Kubo inner product [nln32]

General properties of inner products:

- $\langle A|B\rangle = \langle B|A\rangle^*$,
- $\langle A|A\rangle = ||A||^2 \geq 0$,
- $\langle A|\lambda B\rangle = \lambda\langle A|B\rangle$,
- $\langle A|B{+}C\rangle = \langle A|B\rangle{+}\langle A|C\rangle$.

Kubo inner product for quantum system:[1]

$$\langle A|B\rangle \doteq \frac{1}{\beta}\int_0^\beta d\lambda\,\langle e^{\lambda\mathcal{H}}A^\dagger e^{-\lambda\mathcal{H}}B\rangle,$$

where

$$\langle A\rangle = \frac{1}{Z}\mathrm{Tr}\{e^{-\beta\mathcal{H}}A\}, \qquad Z = \mathrm{Tr}\{e^{-\beta\mathrm{H}}\}, \qquad \beta = \frac{1}{k_BT}.$$

Alternative inner product for quantum systems:[2]

$$\langle A|B\rangle \doteq \frac{1}{2}\langle A^\dagger B + BA^\dagger\rangle.$$

Both inner products have the same classical limit:[3]

$$\langle A|B\rangle \doteq \frac{1}{Z}\int d^nq\,d^np\,e^{-\beta\mathcal{H}(q,p)}A(q,p)B(q,p).$$

Inner products of [nln31] employ...

▷ quantum Liouville operator: $L = \frac{1}{\hbar}[\mathcal{H},\ ]$,

Heisenberg equation of motion: $\frac{dA}{dt} = \frac{\imath}{\hbar}[\mathcal{H},A] = \imath LA$.

▷ classical Liouville operator: $L = \imath\{\mathcal{H},\ \} = \imath\sum_{j=1}^{n}\left(\frac{\partial\mathcal{H}}{\partial q_j}\frac{\partial}{\partial p_j} - \frac{\partial\mathcal{H}}{\partial p_j}\frac{\partial}{\partial q_j}\right)$,

Hamilton's equation of motion: $\frac{dA}{dt} = -\{\mathcal{H},A\} = \imath LA$

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[1] Designed to satisfy classical fluctuation-dissipation theorem in [nln39].

[2] Designed to satisfy quantum fluctuation-dissipation theorem in [nln39].

[3] Option for all inner products: subtract $\langle A^\dagger\rangle\langle B\rangle$.