

Math Diversion Problem 815

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Abstract

This note explores what happens to the Schrödinger Equation when the usual form of the complex function ψ is presented in polar form $\psi = R e^{iS/\hbar}$, and we find a surprising connection to Hamilton-Jacobi theory and its further connection to Bohmian Mechanics.

Chancellor, all presidents are faced with difficult decisions.

It is by their *decisions* that they are judged.

— Cardinal Barusa

[Doctor Who, *Deadly Assassin*]

1 Problem

Investigate the relation of Schrödinger Equation's to the Hamilton-Jacobi equation and Bohmian Mechanics.

2 Introduction

The time-dependent Schrödinger Equation is given by

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{x}, t) + V(\mathbf{x}) \psi(\mathbf{x}, t). \quad (1)$$

Typically, a generic complex function ψ is expressed in terms of its real and imaginary parts by

$$\psi(\mathbf{x}, t) = \psi_{\text{Re}}(\mathbf{x}, t) + i\psi_{\text{Im}}(\mathbf{x}, t). \quad (2)$$

It should be pointed out that most textbook solutions to problems in quantum mechanics avoid breaking up ψ as in the last equation, preferring to exhibit it in complex exponential form. Why? Because quantum mechanics is 'wave mechanics' and waves are efficiently expressed as complex exponentials.

Definition: One of the most important vector identities in quantum mechanics in dealing with the Schrödinger Equation in three-dimensions (1) is what I call **Nickel's Identity**, which is the following:

$$\nabla \cdot (\phi \mathbf{v}) = \mathbf{v} \cdot \nabla \phi + \phi \nabla \cdot \mathbf{v}. \quad (3)$$

So far as I know, this identity has no commonly accepted name. So, don't use the name I gave it in your mathematical writings or papers, because no one will know what you are referring to.

Our goal is to see what happens when we replace ψ in (1) with the 'polar form'

$$\psi = R e^{iS/\hbar}, \quad (4)$$

where R and S are real-valued functions. In the doing, we must put-up with some involved computations, which will be prepared for in advance with a number of lemmas following.

3 Ye Olde Lemmas

Lemma 1: Proof of Nickel's Identity

Here I give a proof of Nickel's Identity, which employs Geometric Calculus. The reader can skip this proof and perhaps find a conventional proof on the Internet.

Proof: For arbitrary arbitrary function ϕ and vector \mathbf{v} :

$$\begin{aligned} \nabla \cdot (\phi \mathbf{v}) &= \langle \nabla(\phi \mathbf{v}) \rangle \\ &= \langle (\nabla \phi) \mathbf{v} \rangle + \langle \phi \nabla \mathbf{v} \rangle \\ &= (\nabla \phi) \cdot \mathbf{v} + \phi \nabla \cdot \mathbf{v} \\ &= \mathbf{v} \cdot \nabla \phi + \phi \nabla \cdot \mathbf{v}. \end{aligned} \quad (5)$$

Lemma 2:

$$\nabla e^{iS/\hbar} = \frac{i}{\hbar} (\nabla S) e^{iS/\hbar}. \quad (6)$$

The trick to proving this is to take the operation of the gradient one component at a time.

Lemma 3:

$$\nabla^2 e^{iS/\hbar} = \left[\frac{i}{\hbar} (\nabla^2 S) - \frac{1}{\hbar^2} (\nabla S)^2 \right] e^{iS/\hbar}. \quad (7)$$

The basic idea of the proof is first to know that $\nabla^2 = \nabla \cdot \nabla$ and then to use Nickel's Identity applied to (6), with $\phi = e^{iS/\hbar}$ and $\mathbf{v} = \nabla S$, and one can let the constant factor i/\hbar slip through the derivative.

Lemma 4: For scalar functions ϕ and λ :

$$\nabla(\phi\lambda) = (\nabla\phi)\lambda + \phi\nabla\lambda. \quad (8)$$

Lemma 5: (Hint: Use the last lemma):

$$\nabla\psi = \nabla(R e^{iS/\hbar}) = \left[\nabla R + \frac{iR}{\hbar}(\nabla S) \right] e^{iS/\hbar}. \quad (9)$$

Lemma 6: Now for the LHS of (1):

$$i\hbar \frac{\partial\psi(\mathbf{x}, t)}{\partial t} = \left[i\hbar \frac{\partial R}{\partial t} - R \frac{\partial S}{\partial t} \right] e^{iS/\hbar}. \quad (10)$$

4 Main Part

Now it's time to put the lemmas to practical use.

$$\begin{aligned} \nabla^2\psi &= \nabla \cdot (\nabla\psi) \\ &= \nabla \cdot (\nabla R e^{iS/\hbar}) \\ &= \nabla \cdot \left\{ \left[\nabla R + \frac{iR}{\hbar}(\nabla S) \right] e^{iS/\hbar} \right\} \\ &= \nabla \cdot \left[(\nabla R) e^{iS/\hbar} \right] + \frac{i}{\hbar} \nabla \cdot \left[R e^{iS/\hbar} (\nabla S) \right]. \end{aligned}$$

At this point, we use Nickel's Identity for both terms on the right:

$$\begin{aligned} \nabla \cdot \left[(\nabla R) e^{iS/\hbar} \right] &= (\nabla R) \cdot \nabla e^{iS/\hbar} + e^{iS/\hbar} \nabla^2 R \\ &= \left[\frac{i}{\hbar} (\nabla R) \cdot (\nabla S) + \nabla^2 R \right] e^{iS/\hbar}. \end{aligned} \quad (11)$$

And

$$\begin{aligned} \frac{i}{\hbar} \nabla \cdot \left[R e^{iS/\hbar} (\nabla S) \right] &= \frac{i}{\hbar} \left[(\nabla S) \cdot \nabla (R e^{iS/\hbar}) + R e^{iS/\hbar} (\nabla^2 S) \right] \\ &= \frac{i}{\hbar} \left[(\nabla S) \cdot \left\{ \nabla R + \frac{iR}{\hbar} (\nabla S) \right\} + R (\nabla^2 S) \right] e^{iS/\hbar} \\ &= \left[\frac{i}{\hbar} (\nabla S) \cdot (\nabla R) - \frac{R}{\hbar^2} (\nabla S)^2 + \frac{i}{\hbar} R (\nabla^2 S) \right] e^{iS/\hbar} \end{aligned} \quad (12)$$

Therefore,

$$\nabla^2\psi = \left[\frac{2i}{\hbar} (\nabla S) \cdot (\nabla R) - \frac{R}{\hbar^2} (\nabla S)^2 + \frac{i}{\hbar} R (\nabla^2 S) + \nabla^2 R \right] e^{iS/\hbar} \quad (13)$$

So, we now know what (1) becomes after we substitute in and cancel the factor $e^{iS/\hbar}$ on both sides:

$$i\hbar \frac{\partial R}{\partial t} - R \frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m} \left[\frac{2i}{\hbar} (\nabla S) \cdot (\nabla R) - \frac{R}{\hbar^2} (\nabla S)^2 + \frac{i}{\hbar} R (\nabla^2 S) + \nabla^2 R \right] + V(\mathbf{x})R. \quad (14)$$

Simplifying this, we get

$$i\hbar \frac{\partial R}{\partial t} - R \frac{\partial S}{\partial t} = -\frac{i\hbar}{m} (\nabla S) \cdot (\nabla R) + \frac{R}{2m} (\nabla S)^2 - \frac{i\hbar}{2m} R (\nabla^2 S) - \frac{\hbar^2}{2m} \nabla^2 R + V(\mathbf{x})R. \quad (15)$$

Lastly, we separate the real and imaginary parts. From the real part, we get:

$$-\frac{\partial S}{\partial t} = \frac{1}{2m} (\nabla S)^2 - \frac{\hbar^2}{2mR} \nabla^2 R + V(\mathbf{x}). \quad (16)$$

From the imaginary part, we get:

$$\frac{\partial R}{\partial t} = -\left[\frac{1}{m} (\nabla S) \cdot (\nabla R) + \frac{1}{2m} R (\nabla^2 S) \right]. \quad (17)$$

Now, I don't know what to make of this last equation, but if we take the classical limit in Eq. (16), by taking $\hbar \rightarrow 0$, we get

$$-\frac{\partial S}{\partial t} = \frac{1}{2m} (\nabla S)^2 + V(\mathbf{x}). \quad (18)$$

This last equation should look vaguely familiar. In Hamilton-Jacobi theory, we have the relations

$$-\frac{\partial S}{\partial t} = H \quad \text{and} \quad \nabla S = \mathbf{p}, \quad (19)$$

where H is the Hamiltonian of the system and \mathbf{p} is the momentum of the particle. Therefore, we have that

$$H = \frac{1}{2m} \mathbf{p}^2 + V(\mathbf{x}). \quad (20)$$

5 Bohmian Mechanics, Anyone?

As I understand the narrative, in 1952, physicist David Bohm was not happy about the Copenhagen interpretation of quantum mechanics and he sought some way to make the wave function correspond to real things and dispense with the collapse of the wave function and superposition. He published his de Broglie-Bohm pilot-wave theory as an alternative to standard quantum mechanics. Was he right? I don't know, but he came up with what we now call Bohmian mechanics, the substance of which is straightforward.

Bohm interpreted Eq. (16) as

$$-\frac{\partial S}{\partial t} = \frac{1}{2m} (\nabla S)^2 + Q + V(\mathbf{x}), \quad (21)$$

where

$$Q \equiv -\frac{\hbar^2}{2mR} \nabla^2 R, \quad (22)$$

and where Q is the so-called ‘quantum potential’. Wikipedia writes Eq. (21) in the following form:

$$\frac{\partial S}{\partial t} = -\left[\frac{1}{2m} (\nabla S)^2 + Q + V(\mathbf{x}) \right], \quad (23)$$

and calls this equation the *Quantum Hamilton-Jacobi equation*.

So far, so good. But this leaves us without an interpretation of the other equation given in (17). I’ll spare the reader the suspense and cut to the chase. Our goal now is to arrive at the *Continuity Equation* for the system, which normally takes the form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (24)$$

where ρ in the Schrödinger equation way of looking at the system is the probability density of the particle. In that way of dealing with the problem, we get ρ as follows:

$$\rho = \tilde{\psi} \psi. \quad (25)$$

If we substitute into this last equation the ψ from (4), we get

$$\rho = R^2. \quad (26)$$

Now, we know that $\mathbf{p} = m\mathbf{v}$ and from (19), we know that $\nabla S = \mathbf{p}$. Therefore, putting these together, we have that

$$\mathbf{v} = m^{-1} \nabla S. \quad (27)$$

We’re now ready to substitute the values of these last two equations into a slightly modified version of the continuity equation,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) = -[\mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v}]. \quad (28)$$

By doing so, we have that

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -[\mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v}], \\ 2R \frac{\partial R}{\partial t} &= -[(m^{-1} \nabla S) \cdot \nabla R^2 + R^2 \nabla \cdot (m^{-1} \nabla S)], \\ 2R \frac{\partial R}{\partial t} &= -\left[\frac{2R}{m} (\nabla S) \cdot \nabla R + \frac{R^2}{m} \nabla \cdot (\nabla S) \right], \\ \frac{\partial R}{\partial t} &= -\left[\frac{1}{m} (\nabla S) \cdot (\nabla R) + \frac{1}{2m} R \nabla^2 S \right], \end{aligned} \quad (29)$$

which is the same as Eq. (17). Very impressive! And Bohmian mechanics does have it’s adherents, though, it has not as yet made much headway into a special relativistic version of the theory.

6 How About a Hyperbolic Version of the Wave Function?

In their paper, “A Representation of the Schrödinger and Klein-Gordon equations obtained using simple hyperbolic numbers,”¹ authors Paul Bracken and James Hayes made the following change to the polar form of the wave function

$$\psi = R e^{\mathbf{j}S/\hbar}, \quad (30)$$

where \mathbf{j} is a hyperbolic number whose square is unity, that is,

$$\mathbf{j}^2 = 1. \quad (31)$$

When they substitute this function into the Schrödinger Equation (1), they are forced to set

$$\frac{\partial S}{\partial t} = \frac{\partial R}{\partial t} = 0, \quad (32)$$

which seems to place the rest of the theory squarely into the time-independent version of the theory.

Now, I am a huge supporter of all things hyperbolic in mathematics (I have written extensively within the framework of the isomorphic Unipodal Numbers), but I don’t know that I can characterize this hyperbolic substitution as more than a curiosity at this point. Time will tell.

7 Conclusion

What began for me as an effort to reveal to my readers the connection of the time-dependent Schrödinger Equation and Hamilton-Jacobi theory accidentally led me to the Bohmian connection, so I decided to include it for completeness.

The ultimate value of Bohm’s program to found physics back on ‘reality’ has come a long way, yet has a long way to go. Whether at this point the progress it has enjoyed since the 1950s is merely meretricious or of fundamental importance is not for me to say.

¹*American Journal of Physics*, Volume 71, No. 7, July 2003, pp. 726–728.