar{\sigma} \cdot \bar{\tau})}$$

$$\langle r + \tau - \bar{\tau} | r \rangle = \delta(\tau - \bar{\tau})$$

$$\Rightarrow = (2\pi\hbar)^{3N} \delta(\sigma - \bar{\sigma}) \delta(\tau - \bar{\tau})$$

$$= \alpha(\bar{\sigma}, \bar{\tau})$$

$$\text{Tr} [e^{i(\sigma \cdot R + \tau \cdot P)/\hbar} e^{-i(\bar{\sigma} \cdot R + \bar{\tau} \cdot P)/\hbar}] = (2\pi\hbar)^{3N} \delta(\sigma - \bar{\sigma}) \delta(\tau - \bar{\tau})$$

$$\alpha(\sigma, \tau) = \text{Tr} [e^{-i(\sigma \cdot R + \tau \cdot P)/\hbar} A(R, P)]$$

Position matrix elements

(2)

$$\begin{aligned} \langle r | A | \bar{r} \rangle &= \int \frac{d\sigma d\tau}{(2\pi\hbar)^{3N}} e^{i\sigma \cdot r / \hbar} \langle r + \tau | \bar{r} \rangle e^{i\sigma \cdot \tau / 2\hbar} \alpha(\sigma, \tau) \\ &= \frac{1}{(2\pi\hbar)^{3N}} \int d\sigma e^{i\sigma \cdot r / \hbar} \underbrace{\langle r + \tau | \bar{r} \rangle}_{\delta(\tau - \bar{r} + r)} e^{i\sigma \cdot (\bar{r} - \tau) / 2\hbar} \alpha(\sigma, \bar{r} - r) \end{aligned}$$

$$\langle r | A | \bar{r} \rangle = \frac{1}{(2\pi\hbar)^{3N}} \int d\sigma e^{i\sigma \cdot (r + \bar{r}) / 2\hbar} \alpha(\sigma, \bar{r} - r)$$

The Wigner equivalent of $A(R, P)$ is defined as

$$\begin{aligned} A_w(r, p) &= \int d\tau e^{ip \cdot \tau / \hbar} \langle r - \tau/2 | A(R, P) | r + \tau/2 \rangle \\ &= \int d\tau e^{ip \cdot \tau / \hbar} \frac{1}{(2\pi\hbar)^{3N}} \int d\sigma e^{i\sigma \cdot r / \hbar} \alpha(\sigma, \tau) \end{aligned}$$

$$A_w(r, p) = \int \frac{d\sigma d\tau}{(2\pi\hbar)^{3N}} e^{i(\sigma \cdot r + \tau \cdot p) / \hbar} \alpha(\sigma, \tau)$$

Thus, we obtain $A_w(r, p)$ by replacing (R, P) with (r, p) in the Weyl expansion of A .

In order to obtain the Weyl components of a product, we must evaluate

$$\alpha\beta(\sigma, \tau) = \text{Tr} \left[e^{-i[\sigma \cdot R + \tau \cdot P] / \hbar} AB \right]$$

$$= \int \frac{d\bar{\sigma} d\bar{\tau}}{(2\pi\hbar)^{3N}} \int \frac{d\bar{\sigma} d\bar{\tau}}{(2\pi\hbar)^{3N}} \alpha(\bar{\sigma}, \bar{\tau}) \beta(\bar{\sigma}, \bar{\tau})$$

$$\rightarrow \text{Tr} \left[e^{-i(\bar{\sigma} \cdot R + \bar{\tau} \cdot P) / \hbar} e^{i(\sigma \cdot R + \tau \cdot P) / \hbar} e^{i(\bar{\sigma} \cdot R + \bar{\tau} \cdot P) / \hbar} \right]$$

$$e^{-i(\sigma \cdot R + \tau \cdot P)/\hbar} \quad e^{i(\bar{\sigma} \cdot R + \bar{\tau} \cdot P)/\hbar} \quad e^{i(\bar{\sigma} \cdot R + \bar{\tau} \cdot P)/\hbar}$$

$$= e^{-i\sigma \cdot R/\hbar} e^{-i\tau \cdot P/\hbar} e^{\frac{i}{2\hbar} \sigma \cdot \tau} e^{i\bar{\sigma} \cdot R/\hbar} e^{i\bar{\tau} \cdot P/\hbar} e^{\frac{i}{2\hbar} \bar{\sigma} \cdot \bar{\tau}}$$

$$\rightarrow \times e^{i\bar{\tau} \cdot P/\hbar} e^{i\bar{\sigma} \cdot R/\hbar} e^{-\frac{i}{2\hbar} \bar{\tau} \cdot \bar{\sigma}}$$

$$= e^{\frac{i}{2\hbar} (\sigma \cdot \tau + \bar{\sigma} \cdot \bar{\tau} - \bar{\tau} \cdot \bar{\sigma})} e^{-\frac{i}{\hbar} \sigma \cdot R} e^{\frac{i}{\hbar} (\bar{\tau} + \bar{\tau} - \tau) \cdot P}$$

$$\rightarrow \times e^{\frac{i}{\hbar} \bar{\sigma} \cdot (e^{-\frac{i}{\hbar} (\bar{\tau} + \bar{\tau}) \cdot P} R e^{\frac{i}{\hbar} (\bar{\tau} + \bar{\tau}) \cdot P})} e^{\frac{i}{\hbar} \bar{\sigma} \cdot R}$$

$R - \bar{\tau} - \bar{\tau}$

$$= e^{\frac{i}{2\hbar} (\sigma \cdot \tau + \bar{\sigma} \cdot \bar{\tau} - \bar{\sigma} \cdot \bar{\tau})} e^{-\frac{i}{\hbar} \sigma \cdot R} e^{\frac{i}{\hbar} (\bar{\tau} + \bar{\tau} - \tau) \cdot P}$$

$$\rightarrow \times e^{\frac{i}{\hbar} \bar{\sigma} \cdot (R - \bar{\tau} - \bar{\tau})} e^{\frac{i}{\hbar} \bar{\sigma} \cdot R}$$

$$= e^{\frac{i}{2\hbar} (\sigma \cdot \tau - \bar{\sigma} \cdot \bar{\tau} - \bar{\sigma} \cdot \bar{\tau})} e^{-\frac{i}{\hbar} \sigma \cdot \bar{\tau}}$$

$$\rightarrow \times e^{-\frac{i}{\hbar} \sigma \cdot R} e^{\frac{i}{\hbar} (\bar{\tau} + \bar{\tau} - \tau) \cdot P} e^{\frac{i}{\hbar} (\bar{\sigma} + \bar{\sigma}) \cdot R}$$

Substituting on p. (2) leads to

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$$\alpha\beta(\sigma, \tau) = \int \frac{d\bar{\sigma} d\bar{\tau}}{(2\pi\hbar)^{3N}} \int \frac{d\bar{\sigma} d\bar{\tau}}{(2\pi\hbar)^{3N}} \alpha(\bar{\sigma}, \bar{\tau}) \beta(\bar{\sigma}, \bar{\tau})$$

$$\rightarrow \times e^{\frac{i}{2\hbar}(\sigma \cdot \tau - \bar{\sigma} \cdot \bar{\tau} - \bar{\sigma} \cdot \bar{\tau})} e^{-\frac{i}{\hbar} \bar{\sigma} \cdot \bar{\tau}}$$

$$\rightarrow \times \int d\bar{\tau} e^{\frac{i}{\hbar}(\bar{\sigma} + \bar{\sigma} - \sigma) \cdot \bar{\tau}} \delta(\tau - \bar{\tau} - \bar{\tau})$$

$$\alpha\beta(\sigma, \tau) = \int \frac{d\bar{\sigma} d\bar{\tau}}{(2\pi\hbar)^{3N}} \alpha(\bar{\sigma}, \bar{\tau}) \beta(\sigma - \bar{\sigma}, \tau - \bar{\tau}) e^{\frac{i}{2\hbar}(\sigma \cdot \bar{\tau} - \bar{\sigma} \cdot \tau)}$$

OK, agrees w/ [6 Apr 14]

Imte et al. don't state this pretty result. Does someone else???

For the Wigner equivalent of AB, we get

$$(AB)_W(\tau, p) = \int \frac{d\bar{\sigma} d\bar{\tau}}{(2\pi\hbar)^{3N}} \int \frac{d\sigma d\tau}{(2\pi\hbar)^{3N}} e^{i[\sigma \cdot \tau + \tau \cdot p]/\hbar} e^{\frac{i}{2\hbar}(\sigma \cdot \bar{\tau} - \bar{\sigma} \cdot \tau)}$$

$$\rightarrow \times \alpha(\bar{\sigma}, \bar{\tau}) \beta(\sigma - \bar{\sigma}, \tau - \bar{\tau}) .$$

Let $\bar{\sigma} = \sigma - \bar{\sigma} \quad ; \quad \bar{\tau} = \tau - \bar{\tau} \quad (\Rightarrow \quad \sigma = \bar{\sigma} + \bar{\sigma} \quad ; \quad \tau = \bar{\tau} + \bar{\tau})$
 $d\bar{\sigma} = d\sigma \quad ; \quad d\bar{\tau} = d\tau .$

$$(AB)_w(r, p) = \int \frac{d\bar{\sigma}}{(2\pi\hbar)^{3N}} \frac{d\bar{\tau}}{(2\pi\hbar)^{3N}} e^{\frac{i}{\hbar} [\bar{\sigma} \cdot r + \bar{\tau} \cdot p]} \alpha(\bar{\sigma}, \bar{\tau})$$

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$$\times e^{\frac{i}{\hbar} [\bar{\sigma} \cdot r + \bar{\tau} \cdot p]} \beta(\bar{\sigma}, \bar{\tau}) e^{\frac{i}{2\hbar} [\bar{\tau} \cdot \bar{\sigma} - \bar{\sigma} \cdot \bar{\tau}]}$$

$$(AB)_w(r, p) = A_w(r, p) e^{\frac{\hbar\Lambda}{2i}} B_w(r, p),$$

where $\Lambda = \overleftarrow{\nabla}_p \cdot \overrightarrow{\nabla}_r - \overleftarrow{\nabla}_r \cdot \overrightarrow{\nabla}_p$ is the Poisson-bracket operator.

According to Imre and co-workers (1967), this expression is due to Groenwold (1946). It's used by Kapral & Cicchetti (1999) to obtain an \hbar -expansion for the partial Wigner transform of a product, and their analysis is in turn the basis for Petit and Subotnik's 2014 surface-hopping treatment of linear absorption.