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Velocity of Propagation in Diffusional Quantum Theory

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An equation of diffusional quantum theory which takes into account the finite velocity of propagation is derived from Kelvin's telegraph equation and Fürth's relation. The equation is then used to derive the ground state of quantum systems and to derive the Sommerfeld–Dirac expression for the ionization potential of hydrogen-like ions.

KEY WORDS: Quantum theory; diffusion; Kelvin's telegraph equation; velocity of propagation.

Many diffusional theories of quantum mechanics involve the notion that atomic properties can be derived by considering the rapid, random, diffusional motion of a point particle.[1–4] It is the purpose of this paper to incorporate the effects of a finite velocity of propagation into a quantum diffusional theory by using Kelvin's telegraph equation, to consider the ground states of quantum systems, and then to derive the Sommerfeld–Dirac expression for the ionization potential of hydrogen-like ions.

The ordinary theory of diffusion is based on the equation

$$\partial n/\partial t = D\,\nabla^2 n \tag{1}$$

where $n(\mathbf{r}, t)$ is the concentration of diffusing particles at position $\mathbf{r}$ and time t, and D is the diffusivity. If N particles are located at the origin at time $t=0$, then (1) has the well-known solution

$$n(\mathbf{r}, t) = (4\pi\,Dt)^{-3/2}\,N \exp(-r^2/4Dt) \tag{2}$$

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Since, according to (2), it is possible to find particles at any position r, no matter how large, and at any time t, no matter how small, we see that the velocity of propagation of the ordinary diffusion equation (1) is infinite.

According to Fürth,[1,2] a procedure for obtaining a relation between diffusion theory and quantum theory consists in introducing the formal equivalence

$$D = i\hbar/2m \tag{3}$$

Within this framework, the Schrödinger equation has the form

$$\frac{\partial\psi}{\partial t} = D\,\nabla^2\psi + \frac{V(\mathbf{r})}{i\hbar}\psi(\mathbf{r}, t) \tag{4}$$

Although (4) has led to many interesting results, it carries the implication that the velocity of propagation is infinite.

A procedure for taking into account that the velocity of propagation cannot exceed the speed of light is to start with the telegraph equation

$$\frac{\partial n}{\partial t} + \frac{D}{v^2}\frac{\partial^2 n}{\partial t^2} = D\,\nabla^2 n \tag{5}$$

instead of the diffusion equation (1), where v is the velocity of the diffusing particle. In the limit where $v \to \infty$ the telegraph equation (5) reduces to the ordinary diffusion equation (1). The telegraph equation has been used in a variety of contexts in which a velocity of propagation is a factor.[5-8] Here we will set $v = c$, where c is the speed of light. Combining Fürth's equation (3) with the telegraph equation yields the corresponding noncovariant quantum equation

$$i\hbar\frac{\partial\psi}{\partial t} - \frac{\hbar^2}{2mc^2}\frac{\partial^2\psi}{\partial t^2} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \tag{6}$$

It is our object to use the quantum equation (6) to consider the ground state and to derive an expression for the ionization potential of hydrogen-like ions with the Coulombic potential $V(r) = -Ze^2/r$. In particular, it will be shown that Kelvin's telegraph equation and Fürth's relation can be used to derive the Sommerfeld–Dirac ionization potential of hydrogen-like ions. The time-independent quantum equation is derived by the usual procedure of setting $\psi(\mathbf{r}, t) = u(\mathbf{r})\exp(-iEt/\hbar)$, where E is the energy of the ground state. We obtain

$$Eu + \frac{E^2}{2mc^2}u = -\frac{\hbar^2}{2m}\nabla^2 u - \frac{Ze^2}{r}u \tag{7}$$

This equation is to be applied only to the ground state. Higher excited states, which involve complex additional phenomena, are not treated in this paper. Using the fact that the lowest eigenvalue of the operator $H = -(\hbar^2/2m)\nabla^2 - Ze^2/r$ is $-Z^2\alpha^2mc^2/2$, where $\alpha = e^2/\hbar c$, we have

$$E + \frac{E^2}{2mc^2} = -\frac{Z^2}{2}\alpha^2 mc^2 \tag{8}$$

Solving (8) for the case of hydrogen-like ions and noting that the ionization potential I is equal to $-E$ yields

$$I = mc^2[1 - (1 - \alpha^2 Z^2)^{1/2}] \tag{9}$$

Equation (9) is identical to the Sommerfeld–Dirac ionization potential for hydrogen-like ions.[9,10]

In summary, Fürth's relation and Kelvin's telegraph equation have been used to derive an equation of diffusional quantum theory which takes into account the finite velocity of propagation. The ground state of a quantum system was considered and the equation was used to derive the Sommerfeld–Dirac expression for the ionization potential of hydrogen-like ions.

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