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Time Evolution

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Some Notes on Time Evolution

E. Schrödinger

After deBroglie introduced the idea that functions describing particles should have waves associated with them, Schrödinger produced the first identification of a *wave function* with a particle. Explicitly, he postulated that a wave funtion Ψ for a particle moving in one dimension in a potential $V(x)$ would satisfy

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t). \tag{1}$$

An earlier postulate had been proposed by a group of physicists working under the direction of Max Born in the German university in Göttingen. Only a few explicit problems had been solved by the Göttingen group, however, because their formulation involved *matrices*, a mathematical construct that was unfamiliar to physicists at that time.

When Schrödinger's equation was published, however, every one recognized that such equations could be solved by *separation of variables*:

{1°} Assume that the solution would have the form

$$\Psi(x,t) = F(x)\cdot G(t) \tag{2}$$

{2°} Rewrite Eq.(1) as

$$i\,\hbar\frac{G'(t)}{G(t)} = \frac{-\frac{\hbar^2}{2m}F''(x) + V(x)\,F(x)}{F(x)} \tag{3}$$

{3°} Recognize that all the terms dependent on t are on the left hand side of Eq(3) while all the terms dependent on x are on the right hand side. So the values of both the left hand side and the right hand side must be independent of both x and t. Let E stand for this constant. Then the problem leads to two independnt problems,

$$E = i\,\hbar\frac{G'(t)}{G(t)} \tag{4}$$

and

$$E = \frac{-\frac{\hbar^2}{2m}F''(x) + V(x)\,F(x)}{F(x)} \tag{5}$$

{4°} Providing the initial condition $G(0) = 1$, the solution to (4) is

$$G(t) = e^{-i\,E\,t/\hbar},$$

and $F(x)$ is some solution to

$$-\frac{\hbar^2}{2m}F''(x) + V(x)\,F(x) = E\,F(x) \tag{6}$$

In practice, Eq.(6) will only have solutions for certain E values, $\{E_j\}_{j=1}^{j_{Limit}}$ so a set of solutions

$$\Psi_j(x,t) = e^{-i\,E_j\,t/\hbar} \cdot F_j(x), \quad j = 1, \ldots, j_{Limit}$$

is found. The general solution is just some linear combination of these solutions.

Since many solutions to equations of the form of E.(6) were known, A flood of solutions to new problems appeared in the literature. The quantization of many phenomena were correctly described.

When operators were introduced into the construction, Hamilton's function $H(p, x)$ was replaced with the operator

$$H(p,x) \to \hat{H}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}, x\right)$$

and Eq.(6) becomes

$$\hat{H}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}, x\right)\,F(x) = E\,F(x) \tag{7}$$

and we now call the allowed E_i values the *energy eigenvalues* and the allowed $F_i(x)$ functions the *energy eigenfunctions*.

The corresponding rendition of Schrödinger's equation is

$$i\,\hbar\frac{\partial}{\partial t}\,\Psi = \hat{H}\,\Psi \tag{8}$$

In three dimensions, this becomes

$$i\,\hbar\frac{\partial}{\partial t}\,\Psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\boldsymbol{r},t) + V(\boldsymbol{r})\psi(\boldsymbol{r},t) \tag{9}$$

The Continuity Equation

If the probability density $|\Psi(\boldsymbol{r},t)|^2$ evolves in time, there must be a *probability flux* in the system. We can identify the probability flux $\boldsymbol{J}(\boldsymbol{r},t)$ by invoking the *continuity* equation

$$\int_{\partial v} d\boldsymbol{S}\cdot\boldsymbol{J}(\boldsymbol{r},t) = -\frac{\partial}{\partial t}\int_{v} d\boldsymbol{r}|\Psi(\boldsymbol{r},t)|^2 \tag{10}$$

with the integral representing the probability the electron is in the volume v at time t. The surface integral is the integral over the surface δv of v.

If $\hat{H}^* = \hat{H}$,

$$i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t)^*\Psi(\boldsymbol{r},t) = \Psi(\boldsymbol{r},t)^*\,\hat{H}\,\Psi(\boldsymbol{r},t) - \Psi(\boldsymbol{r},t)\,\hat{H}\,\Psi(\boldsymbol{r},t)^*$$

$$= -\frac{\hbar^2}{2m}\left[\Psi(\boldsymbol{r},t)\nabla^2\Psi(\boldsymbol{r},t)^* - \Psi(\boldsymbol{r},t)^*\nabla^2\Psi(\boldsymbol{r},t)\right]$$

$$= -\frac{\hbar^2}{2m}\nabla\cdot\left[\Psi(\boldsymbol{r},t)\nabla\Psi(\boldsymbol{r},t)^* - \Psi(\boldsymbol{r},t)^*\nabla\Psi(\boldsymbol{r},t)\right]$$

then Eq.(10) becomes

$$\int_{\partial v} d\boldsymbol{S}\cdot\boldsymbol{J}(\boldsymbol{r},t) = \frac{-i\hbar}{2m}\int_{v} d\boldsymbol{r}\nabla\cdot\left[\Psi(\boldsymbol{r},t)\nabla\Psi(\boldsymbol{r},t)^* - \Psi(\boldsymbol{r},t)^*\nabla\Psi(\boldsymbol{r},t)\right] \tag{11}$$

It follows from Gauss' theorem that

$$\boldsymbol{J}(\boldsymbol{r},t) = \frac{i\hbar}{2m}\left[\Psi(\boldsymbol{r},t)\nabla\Psi(\boldsymbol{r},t)^* - \Psi(\boldsymbol{r},t)^*\nabla\Psi(\boldsymbol{r},t)\right] \tag{12}$$

at all $\boldsymbol{r},t$.

Deduce a Velocity

If $\boldsymbol{J}(\boldsymbol{r},t) = |\Psi(\boldsymbol{r}.t)|^2\,\boldsymbol{V}(\boldsymbol{r},t)$,

$$\boldsymbol{V}(\boldsymbol{r},t) = \frac{i\hbar}{2m}\left[\nabla\ln(\Psi(\boldsymbol{r},t))^* - \nabla\ln(\Psi(\boldsymbol{r},t))\right] \tag{13}$$

which simplifies to

$$\boldsymbol{V}(\boldsymbol{r},t) = \frac{\hbar}{m}\Im\left\{\nabla\ln(\Psi(\boldsymbol{r},t))\right\} \tag{15}$$

As an example, if

$$\Psi(\boldsymbol{r}, t) = Ce^{i\boldsymbol{k}\cdot\boldsymbol{r} - i\omega t}$$

then

$$\boldsymbol{V} = \frac{\hbar\boldsymbol{k}}{m}.$$

Motion is associated with a phase shift of $\Psi(\boldsymbol{r}, t)$ with position in space. To describe a moving system, the wave function must be *complex*. Most energy eigenstates are *real*, in which case they are called *stationary*. Stationary states can always be made *real*.