

For any operator A (e.g., Hamiltonian H or partial derivative operator ∂_θ), the quantum expectation reads:

$$\begin{aligned}
\langle A \rangle &:= \frac{\langle \psi | A | \psi \rangle}{\langle \psi | \psi \rangle} \\
&= \frac{\sum_s \langle \psi | s \rangle \langle s | A | \psi \rangle}{\langle \psi | \psi \rangle} && \text{(insert complete basis)} \\
&= \frac{\sum_s \langle \psi | s \rangle \langle s | \psi \rangle \langle s | A | \psi \rangle}{\langle \psi | \psi \rangle \langle s | \psi \rangle} && \text{(multiply and divide by } \langle s | \psi \rangle \text{)} \\
&= \sum_s \frac{|\langle s | \psi \rangle|^2}{\langle \psi | \psi \rangle} \times \frac{\langle s | A | \psi \rangle}{\langle s | \psi \rangle} \\
&=: \sum_s p(s) A_{\text{loc}(s)} && \text{(Born probability)}
\end{aligned}$$

This recasts the quantum expectation as a classical average over Born probability $p(s)$ with local estimator $A_{\text{loc}}(s) := \frac{\langle s | A | \psi \rangle}{\langle s | \psi \rangle}$.

If $\langle s | \psi \rangle = 0$ for certain configuration s , local estimator diverges:

$$\underbrace{p(s)}_0 \times \underbrace{A_{\text{loc}(s)}}_\infty = \underbrace{\frac{\langle \psi | s \rangle \langle s | A | \psi \rangle}{\langle \psi | \psi \rangle}}_{\text{finite}}$$

The product remains finite, but MC sampling cannot handle this: we would need to sample an infinite value with zero probability. This arises from dividing by $\langle s | \psi \rangle = 0$ in the derivation above, making standard MC biased.