Wavefunctions and the Hamilton-Jacobi Equation

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(Dated: September 8, 2013)

I show how the differential equation governing a distribution over classical trajectories is consistent with the quantum Schrödinger Equation in the $\hbar \to 0$ limit.

In classical mechanics, a change of variables from (q_i, p_i) to (Q_i, P_i) produces equivalent equations of motion when:

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

for a new Hamiltonian K. Let $F = S(q,P,t) - P_i Q_i$, then:

$$p_i \dot{q}_i - H(q,p,t) = -\dot{P}_i Q_i - K + \frac{\partial S}{\partial t} + \frac{\partial S}{\partial q_i}\dot{q}_i + \frac{\partial S}{\partial P_i}\dot{P}_i. \tag{2}$$

Taking (q_i, P_i) as the independent variables means Equation 2 is satisfied for:

$$H = K - \frac{\partial S}{\partial t} \quad p_i = \frac{\partial S}{\partial q_i} \quad Q_i = \frac{\partial S}{\partial P_i}. \tag{3}$$

If $K = 0$, then Q_i and P_i are constants and $H = -\frac{\partial S}{\partial t}$, known as the Hamilton-Jacobi Equation. Here

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \frac{\partial S}{\partial q_i}\dot{q}_i = p_i \dot{q}_i - H = L \tag{4}$$

showing that $S(q,P,t)$ can be thought of as an action. The only dynamic variables are q_i and t. P_i and $Q_i = \frac{\partial S}{\partial P_i}$ are the $2N$ constants needed to specify the trajectory of a classical particle. To solve for the trajectory of a particle using the Hamilton-Jacobi Equation, $S(q,P,t)$ is found and then the constants $Q_i = \frac{\partial S}{\partial P_i}$ provide implicit expressions for $q_i(t)$.

Now consider $e^{i\frac{S}{\hbar}}$, where the constant $\hbar$ makes the phase dimensionless:

$$\begin{aligned} H \cdot e^{i\frac{S}{\hbar}} &= -\tfrac{\partial S}{\partial t} e^{i\frac{S}{\hbar}} = i\hbar \partial_t e^{i\frac{S}{\hbar}} \\ p_j \cdot e^{i\frac{S}{\hbar}} &= \tfrac{\partial S}{\partial q_j} e^{i\frac{S}{\hbar}} = \tfrac{\hbar}{i}\partial_{q_j} e^{i\frac{S}{\hbar}}. \end{aligned} \tag{5}$$

Acting twice on $e^{i\frac{S}{\hbar}}$ with $\hat{p}_j = \frac{\hbar}{i}\partial_{q_j}$ introduces corrections of order $\mathcal{O}(\hbar)$ to the value of $p_j^2 \cdot e^{i\frac{S}{\hbar}}$:

$$\begin{aligned} \hat{p}_j^2 e^{i\frac{S}{\hbar}} = \left(\tfrac{\hbar}{i}\partial_{q_j}\right)^2 e^{i\frac{S}{\hbar}} &= \left[\left(\tfrac{\partial S}{\partial q_j}\right)^2 + \tfrac{\hbar}{i}\tfrac{\partial^2 S}{\partial q_j^2}\right] e^{i\frac{S}{\hbar}} \\ &= \left[p_j^2 + \tfrac{\hbar}{i}\left(\tfrac{\partial p_j}{\partial q_j}\right)_P\right] e^{i\frac{S}{\hbar}} \end{aligned} \tag{6}$$

where the partial derivative of the momentum p_j with respect to the coordinate q_j is non-zero since the transformed momenta P_i are kept constant during differentiation, not the original momenta p_i. In the limit:

$$\left|\hbar \frac{\partial^2 S}{\partial q_j^2}\right| \ll \left(\frac{\partial S}{\partial q_j}\right)^2 \tag{7}$$

multiplying $H(q,p,t) \cdot e^{i\frac{S}{\hbar}}$ can be approximated as acting with the operator $\hat{H}(q, \frac{\hbar}{i}\partial_{q_j}, t)e^{i\frac{S}{\hbar}}$. This gives:

$$i\hbar \partial_t e^{i\frac{S}{\hbar}} \simeq \hat{H}(q, \frac{\hbar}{i}\partial_{q_j}, t) e^{i\frac{S}{\hbar}} \tag{8}$$

which is a linear differential equation that holds for any set of P_i in $S(q,P,t)$. If I define a function:

$$\Phi(q,t) = \int \mathbb{P}(P_i) e^{i\frac{S(q,P,t)}{\hbar}} \mathrm{d}P_i \tag{9}$$

where $\mathbb{P}(P_i)$ is a probability distribution over trajectories that pass through the point (q,t) with different velocities, then $\Phi(q,t)$ also satisfies Equation 8. That equation has the same form as the Schrödinger Equation for the quantum wave function, substituting $\Phi(q,t) \to \Psi(q,t)$.

A function $\Phi(q,t)$ analogous to the quantum wavefunction $\Psi(q,t)$ thus results from taking an array of particles traveling along classical trajectories and weighting the phase $e^{i\frac{S}{\hbar}}$ at each position $\vec{q}$ and time t with a probability distribution for the constants P_i that distinguish trajectories passing through (q,t) with different velocities (see Figure 1).

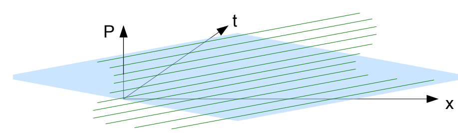

FIG. 1. Set of classical free particle trajectories through different (x,t) on a surface of constant P with $\dot{x} > 0$.

For the case of the free particle, the limit defined in Equation 7 even holds for $\hbar \nrightarrow 0$, since $S = \pm\sqrt{2mP}x - Pt$ has a zero second derivative with respect to x. The function $\Phi(q,t)$ is thus a superposition of plane waves. The free-particle solution is often used as a basis for motivating the quantum Schrödinger Equation and we see here that classical mechanics gives the same result.

In the free particle example, the constant of motion P is identified with the energy of the particle. While a single classical trajectory in N dimensions can be specified with $2N$ constants, the expression for S depends on only N constants. This is analogous to the number of independent quantum numbers that can be used to describe spatial wavefunctions: ex. E in one dimension, $\{E, L_z\}$ in two dimensions, and $\{E, L, L_z\}$ in three dimensions. Since, for one dimension, the energy can be used as the constant P, weighting with $\mathbb{P}(P)$ can be compared to using a Boltzmann factor to weight an ensemble of classical states based on their energy.