A Classical Approach to the Schrődinger Equation for a Particle in a Force Field

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Abstract

A common approach to the Schrődinger equation is to start with a well known wave function solution to a specific problem, apply the corresponding Schrődinger equation and show that the result is equivalent to the classical Hamiltonian energy equation. In this paper the starting point is the classical Hamiltonian energy equation for a free particle under influence of a force potential. An appropriate variable transformation is applied, and the equation for the corresponding generator function that solves the problem is identified. The relationship between the wave function and the generator function is found by studying the momentum in the two formalisms. Assumptions necessary to approach the Schrődinger equation are identified. The approach shown here leads to an equation that is close to the Schrődinger equation, differing only by the appearance of a term containing the total time derivative of the probability density.

The Schrődinger equation

The well known Schrődinger equation describes the time evolution of the wave function, Ψ, of a quantum mechanical system. According to this theory, the wave function squared, $|\Psi|^2$, describes the probability, P, of finding the system in a given state at a given time.

The Schrődinger equation may be written as

$$\left(\bar{H} - \bar{E}\right)\Psi \quad = \quad 0$$

where $\bar{H}$ and $\bar{E}$ are "operators". If the Schrődinger equation is applied to a one dimensional system consisting of a particle in a force field, we get

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial q^2}\right)_{qt} + U(\mathbf{r})\Psi \quad = \quad i\hbar\left(\frac{\partial\Psi}{\partial t}\right)_{qt} \tag{1}$$

where $U(\mathbf{r})$ is the force potential, $\mathbf{r}(q)$ is the position vector, q is the (canonical) coordinate, $i^2 = -1$ and $\hbar$ is the Planck constant (divided by 2π). The subscript in the partial derivative expression indicates the functional dependency of Ψ. In this formalism, the momentum, p, is given by the equation

$$p \quad = \quad -i\hbar\frac{1}{\Psi}\left(\frac{\partial\Psi}{\partial q}\right)_{qt}. \tag{2}$$

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A Classical Approach

Let us study a classical system where the classical momentum, p, is constrained to being a function of the coordinate, q. Our system consists of a particle in a force field, so that the state of the system is given by $\{q, p(q)\}$. We know from [Tveter 1998] that generator functions may be assigned directly to variable systems according to the equation

$$L - p\dot{q} + K - \frac{dS}{dt} = 0, \tag{3}$$

where L is the Lagrange function for the system, S is the assigned generator function and K is the Hamiltonian. Note that the value of the Lagrange function is independent of the variable set (unlike the value of the Hamilton function). We also know from [Tveter 1998] that if the assigned generator function S is a constant in time, then the position vector can only be a function of the coordinate (i.e. $\mathbf{r}(q)$). In this case we may write (3) as

$$L - p\dot{q} + K = 0. \tag{4}$$

A variable set where the position vector, $\mathbf{r}$, only is a function of the coordinate (i.e. $\mathbf{r}(q)$) is usually easy to find for a given problem. These variable sets are the sets in which we *describe* the problem.

If the Hamiltonian K is zero for a variable set, then the time derivatives of the variables in the variable set is also zero ($\dot{Q} = \dot{P} = 0$, where $\{Q, P\}$ is the variable set). For these variable sets (3) becomes

$$L - \frac{dS_2}{dt} = 0, \tag{5}$$

with a solution where $S_2 = \int L dt$ (action integral over the Lagrange function). Variable sets with this generator function therefore represent the *solution* to the problem.

Eliminating the Lagrange function from (4) and (5) gives

$$-p\dot{q} + K = -\frac{dS_2}{dt}.$$

Next we place a constraint on the system by forcing the generator function S_2 to be a function of only $\{qt\}$ (i.e. $S_2(\mathbf{r}(q), t)$). We may then write

$$-p\dot{q} + K = -\frac{dS_2}{dt} = -\left(\frac{\partial S_2}{\partial q}\right)_{qt} \dot{q} - \left(\frac{\partial S_2}{\partial t}\right)_{qt},$$

which has a solution given by

$$p = \left(\frac{\partial S_2}{\partial q}\right)_{qt} \tag{6}$$

$$K = -\left(\frac{\partial S_2}{\partial t}\right)_{qt}. \tag{7}$$

Note that by forcing S_2 to only be a function of the coordinate (i.e. $S_2(\mathbf{r}(q),t)$), the momentum, p, is forced to also be a function of the coordinate (i.e. $p(q,t)$).

By comparing Eqs. (2) and (6) we see that we must have

$$S_2 = -i\hbar \ln \Psi\Psi_t$$

where Ψ_t is a function of t only and determined by the constraints. This term can be eliminated by redefining the wave function, Ψ, appropriately. Taking the derivative gives

$$\begin{aligned}
\left(\frac{\partial S_2}{\partial t}\right)_{qt} &= -i\hbar\frac{1}{\Psi}\left(\frac{\partial \Psi}{\partial t}\right)_{qt} && (8)\\
\left(\frac{\partial S_2}{\partial q}\right)_{qt} &= -i\hbar\frac{1}{\Psi}\left(\frac{\partial \Psi}{\partial q}\right)_{qt} \\
\left(\frac{\partial S_2}{\partial q}\right)^2_{qt} &= -\hbar^2\frac{1}{\Psi^2}\left(\frac{\partial \Psi}{\partial q}\right)^2_{qt} && (9)\\
\left(\frac{\partial^2 S_2}{\partial q^2}\right)_{qt} &= i\hbar\frac{1}{\Psi^2}\left(\frac{\partial \Psi}{\partial q}\right)^2_{qt} - i\hbar\frac{1}{\Psi}\left(\frac{\partial^2 \Psi}{\partial q^2}\right)_{qt} && (10)
\end{aligned}$$

Let us study a single particle in a force field given by the force potential $U(q)$. For this system we have [Goldstein 1981]

$$\begin{aligned}
K(q,p,t) &= \frac{p^2}{2m} + U(q), && (11)\\
\dot{q} &= \left(\frac{\partial K}{\partial p}\right)_{qpt} = \frac{p}{m},
\end{aligned}$$

where m is the particle mass. Using Eqs. (6), (7) and (11) gives

$$\frac{1}{2m}\left(\frac{\partial S_2}{\partial q}\right)^2_{qt} + U(q) = -\left(\frac{\partial S_2}{\partial t}\right)_{qt}. \qquad (12)$$

Let us call this the "action equation", since a solution to this equation gives an S_2 that is equal to the Lagrange action integral (which represents the transformation that will solve the problem).

Next we need to study the probability density function, P, for the particle. Simple particle flow density conservation considerations give us

$$\frac{d\ln P}{dt} = -\left(\frac{\partial \dot{q}}{\partial q}\right)_{qpt} = -\frac{1}{m}\left(\frac{\partial^2 S_2}{\partial q^2}\right)_{qt}. \qquad (13)$$

Using Eqs. (9), (10) and (13) gives

$$\frac{1}{2m}\left(\frac{\partial S_2}{\partial q}\right)^2_{qt} = -\frac{1}{2m}\hbar^2\frac{1}{\Psi}\left(\frac{\partial^2 \Psi}{\partial q^2}\right)_{qt} - i\hbar\frac{1}{2}\frac{d\ln P}{dt} \qquad (14)$$

Combining Eq. (8), (12) and (14) gives

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial q^2}\right)_{qt} + \Psi U(q) \quad = \quad i\hbar\left(\frac{\partial\Psi}{\partial t}\right)_{qt} + i\hbar\Psi\frac{d\ln\sqrt{P}}{dt} \tag{15}$$

We observe that Eq. (15) differs from Eq. (1) on the right hand side, by the appearance of an extra term. The extra term involves the total time derivative of the probability density. When the probability density of the particle does not change as we follow the particle (i.e. constant momentum), this term is zero, and the resulting equation then corresponds to the Schrődinger Equation.

Conclusions

This paper has demonstrated how it is possible to start from the classical Hamilton energy equation and arrive at the Schrődinger equation when several assumptions are applied. The greatest assumption used here is that the total time derivative of the probability density is zero, which is clearly not the case for most systems. A second important assumption is that the classical momentum is given by Eq. (2), and a third assumption is that the probability density changes according to Eq. (13). For instance a free particle with uniform distribution probability and not under the influence of any force potential, obeys all of the assumptions above, and the probability density derived from the Schrődinger equation, $\Psi \sim e^{i\frac{p}{\hbar}x - i\frac{E}{\hbar}t}$, will in this case be in agreement with results from classical mechanics.

References

[Goldstein 1981] H. Goldstein 1981, Classical Mechanics Second ed., Addison-Wesley, USA.

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