Schrodinger Equation and Geometric Algebra

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Abstract

These notes recast the spinless Schrodinger equation in geometric algebra terms, following the approach of *Geometric Algebra for Physicists*, by Chris Doran and Anthony Lasenby.

3D Euclidean Geometric Algebra Basis

Three dimensional Euclidean geometrical algebra has a scalar (1), three vectors (e_x, e_y and e_z), three bivectors ($e_x e_y$, $e_z e_x$, and $e_y e_z$), and one trivector ($e_x e_y e_z$) defining the geometry. Multivector multiplication is associative, but not necessarily commutative.

In 3D Euclidean space, by definition, the three vector elements individually square to +1.

$$\begin{aligned} e_x * e_x &= e_x e_x = 1 \\ e_y * e_y &= e_y e_y = 1 \\ e_z * e_z &= e_z e_z = 1 \end{aligned}$$

In contrast to the cross product, the product of different vector basis is an anti-commutating bivector.

$$\begin{aligned} e_x * e_y &= e_x e_y = -e_y e_x \\ e_y * e_z &= e_y e_z = -e_z e_y \\ e_z * e_x &= e_z e_x = -e_x e_z \end{aligned}$$

These bivectors square to -1, as illustrated by

$$\begin{aligned}(e_x e_y) * (e_x e_y) &= e_x e_y e_x e_y \\ &= -e_y e_x e_x e_y \\ &= -e_y 1 e_y = -e_y e_y \\ &= -1\end{aligned}$$

The trivector $e_x e_y e_z$ squares to negative one, and commutes will all multivector components. This trivector, mimicing the behavior of i, is commonly written as I, sometimes as i, sometimes as j in the literature. In our case, whenever I see an i in a parent equation prior geometric algebra, I will suspect this to translate into the trivector in the post geometric algebra format. When I want to emphasize the correlation to older equations, I will use the capital $I = e_x e_y e_z$.

With our bivectors, I have a preference to use $e_x e_y, e_y e_z, e_z e_x$ as the preferred order of products, which leads to component equations with obvious dot product and couple terms.

In multiplication table format, the order-sensitive multiplication among these elements, with prefactors on the left column and postfactors on top row, is

	1	e_x	e_y	e_z	$e_x e_y$	$e_z e_x$	$e_y e_z$	$e_x e_y e_z$
1	1	e_x	e_y	e_z	$e_x e_y$	$e_z e_x$	$e_y e_z$	$e_x e_y e_z$
e_x	e_x	1	$e_x e_y$	-$e_z e_x$	e_y	$-e_z$	$e_x e_y e_z$	$e_y e_z$
e_y	e_y	$-e_x e_y$	1	$e_y e_z$	$-e_x$	$e_x e_y e_z$	e_z	$e_z e_x$
e_z	e_z	$e_z e_x$	$-e_y e_z$	1	$e_x e_y e_z$	e_x	$-e_y$	$e_x e_y$
$e_x e_y$	$e_x e_y$	$-e_y$	e_x	$e_x e_y e_z$	-1	$e_y e_z$	$-e_z e_x$	$-e_z$
$e_z e_x$	$e_z e_x$	e_z	$e_x e_y e_z$	$-e_x$	$-e_y e_z$	-1	$e_x e_y$	$-e_y$
$e_y e_z$	$e_y e_z$	$e_x e_y e_z$	$-e_z$	e_y	$e_z e_x$	$-e_x e_y$	-1	$-e_x$
$e_x e_y e_z$	$e_x e_y e_z$	$e_y e_z$	$e_z e_x$	$e_x e_y$	$-e_z$	$-e_y$	$-e_x$	-1

Some Basics

In 1901 (On the Law of the Distribution of Energy in the Normal Spectrum), Max Planck deduced that the energy of photons was related to frequency by $E = h\nu$, with $h = 6.26 \cdot 10^{-34}$ kg m^2/s. Modern practice prefers a slightly different notation, where Planck's constant and frequency are both scaled by 2π, to use the form $E = \hbar\omega = \hbar(2\pi f)$ where $\hbar = h/(2\pi)$ and $f = \nu$. Engineers and physicists who have been exposed to the Fourier transform and circuit theory recognize the linear dependence on frequency as indicating the presense of a time derivative. Clearly, the energy of a photon is the time derivative of some harmonic oscillator of some type. Looking at units, energy in Joules is the derivative of action in Joule seconds. In electrical units, a Coulomb volt is a Joule, and this, in turn, gives rise to units of action being expressible as Coulomb volt seconds, or Coulombs times magnetic flux.

In addition to energy, photons exhibit a fixed angular momentum. By analogy to a rotating object with energy $E = \frac{1}{2}I\omega^2$ and angular momentum $J = I\omega$, we can see that fixed angular momentum and linear energy with frequency is consistent with a rotational energy model. $E = \frac{1}{2}I\omega^2 = \hbar\omega$ implies that $I\omega = 2\hbar =$ constant, or that the angular momentum of this rotator is constant. We can also turn this around, and assert that constant angular momentum implies a linear frequency relationship for energy.

Schrodinger Equation with Electromagnetism

I understand Schrodinger's equation to be descended from the Hamilton-Jacobi equation, with modifications to the relationship between amplitude and phase removing non-linearities from the Hamilton-Jacobi equation, allowing linear superposition of states. [5]

As usually taught, we have a process to generate the appropriate Schrodinger's equation from classical formulas.

In QM, energy and momentum are changed to become operators acting on a wavefunction ψ

$$\begin{aligned} E &= i\hbar\frac{\partial}{\partial t} \\ E\psi &= \frac{\partial}{\partial t}(i\hbar\psi) \\ \vec{p} &= -i\hbar\vec{\nabla} \\ \vec{p}\psi &= -i\hbar\vec{\nabla}\psi \end{aligned}$$

In the macroscopic world, the kinetic energy relationship for a free particle

$$E = \frac{p^2}{2m} = \frac{\vec{p}\cdot\vec{p}}{2m}$$

translates to the microscopic world as

$$\begin{aligned} E(\psi) &= \frac{\vec{p}\cdot\vec{p}}{2m}(\psi) \\ i\hbar\frac{\partial}{\partial t}\psi &= \frac{(-i\hbar\vec{\nabla})^2}{2m}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi \end{aligned}$$

Electromagnetic fields possess both energy $q\phi$ and momentum $q\vec{A}$. When using the Schrodinger equation with electromagnetic fields, the canonical energy becomes $E - q\phi$, and the canonical momentum becomes $\vec{p} - q\vec{A}$. For a spinless charged particle in a electromagnetic field $(\phi, \vec{A})$, the Schrodinger equation is

$$\begin{aligned} (E - q\phi)\psi &= \frac{(\vec{p} - q\vec{A})^2}{2m}(\psi) \\ E\psi &= \frac{(\vec{p} - q\vec{A})^2}{2m}(\psi) + q\phi\psi \\ i\hbar\frac{\partial}{\partial t}\psi &= \left(\frac{\left(\vec{p} - q\vec{A}\right)^2}{2m} + q\phi\right)\psi \\ i\hbar\frac{\partial}{\partial t}\psi &= \left(\frac{\left(-i\hbar\vec{\nabla} - q\vec{A}\right)^2}{2m} + q\phi\right)\psi \end{aligned}$$

Expanding out this equation, with the square terms being a dot product, as implied by the classical formula, we have

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi &= \left(\frac{\left(-i\hbar\vec{\nabla} - q\vec{A}\right)^2}{2m} + q\phi\right)\psi \\ 2mi\hbar\frac{\partial}{\partial t}\psi &= \left(-i\hbar\vec{\nabla} - q\vec{A}\right)\cdot\left(-i\hbar\vec{\nabla} - q\vec{A}\right)\psi + 2mq\phi\psi \\ &= \left(i\hbar\vec{\nabla} + q\vec{A}\right)\cdot\left(i\hbar\vec{\nabla} + q\vec{A}\right)\psi + 2mq\phi\psi \end{aligned}$$

As we apply our operators, we need to go one step at a time to avoid subtle errors.

$$
\begin{aligned}
2mi\hbar\frac{\partial}{\partial t}\psi &= \left(i\hbar\vec{\nabla} + q\vec{A}\right)\cdot\left(i\hbar\vec{\nabla} + q\vec{A}\right)\psi + 2mq\phi\psi \\
&= \left(i\hbar\vec{\nabla} + q\vec{A}\right)\cdot\left(i\hbar\vec{\nabla}\psi + q\vec{A}\psi\right) + 2mq\phi\psi \\
&= +i\hbar\vec{\nabla}\cdot(i\hbar\vec{\nabla}\psi) + i\hbar\vec{\nabla}\cdot(q\vec{A}\psi) + q\vec{A}\cdot(i\hbar\vec{\nabla}\psi) + q\vec{A}\cdot(q\vec{A}\psi) + 2mq\phi\psi
\end{aligned}
$$

Now $i\hbar\vec{\nabla}\cdot(q\vec{A}\psi) = iq\hbar(\vec{A}\cdot(\vec{\nabla}\psi)) + iq\hbar(\vec{\nabla}\cdot\vec{A})\psi$, so

$$
2mi\hbar\frac{\partial}{\partial t}\psi = -\hbar^2\vec{\nabla}^2\psi + 2iq\hbar(\vec{A}\cdot(\vec{\nabla}\psi)) + iq\hbar(\vec{\nabla}\cdot\vec{A})\psi + q^2A^2\psi + 2mq\phi\psi
$$

Moving my factor of $2m$ back, now that most of the algebra is done, yields

$$
i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + \frac{iq\hbar}{m}(\vec{A}\cdot\vec{\nabla})\psi + \frac{iq\hbar}{2m}(\vec{\nabla}\cdot\vec{A})\psi + \frac{q^2}{2m}A^2\psi + q\phi\psi
$$

Complex Wavefunction

The spin-free wavefunction $\psi = \psi_r + i\psi_i$ is a complex field. In three dimensional geometric algebra, this maps to a scalar plus trivector combination. As a multivector this is missing vector and bivector terms. We are not surprised however, as this is an incomplete, simplest model. Adding spin, as in the Pauli and Dirac equations, will fill out this multivector.

Writing out the wavefunction in component form, illustrating the missing terms, we have

$$
\psi = (\psi_r, 0, 0, 0, 0, 0, 0, \psi_i)
$$

Returning to our Scrodinger equation, we now separate out the real and imaginary components for ψ.

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi &= -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + \frac{iq\hbar}{m}(\vec{A}\cdot\vec{\nabla})\psi + \frac{iq\hbar}{2m}(\vec{\nabla}\cdot\vec{A})\psi + \frac{q^2}{2m}A^2\psi + q\phi\psi \\
i\hbar\frac{\partial}{\partial t}(\psi_r + i\psi_i) &= -\frac{\hbar^2}{2m}\vec{\nabla}^2(\psi_r + i\psi_i) + \frac{iq\hbar}{m}(\vec{A}\cdot\vec{\nabla})(\psi_r + i\psi_i) + \frac{iq\hbar}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_r + i\psi_i) \\
&\quad + \frac{q^2}{2m}A^2(\psi_r + i\psi_i) + q\phi(\psi_r + i\psi_i)
\end{aligned}
$$

We separate our real and imaginary terms, forming two coupled sets of equations. Repeating our equation from the previous page,

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}(\psi_r + i\psi_i) &= -\frac{\hbar^2}{2m}\vec{\nabla}^2(\psi_r + i\psi_i) + \frac{iq\hbar}{m}(\vec{A}\cdot\vec{\nabla})(\psi_r + i\psi_i) + \frac{iq\hbar}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_r + i\psi_i) \\
&\quad + \frac{q^2}{2m}A^2(\psi_r + i\psi_i) + q\phi(\psi_r + i\psi_i)
\end{aligned}
$$

Separating out parts,

$$
\begin{aligned}
-\hbar\frac{\partial}{\partial t}\psi_i &= -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_r - \frac{q\hbar}{m}(\vec{A}\cdot\vec{\nabla}\psi_i) - \frac{q\hbar}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_i) + \frac{q^2}{2m}A^2(\psi_r) + q\phi(\psi_r) \\
+i\hbar\frac{\partial}{\partial t}\psi_r &= -i\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_i + i\frac{q\hbar}{m}(\vec{A}\cdot\vec{\nabla}\psi_r) + i\frac{q\hbar}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_r) + i\frac{q^2}{2m}A^2(\psi_i) + iq\phi(\psi_i)
\end{aligned}
$$

Clearing out common factors,

$$
\begin{aligned}
\frac{\partial}{\partial t}\psi_i &= \frac{\hbar}{2m}\vec{\nabla}^2\psi_r + \frac{q}{m}(\vec{A}\cdot\vec{\nabla}\psi_i) + \frac{q}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_i) - \frac{q^2}{2\hbar m}A^2(\psi_r) - \frac{q\phi}{\hbar}(\psi_r) \\
\frac{\partial}{\partial t}\psi_r &= -\frac{\hbar}{2m}\vec{\nabla}^2\psi_i + \frac{q}{m}(\vec{A}\cdot\vec{\nabla}\psi_r) + \frac{q}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_r) + \frac{q^2}{2\hbar m}A^2(\psi_i) + \frac{q\phi}{\hbar}(\psi_i)
\end{aligned}
$$

Organizing by variables

$$
\begin{aligned}
\frac{\partial}{\partial t}\psi_r &= +\frac{q}{m}(\vec{A}\cdot\vec{\nabla}\psi_r) + \frac{q}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_r) - \frac{\hbar}{2m}\vec{\nabla}^2\psi_i + \frac{q^2}{2\hbar m}A^2(\psi_i) + \frac{q\phi}{\hbar}(\psi_i) \\
\frac{\partial}{\partial t}\psi_i &= \frac{\hbar}{2m}\vec{\nabla}^2\psi_r - \frac{q^2}{2\hbar m}A^2(\psi_r) - \frac{q\phi}{\hbar}(\psi_r) + \frac{q}{m}(\vec{A}\cdot\vec{\nabla}\psi_i) + \frac{q}{2m}(\vec{\nabla}\cdot\vec{A})(\psi_i)
\end{aligned}
$$

At this point, I've written the Schrodinger equations for electromagnetics without spin in component form. I don't pick up much insight on the relationships between the wavefunction and electromagnetics at this point. (I am looking for association of the wavefunction with magnetic flux density, as in $A = \nabla\psi_r$ or such.)

Next steps are the Pauli and Dirac equations.

References

[1] David J. Griffiths, *Introduction to Electrodynamics* 1981 Prentice Hall, ISBN 0-13-481374-X

[2] Chris Doran and Anthony Lasenby, *Geometric Algebra for Physicists* Cambridge University Press, ISBN 978-0-521-71595-9

[3] Anthony Lasenby and Chris Doran, *Lectures and Handouts 1999* `http://www.mrao.cam.ac.uk/clifford/ptIIIcourse/`

[4] Eric Langyel, Game Developers Conference 2012 Slideset `http://www.terathon.com/lengyel/`

[5] Wolfgang P. Schleich, Marlon O. Scully, "Schrodinger Equation Revisited", Proceedings of the National Academy of Science (US), vol 110, no. 14