Expectation Values from the Hamilton-Jacobi Equation

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I use the classical Hamilton-Jacobi Equation to formulate a definition for operator expectation values consistent with those for quantum operators.

In "Wavefunctions and the Hamilton-Jacobi Equation," I showed that performing a canonical change of variables from (q_i, p_i) to constants (Q_i, P_i):

$$p_i \dot{q}_i - H(q,p,t) = P_i \dot{Q}_i - K(Q,P,t) + \frac{dF}{dt} \tag{1}$$

for $F = S(q,P,t) - P_i Q_i$, gave:

$$H = -\frac{\partial S}{\partial t} \quad p_i = \frac{\partial S}{\partial q_i} \quad Q_i = \frac{\partial S}{\partial P_i}. \tag{2}$$

when $K = 0$. Here $\frac{dS}{dt} = L$ and the function $e^{i\frac{S}{\hbar}}$ had the property that ordinary multiplication by the value of H or p_j was equivalent to acting with a differential operator:

$$\begin{aligned} H \cdot e^{i\frac{S}{\hbar}} &= -\tfrac{\partial S}{\partial t} e^{i\frac{S}{\hbar}} = i\hbar \partial_t e^{i\frac{S}{\hbar}} \\ p_j \cdot e^{i\frac{S}{\hbar}} &= \tfrac{\partial S}{\partial q_j} e^{i\frac{S}{\hbar}} = \tfrac{\hbar}{i}\partial_{q_j} e^{i\frac{S}{\hbar}}. \end{aligned} \tag{3}$$

In that paper, I went on to study how classical equations differ by a term of order $\hbar$. Here, I will focus on the one-dimensional case and instead look at a new definition for the expectation value of an operator:

$$\langle \hat{\mathcal{O}} \rangle \equiv \frac{\int \mathbb{P}(P) \mathrm{d}P \mathrm{d}q \left\{ e^{-i\frac{S(q,P,t)}{\hbar}} \hat{\mathcal{O}} e^{i\frac{S(q,P,t)}{\hbar}} \right\}}{\int \mathrm{d}q} \tag{4}$$

where $\mathbb{P}(P)$ is a normalized, real probability distribution over the classical constant P, S is real, and $\hat{\mathcal{O}}$ is a hermitian operator found by promoting the classical function $\mathcal{O}(q,p)$ to $\mathcal{O}(q, \frac{\hbar}{i}\partial_q)$.

I. QUADRATIC TERMS

Since S is defined so that $p = \frac{\partial S}{\partial q}$, one finds that:

$$\begin{aligned} \langle \hat{p}^2 \rangle &= \frac{\int \mathbb{P}(P)\mathrm{d}P\mathrm{d}q \left\{ e^{-i\frac{S(q,P,t)}{\hbar}} (\frac{\hbar}{i}\frac{\partial}{\partial q})^2 e^{i\frac{S(q,P,t)}{\hbar}} \right\}}{\int \mathrm{d}q} \\ &= \frac{\int \mathbb{P}(P)\mathrm{d}P\mathrm{d}q \frac{\hbar}{i}\frac{\partial}{\partial q} \left\{ e^{-i\frac{S(q,P,t)}{\hbar}} \frac{\hbar}{i}\frac{\partial}{\partial q} i^{\frac{S(q,P,t)}{\hbar}} \right\}}{\int \mathrm{d}q} \\ &\quad - \frac{(\frac{\hbar}{i}\frac{\partial}{\partial q} e^{-i\frac{S(q,P,t)}{\hbar}})(\frac{\hbar}{i}\frac{\partial}{\partial q} e^{i\frac{S(q,P,t)}{\hbar}})}{\int \mathbb{P}(P)\mathrm{d}P\mathrm{d}q} \\ &= \frac{-\frac{\hbar}{i}\int \mathbb{P}(P)\mathrm{d}P \frac{\partial S(q,P,t)}{\partial q}\Big|_{q=-\infty}^{q=+\infty}}{\int \mathrm{d}q} \\ &\quad + \frac{\int \mathbb{P}(P)\mathrm{d}P\mathrm{d}q (\frac{\partial S(q,P,t)}{\partial q})^2}{\int \mathrm{d}q} \end{aligned} \tag{5}$$

Under certain conditions for S, the boundary term can cancel or vanish. The suppression by $\int \mathrm{d}q$ in the denominator, however, can eliminate this term even for finite $\frac{\partial S}{\partial q}$, when the range of q is taken to infinity. The result is that $\langle \hat{p}^2 \rangle = \langle p^2 \rangle$. At any time, the operator expectation value for $\hat{p}^2$, as defined in Equation 4, is equal to the classical spatial average of the momentum squared for particles distributed with probability $\mathbb{P}(P)$ over classical orbits with constant P.

Higher powers of $\hat{p}$ will give similar boundary terms when integrated by parts, so that $\langle \hat{p}^n \rangle = \langle p^n \rangle$. Products of $\hat{p}$ with q include extra terms. For instance:

$$\begin{aligned} \langle q\hat{p} - \hat{p}q \rangle &= \frac{\int \mathbb{P}(P)\mathrm{d}P\mathrm{d}q \left\{ e^{-i\frac{S(q,P,t)}{\hbar}} (q\frac{\hbar}{i}\frac{\partial}{\partial q} - \frac{\hbar}{i}\frac{\partial}{\partial q} q) e^{i\frac{S(q,P,t)}{\hbar}} \right\}}{\int \mathrm{d}q} \\ &= \frac{\int \mathbb{P}(P)\mathrm{d}P\mathrm{d}q \left\{ e^{-i\frac{S(q,P,t)}{\hbar}} (q\frac{\hbar}{i}\frac{\partial}{\partial q} - \frac{\hbar}{i} - q\frac{\hbar}{i}\frac{\partial}{\partial q}) e^{i\frac{S(q,P,t)}{\hbar}} \right\}}{\int \mathrm{d}q} \\ &= i\hbar \end{aligned} \tag{6}$$

which agrees with the quantum commutation relation $[\hat{q}, \hat{p}] = i\hbar$ for the position and momentum operators.

II. HERMITICITY REQUIREMENT

A classical observable which does not depend explicitly on time can be described as a function of position and momentum: $\mathcal{O}(q,p) = \mathcal{O}(q, \frac{\partial S}{\partial q})$. The exponentials on either side of $\hat{\mathcal{O}}$ in Equation 4 allow one to replace $\frac{\partial S}{\partial q}$ in $\mathcal{O}$ with a partial derivative $\frac{\hbar}{i}\frac{\partial}{\partial q}$ on either the left or the right.

The differential operator $\hat{\mathcal{O}}$ must be Hermitian to be consistent, i.e. the expectation value of the operator $\frac{1}{2}(q^n \hat{p}^m + \hat{p}^m q^n)$ needs both terms to agree with the classical $\langle q^n p^m \rangle$. Consider $\hat{\mathcal{O}} = -\hbar^2[f(q)\frac{\partial^2}{\partial q^2} + \frac{\partial^2}{\partial q^2} f(q)]$:

$$
\begin{aligned}
\langle\hat{\mathcal{O}}\rangle &= \frac{-\hbar^2\int\mathbb{P}(P)\mathrm{d}P\mathrm{d}q\Big\{e^{-i\frac{S(q,P,t)}{\hbar}}[f(q)\frac{\partial^2}{\partial q^2}+\frac{\partial^2}{\partial q^2}f(q)]e^{i\frac{S(q,P,t)}{\hbar}}\Big\}}{\int\mathrm{d}q}\\
&= \frac{\hbar^2\int\mathbb{P}(P)\mathrm{d}P\mathrm{d}q\Big\{\frac{\partial}{\partial q}[e^{-i\frac{S(q,P,t)}{\hbar}}f(q)]\frac{\partial}{\partial q}e^{i\frac{S(q,P,t)}{\hbar}}\Big\}}{\int\mathrm{d}q}\\
&+\frac{\hbar^2\int\mathbb{P}(P)\mathrm{d}P\mathrm{d}q\Big\{\frac{\partial}{\partial q}e^{-i\frac{S(q,P,t)}{\hbar}}\frac{\partial}{\partial q}[f(q)e^{i\frac{S(q,P,t)}{\hbar}}]\Big\}}{\int\mathrm{d}q}\\
&= \frac{\int\mathbb{P}(P)\mathrm{d}P\mathrm{d}q\Big\{(\frac{\partial S(q,P,t)}{\partial q})^2f(q)+i\hbar\frac{\partial S(q,P,t)}{\partial q}f'(q)\Big\}}{\int\mathrm{d}q}\\
&+\frac{\int\mathbb{P}(P)\mathrm{d}P\mathrm{d}q\Big\{(\frac{\partial S(q,P,t)}{\partial q})^2f(q)-i\hbar\frac{\partial S(q,P,t)}{\partial q}f'(q)\Big\}}{\int\mathrm{d}q}\\
&= \langle 2f(q)(\frac{\partial S(q,P,t)}{\partial q})^2\rangle
\end{aligned}
\tag{7}
$$

where the symmetry of $\hat{\mathcal{O}}$ led to the cancellation of terms depending on $f'(q)$.

III. POISSON BRACKET TO COMMUTATOR

One often considers the promotion of a poisson bracket (when there are no constraints) to a quantum commutator as a rule of thumb. In the context of the expectation values considered here, one sees that this association comes in two steps: first, the canonical commutation relations allowed me to construct the classical function $S(q,P,t)$; second, the expectation value defined in Equation 4 allowed me to promote classical multiplication to a differential operator.

For functions that can be Taylor expanded in q and p:

$$
\begin{aligned}
\langle\{q^np^m,q^rp^s\}\rangle &= (ns-mr)\langle q^{n+r-1}p^{m+s-1}\rangle\\
&= \frac{-i}{4\hbar}\langle[q^n\hat{p}^m+\hat{p}^mq^n,q^r\hat{p}^s+\hat{p}^sq^r]\rangle
\end{aligned}
\tag{8}
$$

the expectation value of the Poisson bracket is proportional to the expectation value of the commutator of the associated Hermitian operators.

As a result, I can use the classical equations of motion to compute the time derivative of a classical operator:

$$\frac{d}{dt}\mathcal{O}(q,p)=\{\mathcal{O},H\} \tag{9}$$

and, from Equation 8, conclude that:

$$\frac{d}{dt}\langle\hat{\mathcal{O}}\rangle=\frac{-i}{\hbar}\langle[\hat{\mathcal{O}},\hat{H}]\rangle \tag{10}$$

since the time derivatives of the exponential factors cancel. Equation 10 is known as Ehrenfest's Theorem.

IV. COMPLEX PHASE VS. REAL EXPONENTIAL

Up until this point, the meaning of the constant $\hbar$ has been unspecified. Its units are required to be the same as Planck's constant. The definition of the phase factors was designed to make the results consistent with quantum mechanics. The $e^{i\frac{S(q,P,t)}{\hbar}}$ is reminiscent of $e^{-i\frac{Ht}{\hbar}}$. Note that the classical hamiltonian is given by $H=-\frac{\partial S}{\partial t}$.

One could opt to consider only real functions, as opposed to complex ones, by taking $\hbar\to -i\epsilon$. This changes $e^{i\frac{S(q,P,t)}{\hbar}}$ to $e^{-\frac{S(q,P,t)}{\epsilon}}$, which is reminiscent of Wick rotating the time dimension when computing path integrals.

While having $\hbar$ be real makes the expectation value look like it involves a unitary transformation of $\hat{\mathcal{O}}$, imaginary $\hbar$ gives something similar to a statistical mechanics partition function.