Relativistic origins of the Schrödinger equation.

Originally appeared at:
http://sites.google.com/site/peeterjoot/math2009/relwave.pdf

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June 18, 2009

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1. Goals and approach.

Most introductory Quantum texts present some attempt to motivate Schrödinger's equation. The quality, size and approach of each of these ranges widely.

Pauli's Wave Mechanics ([1]) differs from most of these, utilizing relativistic arguments to motivate the Schrödinger equation. His little quantum book starts off, not with the Bohr model or black bodies, but with a lighting fast two page treatment of special relativity.

The Wikipedia Klein-Gordon article ([2]) indicates that this is also the historical approach used initially by Schrödinger.

This blog entry follows Pauli's treatment closely. The starting point will not be "see optics", but an attempt at a logic progression building on basic results of electromagnetism, Fourier techniques, and Lorentz invariance.

From special relativity the Lorentz invariant for energy and momentum $E^2 - c^2\mathbf{p}^2 = (mc^2)^2$ is required. An optional review of how this follows from the definition of Lorentz invariant length is included below. For any sort of complete coverage of special relativity other sources should be consulted.

Fourier transforms will be used to find general solutions of the wave equation for components of the electric or magnetic fields in vacuum

$$\square\mathbf{E} \equiv \frac{1}{c^2}\frac{\partial^2 \mathbf{E}}{\partial t^2} - \boldsymbol{\nabla}^2\mathbf{E} = 0 \tag{1}$$

$$\square\mathbf{B} \equiv \frac{1}{c^2}\frac{\partial^2 \mathbf{B}}{\partial t^2} - \boldsymbol{\nabla}^2\mathbf{B} = 0 \tag{2}$$

Fixing notation, the symmetric transform pair convention will be used

$$\mathcal{F}(f(\mathbf{x})) = \hat{f}(\mathbf{k}) = \frac{1}{(\sqrt{2\pi})^3}\int f(\mathbf{x})\exp\left(-i\mathbf{k}\cdot\mathbf{x}\right)d^3x \tag{3}$$

$$\mathcal{F}^{-1}(f(\mathbf{k})) = f(\mathbf{x}) = \frac{1}{(\sqrt{2\pi})^3}\int \hat{f}(\mathbf{k})\exp\left(i\mathbf{k}\cdot\mathbf{x}\right)d^3k \tag{4}$$

As with Fourier solutions of the heat equation ([3]), the wave equation when expressed in the wave number domain will be a much simpler equation to solve.

A relation between the invariant length of the energy momentum four vector for light and the electrodynamic wave equation solution will be observed. Using this observation, as well as the quantization by frequency from the photoelectric effect, and the DeBroglie hypothesis will allow for formation of a natural relativistic matter wave equation (ie: the Klein-Gordon equation).

Finally, a Taylor expansion of wave function solutions to the Klein-Gordon equation around the rest angular frequency will be made. The end result will be finding the traditional introductory form of the Schrödinger's equation hiding in this relativistic matter wave equation.

2. **Relativity prerequisites.**

In these notes the space time trajectory of a particle will be represented as the pair of locally observable quantities or a column vector equivalent

$$X = (ct, \mathbf{x}) \tag{5}$$

In analogy to the distance invariance with respect to rotation in Euclidean space, the invariant (squared) length of a four vector with respect to Lorentz transformation is

$$X^2 \equiv c^2t^2 - \mathbf{x}^2 \equiv c^2t^2 - \mathbf{x}\cdot\mathbf{x} \tag{6}$$

One can verify without any trouble that such a generalized length is unchanged by rotation

$$\begin{bmatrix} ct' \\ x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\theta & \sin\theta \\ 0 & 0 & -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} ct \\ x \\ y \\ z \end{bmatrix} \tag{7}$$

And also unchanged by Lorentz boost

$$\begin{bmatrix} ct' \\ x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cosh\alpha & -\sinh\alpha & 0 & 0 \\ -\sinh\alpha & \cosh\alpha & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} ct \\ x \\ y \\ z \end{bmatrix} \tag{8}$$

Although the Lorentz length of a four vector does not change under rotation or boost (or composition of the two), that does not mean that this length is a constant. Consider the worldline of a particle at rest at the origin of the observer frame

$$X = (ct, 0) \tag{9}$$

The Lorentz length in this frame is c^2t^2. In general the Lorentz length will be a function of all the coordinates.

Those vectors that have constant length are particularly useful, and can be constructed from scalar multiples of unit vectors. In particular for the time evolution of a particle's worldline from an observer frame one has

$$\frac{dX}{dt} = \left(c, \frac{d\mathbf{x}}{dt}\right) \tag{10}$$

Writing $\mathbf{v} = d\mathbf{x}/dt$, the Lorentz length and corresponding unit vector $V \equiv \frac{dX}{dt}/\sqrt{\left(\frac{dX}{dt}\right)^2}$ are then, respectively,

$$\left(\frac{dX}{dt}\right)^2 = c^2 - \mathbf{v}^2 \tag{11}$$

$$V = \frac{1}{\sqrt{1 - \mathbf{v}^2/c^2}} (1, \mathbf{v}/c) \tag{12}$$

Finally, a scaling by mc of this dimensionless "proper" velocity V yields a vector with dimensions of momentum, the relativistic energy momentum vector (a definition). This vector and its Lorentz length are

$$P \equiv mcV = \frac{1}{\sqrt{1 - \mathbf{v}^2/c^2}} \left(mc^2/c, m\mathbf{v}\right) = (E/c, \mathbf{p}) \tag{13}$$

$$E^2/c^2 - \mathbf{p}^2 = m^2c^2 \tag{14}$$

When the particle is observed at rest ($\mathbf{p} = 0$), the Lorentz length (14) provides the familiar $E = mc^2$ relation. Observe that for the Lorentz length of this energy momentum pairing to come out so nicely constant, the relativistic definitions of energy and momentum are required

$$E \equiv \frac{mc^2}{\sqrt{1 - \mathbf{v}^2/c^2}} = mc^2 + \frac{1}{2}m\mathbf{v}^2 + \cdots \tag{15}$$

$$\mathbf{p} \equiv \frac{m\mathbf{v}}{\sqrt{1 - \mathbf{v}^2/c^2}} = m\mathbf{v} + \frac{1}{2}m\mathbf{v}^3/c^2 + \cdots \tag{16}$$

Only in the small velocity limits are the Newtonian kinetic energy $m\mathbf{v}^2/2$ and momentum $m\mathbf{v}$ the only significant portions of the Taylor series.

3. Light quantization and DeBroglie hypothesis

The notion that light is quantized coming in discrete frequency dependent packets of energy and momentum, a photon, is now a familiar one. In symbols

$$E = h\nu = \hbar\omega \tag{17}$$

With zero mass for a photon, the invariance relation (14) implies that the magnitude of the photon momentum is not independent of ω and in fact must be

$$|\mathbf{p}| = \frac{\hbar\omega}{c} \tag{18}$$

It is customary to write

$$\mathbf{p} = \hbar \mathbf{k} \tag{19}$$

so that the energy momentum four vector for a photon is

$$P = \hbar(\omega/c, \mathbf{k}) \tag{20}$$

DeBroglie's extension ([4]) of the quantum relation for photon energy was to write for non-massless particles

$$h\nu = \frac{mc^2}{\sqrt{1 - \mathbf{v}^2/c^2}} \tag{21}$$

This, together with (14), provides a quantized invariant relation for energy momentum

$$\hbar^2 \left(\frac{\omega^2}{c^2} - \mathbf{k}^2 \right) = m^2 c^2 \tag{22}$$

Once the solution of the wave equation for light (i.e. electromagnetic fields) has been examined, this invariant can be used directly to construct a relativistic wave equation for matter (the Klein-Gordon equation), which is the next step along this path to the traditional non-relativistic Schrödinger equation.

4. **Solution of the relativistic wave equation.**

The next order of business is the solution of the wave equations for the six equations (1), and (2). Writing ψ for one of the components of $\mathbf{E}$ or $\mathbf{B}$ one is left with a scalar homogeneous equation to solve

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2 \right) \psi(t, \mathbf{x}) = 0 \tag{23}$$

Let's begin the attack, applying the transform (3) to both terms of the wave equation

$$\frac{1}{(\sqrt{2\pi})^3} \int \frac{1}{c^2} \frac{\partial^2 \psi(t, \mathbf{x})}{\partial t^2} \exp\left(-i\mathbf{k} \cdot \mathbf{x}\right) d^3x = \sum_{m=1}^{3} \frac{1}{(\sqrt{2\pi})^3} \int \frac{\partial^2 \psi(t, \mathbf{x})}{\partial {x_m}^2} \exp\left(-i\mathbf{k} \cdot \mathbf{x}\right) d^3x \tag{24}$$

Now send the Rigor police on vacation, demanding of ψ that it and its derivatives vanish at the boundaries of the integration region, and that sufficient continuity exists that the time derivatives can be pulled out of the LHS integral. With this demand of good behavior made, pull the time differentiation out of the integral on the LHS and integrate by parts twice on the RHS for

$$\frac{1}{c^2} \frac{\partial^2 \hat{\psi}(t, \mathbf{k})}{\partial t^2} = (-i)^2 \mathbf{k}^2 \hat{\psi}(t, \mathbf{k}) \tag{25}$$

With the exception that integration constant may be a function of $\mathbf{k}$ due to the time partials, this is the harmonic oscillator equation with solution

$$\hat{\psi}_{\pm}(t, \mathbf{k}) = D_{\pm}(\mathbf{k}) \exp(\pm ic|\mathbf{k}|t) \tag{26}$$

Evaluation at $t = 0$ eliminates the exponential, so by (4) the integration constants $D_{\pm}(\mathbf{k})$ may be expressed in terms of the initial time Fourier transforms of the wave function.

$$D_{\pm}(\mathbf{k}) = \hat{\psi}_{\pm}(0, \mathbf{k}) = \frac{1}{(\sqrt{2\pi})^3} \int \psi_{\pm}(0, \mathbf{x}) \exp\left(-i\mathbf{k} \cdot \mathbf{x}\right) d^3x \tag{27}$$

Writing the inverse Fourier transformation (4) now completely specifies the time evolution of these wave function solutions given the initial time field

$$\psi_{\pm}(t, \mathbf{x}) = \frac{1}{(2\pi)^3} \int \psi_{\pm}(0, \mathbf{x}') \exp\left(-i\mathbf{k} \cdot (\mathbf{x}' - \mathbf{x}) \pm ic|\mathbf{k}|t\right) d^3x' d^3k \tag{28}$$

Many interesting things can be done with this result and most will be ignored here. Instead put the evaluational integration into a black box, avoiding any explicit statement of the initial conditions (the Rigor police are still on vacation and they can't catch this blatant disregard for integration order). Dropping explicit $\pm$ subscripts for the $\mathbf{k}$ dependent function of the integral the wave function is now

$$A(\mathbf{k}) = \frac{1}{(2\pi)^3} \int \psi(0, \mathbf{x}') \exp\left(-i\mathbf{k} \cdot \mathbf{x}'\right) d^3x' \tag{29}$$

$$\psi(t, \mathbf{x}) = \int A(\mathbf{k}) \exp\left(i\mathbf{k} \cdot \mathbf{x} \pm ic|\mathbf{k}|t\right) d^3k \tag{30}$$

Inspection shows that $c|\mathbf{k}|$ has the appearance of angular velocity, and a slightly more conventional looking form can be achieved by making this explicit

$$\omega = c|\mathbf{k}| \tag{31}$$

$$\psi(t, \mathbf{x}) = \int A(\mathbf{k}) e^{i(\mathbf{k} \cdot \mathbf{x} \pm \omega t)} d^3k \tag{32}$$

This (constrained) superposition of fundamental harmonics represents a general solution to the wave equation for the components of the electromagnetic field.

Forgetting temporarily the lightlike constraint (31) on angular frequency observe the effect of applying the wave equation operator to (32)

$$\Box\psi(t, \mathbf{x}) = -\int A(\mathbf{k}) \left(\frac{\omega^2}{c^2} - \mathbf{k}^2\right) e^{i(\mathbf{k} \cdot \mathbf{x} \pm \omega t)} d^3k \tag{33}$$

It is clear that functions of the form $f(\mathbf{k}\cdot\mathbf{x} \pm c|\mathbf{k}|t)$ explicitly encode the null vector properties required for light-like worldline trajectories. If this strict proportionality between angular frequency and wave number is relaxed then it is reasonable to assume that such a wave function could then describe phenomena (for massive particles) within the light cone.

In particular observe the effect in (33) if the DeBroglie invariant (22) is applied to (32)

$$\Box\psi(t,\mathbf{x}) = -\frac{m^2c^2}{\hbar^2}\psi \tag{34}$$

This modified wave equation (the Klein-Gordon equation) still describes electric and magnetic fields since photons are massless, but it additionally is not unreasonable seeming as a wave equation for particles with mass.

5. Taylor expansion of the Klein-Gordon equation around the rest angular frequency.

To transition from the covariant Klein-Gordon equation to one with an explicit spacetime split, consider an angular momentum approximation similar to that used for Kinetic energy in (15). From the DeBroglie invariant (22) rearrange for the angular frequency

$$\omega = \frac{mc^2}{\hbar}\sqrt{1+\frac{\hbar^2\mathbf{k}^2}{m^2c^2}} \tag{35}$$

If $(\hbar^2\mathbf{k}^2)/(m^2c^2) < 1$ is small enough a Taylor expansion is possible

$$\omega = \frac{mc^2}{\hbar} + \frac{\hbar\mathbf{k}^2}{2m} + \cdots \tag{36}$$

With the zeroth order term factored out the wave function integral (32) becomes

$$\psi(t,\mathbf{x}) = e^{\pm imc^2t/\hbar}\int A(\mathbf{k})\exp\left(i\left(\mathbf{k}\cdot\mathbf{x} \pm \left(\frac{\hbar\mathbf{k}^2}{2m} + \cdots\right)\right)\right)d^3k \tag{37}$$

It is natural to bundle the integral into a helper variable

$$\psi(t,\mathbf{x}) = e^{\pm imc^2t/\hbar}\psi'(t,\mathbf{x}) \tag{38}$$

Note that there is not actually any requirement to drop the quadratic and higher order terms here. If doing so, one could call this a small momentum approximation. A more accurate description is probably a Taylor expansion around the rest frequency $mc^2/\hbar$.

Application of the wave equation operator to the product (38) is now possible. Let's do this in pieces, starting with the time derivatives

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\left(e^{\pm imc^2t/\hbar}\psi'\right) = \frac{1}{c^2}\frac{\partial}{\partial t}\left(\left(\pm\frac{imc^2}{\hbar}\psi' + \frac{\partial\psi'}{\partial t}\right)e^{\pm imc^2t/\hbar}\right) \tag{39}$$

Second partials give

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}e^{\pm imc^2t/\hbar}\psi' = \frac{1}{c^2}\left(-\left(\frac{mc^2}{\hbar}\right)^2\psi' \pm \frac{2imc^2}{\hbar}\frac{\partial \psi'}{\partial t} + \frac{\partial^2 \psi'}{\partial t^2}\right)e^{\pm imc^2t/\hbar} \tag{40}$$

And finally for the entire wave equation

$$0 = \left(\Box + \frac{m^2c^2}{\hbar^2}\right)\psi = \frac{1}{c^2}\left(\left(\pm 2i\frac{mc^2}{\hbar}\frac{\partial \psi'}{\partial t} + \frac{\partial^2 \psi'}{\partial t^2}\right) - \boldsymbol{\nabla}^2\psi'\right)\exp\left(i\frac{mc^2}{\hbar}t\right) \tag{41}$$

A final rearrangement produces something quite close to the Schrödinger equation as it is probably first seen in the (less general) non-Hamiltonian form

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi' = \mp i\hbar\frac{\partial \psi'}{\partial t} - \frac{\hbar^2}{2mc^2}\frac{\partial^2 \psi'}{\partial t^2} \tag{42}$$

There are two notable differences, one is the sign and the other is the second order time partial. Comparisons in size for coefficients of this wave equation have to be made relative to the other coefficients since $\hbar$ is already a small quantity, however, if m is the mass of an electron this second time partial coefficient is of the order $\hbar/(m_e c^2) \approx 10^{-21}$ (seconds). This is small enough that omitting it is justifiable.

Once that term is dropped two equations are left, one of which is the three dimensional potential free Schrödinger's equation.

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi' = \mp i\hbar\frac{\partial \psi'}{\partial t} \tag{43}$$

The alternation in sign is suggestive of conjugate behavior, but it is helpful to know to expect this in the first place!

This presentation attempts to show that the Schrödinger equation (43) has some deeply rooted relativistic origins. When the spatial and time derivatives in the Schrödinger equation aren't even of the same order it isn't obvious that quantum mechanics and relativity have any sort of association with each other. This is reflected in treatments of Quantum mechanics, where many introductory QM texts will not mention relativity at all, except perhaps to note that the Schrödinger equation is not valid at speeds where v/c is significant. Finding a statement like "There is no inherent connection between special relativity and quantum mechanics" ([5]), shows that this apparent disconnect goes both ways.

There are obvious deficiencies in this treatment. In particular the quantization of light was glossed over, and if it had been pursued, would be grossly wrong. Part of the problem is that solutions of Maxwell's equations in vacuum are not entirely equivalent to six independent wave equations for the components of the fields. Additional constraints are also imposed by Maxwell equations, introducing a coupling between the field components. For example in a linearly polarized plane wave one has $\mathbf{B} = \hat{\mathbf{k}} \times \mathbf{E}$, and the triplet of $\mathbf{E}$, $\mathbf{B}$, and $\hat{\mathbf{k}}$ (the propagation direction) form a set of mutually perpendicular vectors ([6]). An expectation calculation based on a quantized light equation that neglects this coupling cannot possibly recover Maxwells equations. One could perhaps start with the simpler four vector potential Maxwell wave equations $\partial_\mu \partial^\mu A^\nu = 0$ under the Lorentz gauge $\partial_\mu A^\mu = 0$. That would reduce the problem to dealing with only four coupled equations intead of six, and the coupling is considerably simpler. Perhaps if this were pursued more carefully one would end up with QFT. Thats an interesting potential digression, but not the goal here and now.

As mentioned previously the goal was really to highlight some of the relativistic connections of quantum mechanics. A secondary goal was personal, having never seen any single completely satisfying attempt to motivate the Schrödinger equation, it seemed reasonable to attempt enunciation of this myself. Given my current point in time understanding of mathematics and physics, Pauli's SR based motivation was found to be one of the most logical, had no steps that were particularly surprising, but suffered from too much brevity. This made it a good starting point, and perhaps the result is slightly more accessible.

Somebody who knows Quantum Mechanics well (or Quantum field theory) would likely consider these notes completely backwards. One can logically go from Quantum to classical, but going the other way around is impossible. That is quite likely true, however to somebody like this author, just starting to learn QM, pointing this out is not particularly helpful seeming.

6. Some other approaches for motivating the Schrödinger's equation to compare with.

Many other methods of motivating the Schrödinger equation are considerably simpler and shorter that this one, however this may however come at the expense of a corresponding excess of magic steps.

French and Taylor ([7]), arrives at the specialization of Schrödinger's equation for a particle in a one dimensional potential

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar\frac{\partial \psi}{\partial t} \tag{44}$$

in only seven pages with no mathematics or physics unfamiliar to second year engineering undergrads (this is a remarkable success IMO). It is worth noting that they include a disclaimer upfront "we ... simply try to make the form of the equation plausible". The plausibility arguments found in this text are not uncommon, and can be found for example (without the surrounding discussion of the text) in the "Short heuristic derivation" of the Wikipedia's Schrödinger's equation article ([8]).

Calling these derivations is justifiably debatable and is perhaps the origin of statements like "Schrödinger's equation cannot be derived" ([9]).

Considerable care is required to construct logically consistent arguments that motivate the quantum wave equation in a fashion that is not simply playing the equation in reverse. Bohm's Quantum Theory ([10]) contains such a carefully crafted treatment. The cost of this presentation is that it takes nine chapters and two hundred pages to get to the starting point of many other introductory Quantum texts.

Heisenberg apparently was able to build his matrix mechanics using observational data (spectral measurements) as a starting point. That would be a desirable motivational attempt, but there also appears to be agreement that his construction was something that nobody else in the right mind would have thought of. Susskind even says in one of his lectures of this "I don't know what he was smoking"!

Susskind's method of teaching QM goes straight to the point, and he uses nothing but Dirac's axiomatic formulation. There's a lot of abstraction in that approach and it is perhaps not the most palatable technique available to a new learner.

Perhaps agreeing with a it cannot be derived opinion, the text of Liboff ([11]) appears to take a "let's calculate approach". There is little attempt to motivate the equation, instead presenting the equation rather abstractly as an operatorizing of the Hamiltonian. This requires the magic identification $\mathbf{p} \sim -i\hbar\boldsymbol{\nabla}$, something harder to make plausible in a classical context. Instead one is left to learn its characteristics by using it. This engineering approach has some merits but must also contribute to much of the mystery and confusion surrounding the subject. The most classic example of this is Feynman's famous quote "I think I can safely say that nobody understands quantum mechanics".

References

[1] W. Pauli. *Wave Mechanics*. Courier Dover Publications, 2000.

[2] Wikipedia. Klein-gordon equation — wikipedia, the free encyclopedia [online]. 2009. [Online; accessed 5-May-2009]. Available from: `http://en.wikipedia.org/w/index.php?title=Klein%E2%80%93Gordon_equation&oldid=288115284`.

[3] Prof. Brad Osgood. The Fourier Transform and its Applications. [online]. Available from: `http://www.stanford.edu/class/ee261/book/all.pdf`.

[4] A. F. Kracklauer. Louis de Broglie (Thesis): On the theory of Quanta [online]. Available from: `http://www.ensmp.fr/aflb/LDB-oeuvres/De_Broglie_Kracklauer.pdf` [cited 19 June 2009].

[5] H. Goldstein. *Classical mechanics*. Cambridge: Addison-Wesley Press, Inc, 1st edition, 1951.

[6] JD Jackson. *Classical Electrodynamics Wiley*. 2nd edition, 1975.

[7] A.P. French and E.F. Taylor. *An Introduction to Quantum Physics*. CRC Press, 1998.

[8] Wikipedia. Schrdinger equation (short heuristic derivation) — wikipedia, the free encyclopedia [online]. 2009. [Online; accessed 29-June-2009]. Available from: `http://en.wikipedia.org/w/index.php?title=Schr%C3%B6dinger_equation&oldid=299325461`.

[9] Carl R. (Rod) Nave. Free particle approach to the Schrodinger equation [online]. Available from: `http://hyperphysics.phy-astr.gsu.edu/Hbase/quantum/Schr2.html` [cited 19 June 2009].

[10] D. Bohm. *Quantum Theory*. Courier Dover Publications, 1989.

[11] R. Liboff. *Introductory quantum mechanics*. 2003.