Quantum mechanics in space and time

Tunneling

Wave packet spreading

What is quantum mechanics?

“Framework”

Standard model

Hopeful models

Probability Density Versus $|\psi(x)|^2$

They’re not the same, and it’s interesting

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(1) A Motivating Example

Non-relativistic limit of Dirac electron

The relativistic (Dirac) theory suggests a correction of to probability density in the effective description of non-relativistic electrons:

$$\rho(x) = \Psi^{\dagger}(x)\Psi(x)$$

$$\Psi \approx \left(\psi, \frac{\sigma \cdot p}{2m}\psi\right)^{T}$$

$$\rho \rightarrow \psi^{*}\psi + \frac{1}{4m^{2}}\nabla\psi^{*}\nabla\psi$$

The correction term is of order v^2/c^2. It is usually - but not always? - quite small for practical purposes.

It removes “dead spots”, gets more competitive near steep potential gradients, comes into highly excited states …

… raises conceptual issues … and maybe suggests opportunities.

(1a) Addendum

Non-relativistic limit of Dirac electron, made simple

$$i(\gamma^0\partial_0 - \vec{\gamma}\cdot\vec{\nabla} - m)\Psi \;=\; 0$$

$$\begin{pmatrix} i\nabla_0 - m & -i\sigma\cdot\nabla \\ i\sigma\cdot\nabla & -i\nabla_0 - m \end{pmatrix} \begin{pmatrix} \tilde{\psi} \\ \tilde{\lambda} \end{pmatrix}$$

$$(\psi,\lambda) \;\equiv\; e^{-imt}(\psi,\lambda)$$

N. B. It might be better to take out $m + A_0$

$$\begin{aligned} i\nabla_0\psi - i\sigma\cdot\nabla\lambda &= 0 \\ i\sigma\cdot\nabla\psi + (-i\nabla_0 - 2m))\lambda &= 0 \end{aligned}$$

$$
\begin{aligned}
i\nabla_0\psi - i\sigma\cdot\nabla\lambda &= 0 \\
i\sigma\cdot\nabla\psi + (-i\nabla_0 - 2m))\lambda &= 0
\end{aligned}
$$

$$
\begin{aligned}
\lambda &= \lambda_0 + \lambda_1 \\
\lambda_0 &= \frac{i\sigma\cdot\nabla\psi}{2m + A_0}
\end{aligned}
$$

Substituting for λ_0 and dropping λ_1, for $A_0 << m$ the first line becomes the Pauli equation (Schrödinger + magnetic moment).

To next order in $\frac{A_0}{m}$ we get a spin-orbit term and a "Darwin" term $\propto iE\cdot p$ *.

$$-i\partial_t\lambda_0 - i\nabla_0\lambda_1 - 2m\lambda_1 \;=\; 0$$

$$\lambda_1 \;\approx\; -i\frac{1}{2m+A_0}\nabla_0\frac{i\sigma\cdot\nabla\psi}{2m+A_0}$$

$$i\nabla_0\psi - i\sigma\cdot\nabla\Big(\frac{i\sigma\cdot\nabla\psi}{2m+A_0} - i\frac{1}{2m+A_0}\nabla_0\frac{i\sigma\cdot\nabla\psi}{2m+A_0}\Big) \approx 0$$

With $\overrightarrow{A} = 0$ and $A_0 << m$ we get the modified Schrödinger equation we'll be focusing on.

It is straightforward in principle to relax those conditions.

The next correction to λ brings in second-order time derivatives of ψ, which modify the initial value problem.

Those can probably be handled sensibly, though it's not straightforward. But at some point we have to ask ourselves why we're not just solving the Dirac equation. (See Lecture 3.)

(2) A Basic Question

What's a Point?

Textbooks on basic quantum mechanics, when come to make contact with the empirical world, tend to postulate that there is such a thing as a particle that has amplitudes at different times and places - i.e., a wave-function $\psi(x, t)$ - and that $\psi^*\psi$ represents the probability density for it to “be there then”.

Here's how an argument might go:

1. A particle is associated with a dynamical variable x, its position. We can diagonalize it, and then label particle states by their coefficients in that basis, using the wave-function $\psi(x)$ in

$$|\psi\rangle = \int dx\, \psi(x)\, |x\rangle$$

2. Assuming that the wave function for the ket $\langle\psi|$ associated with $|\psi\rangle$ is ψ^*, the amplitude to observe the eigenvalue x_0 is then proportional to

$$\langle\psi|\,\delta(x-x_0)\,|\psi\rangle \;=\; \int\int dx_2 dx_1 \psi^*(x_2)\delta(x_1-x_0)\psi(x_1)\langle x_2|x_1\rangle$$

3. If we make the "obvious" choice for a structureless point

$$\langle x_2|x_1\rangle_s \;=\; \delta(x_2-x_1)$$

then the integral reduces to $\psi^*(x_0)\,\psi(x_0)$

We will challenge assumption 3. We could (alternatively) challenge 2.

But we can contemplate other possibilities. An interesting possibility that preserves locality, translation symmetry, and parity is

$$\langle x_2 | x_1 \rangle \;=\; (1 - a\partial_{x_2}^2)\,\delta(x_2 - x_1)$$

This amounts to a choice of measure.

It leads (in 3D) to

$$\langle \psi | \,\delta(x - x_0)\, | \psi \rangle \;=\; \psi^* \psi \;+\; a\,\nabla\psi^* \cdot \nabla\psi$$

In this way, we've reverse-engineered the Dirac-inspired form.

In other parts of the textbooks, it is emphasized that we should be careful about assigning physical reality to things that we don't measure.

Many practical measurements ultimately come down to interactions with electromagnetic fields. "Electron position" offers a convenient way to discuss charge density. From this perspective electron probability density is a secondary rather than a primary concept. The fundamental object is the charge density associated with a $U(1)$ symmetry and a conserved current.

(3) Derivation from Lagrangian

Modified Schrödinger Equation and Conserved Current

The a term arises within a broader “philosophy”:

1. Quantum theory can/should be built up from Lagrangians

2. Symmetry, locality and simplicity* guide us in selecting interesting Lagrangians

3. *Polynomial terms of small degree / low mass dimension are especially worthy of consideration.

These considerations apply to other kinds of particles and quasiparticles, besides electrons.

Let’s see what the equations this philosophy suggests tell us:

$$0 = \frac{\delta L}{\delta \psi}\psi + \frac{\delta L}{\delta \partial_t \psi}\partial_t \psi + \frac{\delta L}{\delta \nabla \psi}\nabla \psi + \frac{\delta L}{\delta \partial_t \nabla \psi}\partial_t \nabla \psi - (\psi \to \psi^*)$$

U(1) Symmetry

$$0 = \frac{\delta L}{\delta \psi} - \partial_t \frac{\delta L}{\delta \partial_t \psi} - \nabla \frac{\delta L}{\delta \nabla \psi} + \partial_t \nabla \frac{\delta L}{\delta \partial_t \nabla \psi}$$

Equation of Motion

$$0 = (\partial_t \frac{\delta L}{\delta \partial_t \psi} + \nabla \frac{\delta L}{\delta \nabla \psi} - \partial_t \nabla \frac{\delta L}{\delta \partial_t \nabla \psi})\psi$$

$$+ \frac{\delta L}{\delta \partial_t \psi}\partial_t \psi + \frac{\delta L}{\delta \nabla \psi}\nabla \psi + \frac{\delta L}{\delta \partial_t \nabla \psi}\partial_t \nabla \psi - (\psi \to \psi^*)$$

$$= \partial_t(\frac{\delta L}{\delta \partial_t \psi}\psi) + \nabla(\frac{\delta L}{\delta \nabla \psi}\psi)$$

$$= \partial_t(\frac{\delta L}{\delta \partial_t \nabla \psi}\nabla \psi) - \nabla(\partial_t \frac{\delta L}{\delta \partial_t \nabla \psi}\psi)$$

$$\mathrm{Im}\left(\quad + \quad \right) = 0$$

Conservation Law

The usual Schrödinger equation can be derived from the Lagrangian

$$L^{(0)} = \frac{i}{2}\psi^* \overset{\leftrightarrow}{\partial_t} \psi + \frac{1}{2m}\nabla\psi^*\nabla\psi - V\psi^*\psi$$

It supports a conserved probability current

$$\mathrm{Im}\Big(\frac{\delta L}{\delta\partial_t\psi}\psi + \frac{\delta L}{\delta\partial_t\nabla\psi}\nabla\psi, \frac{\delta L}{\delta\nabla\psi}\psi - \partial_t\frac{\delta L}{\delta\partial_t\nabla\psi}\psi\Big)$$

whose 0 component is the probability density $\boldsymbol{\psi^*\psi}$.

The a term in probability density arises from adding to $L^{(0)}$ the term

$$L^{(1)} = \frac{ia}{2} \nabla\psi^* \overset{\leftrightarrow}{\partial_t} \nabla\psi$$

(The modification suggested by the Dirac equation corresponds to $a = \frac{1}{4m^2}$.)

Having the Lagrangian, we can shift from assumption to deduction.

From $L^{(0)} + L^{(1)}$ we derive the modified Schrödinger equation (equation of motion)

$$i(\partial_t \psi - a\partial_t \nabla^2 \psi) = -\frac{1}{2m}\nabla^2\psi + V\psi$$

and the probability current

$$\left(\psi^*\psi + a\nabla\psi^* \cdot \nabla\psi,\ \mathrm{Im}\,(\frac{1}{2m}\nabla\psi^*\psi - \frac{a}{2}\partial_t(\psi\nabla\psi^*))\right)$$

Note that the equation of motion and the number conservation equation are not independent.

When the dynamics follows the modified Schrödinger equation, $\psi^*\psi$ is not conserved, and cannot be interpreted as a probability density.

Given the modified Schrödinger equation, or the Lagrangian it came from, the modified probability density is mandatory.

(4) Basic Examples

Some Surprising Dynamics

For stationary states, with $\psi(x,t) = \psi(x)e^{-iEt}$, the a term the modified Schrödinger equation becomes*

$$E(1 - a\nabla^2)\,\psi = -\frac{1}{2m}\nabla^2\psi + V\psi$$

Thus, the a term has the same form as the mass term. We capture its influence in an effective mass

$$\frac{1}{2m_{\text{eff.}}} = \frac{1}{2m} - aE$$

$$m_{\text{eff.}} = \frac{m}{1 - 2amE}$$

*Note: Here we have coupled V to $\psi^*\psi$. It would be interesting - and maybe more “photon-like” - to consider coupling to the conserved density. We’re doing that.

This enables us, when we have a formula for how energy ϵ depends on m in the ordinary ($a = 0$) Schrödinger equation, to infer E in the general situation.

For the harmonic oscillator, after some algebra we find the discrete spectrum

$$E_n = \epsilon_n(\sqrt{1 + (\epsilon_n am)^2} - \epsilon_n am)$$

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$$\epsilon_n = (n + \frac{1}{2})\,\omega$$

- The energy levels are no longer equally spaced
- The corrections become more significant as n grows
- There is a limiting energy

$$E_{\text{ion.}} = \frac{1}{2am}$$

for the discrete spectrum!

That last fact has a clear and remarkable explanation.

As the energy grows, the effective mass also grows, until at $E_{\text{ion.}}$ it diverges. Then it becomes negative.

Note that in a sense infinitely large positive and infinitely large negative mass are close to one another, since it is m^{-1} that appears in the Schrödinger equation.

Classically, a negative mass particle will *accelerate into* a rising potential.

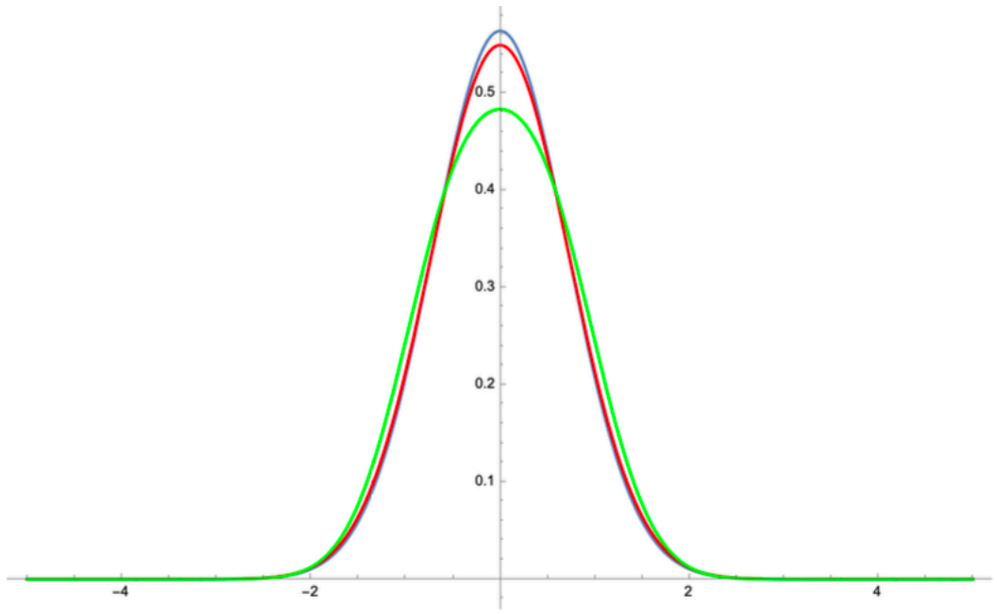
Quantum mechanically we find, from $E - V \sim \frac{k^2}{2m}$, that when $m < 0$ forbidden regions (where $V > E$) are associated with real values of k — that is, with oscillatory behavior ..

.. and the more forbidden, the faster the oscillation! This corresponds beautifully to the acceleration suggested classically.

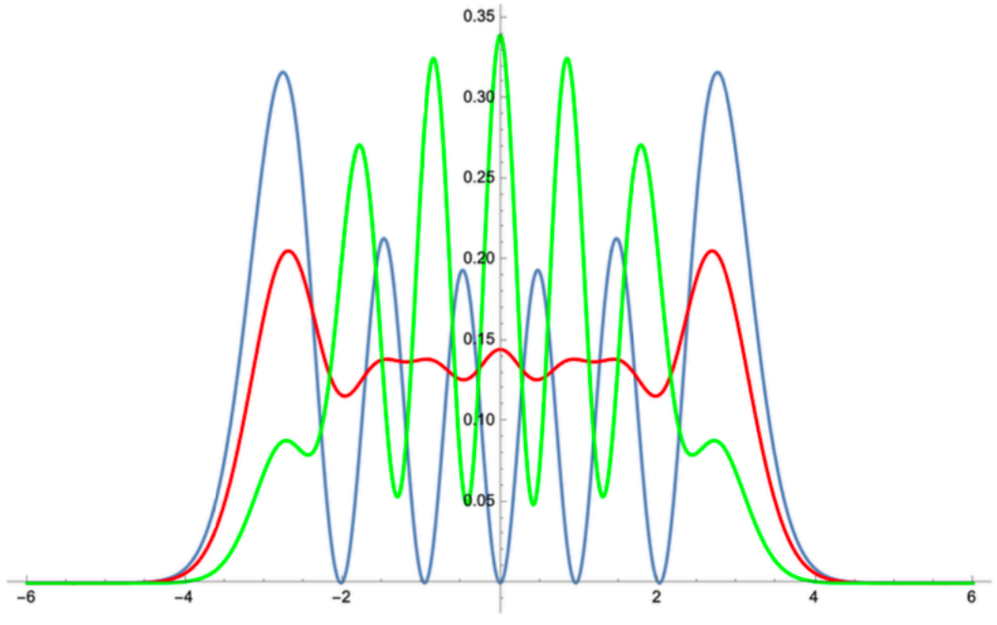
Thus, the modified Schrödinger equation allows a particle to “ionize” its way out of an harmonic oscillator potential!

This under-barrier behavior is reminiscent of the famous Klein paradox. (See Supplement 4a.)

Here it is occurring in the framework of a fully consistent set-up, where in particular energy is bounded below, so maybe we should try to take it seriously



(a) Ground state



(b) Fifth excited state

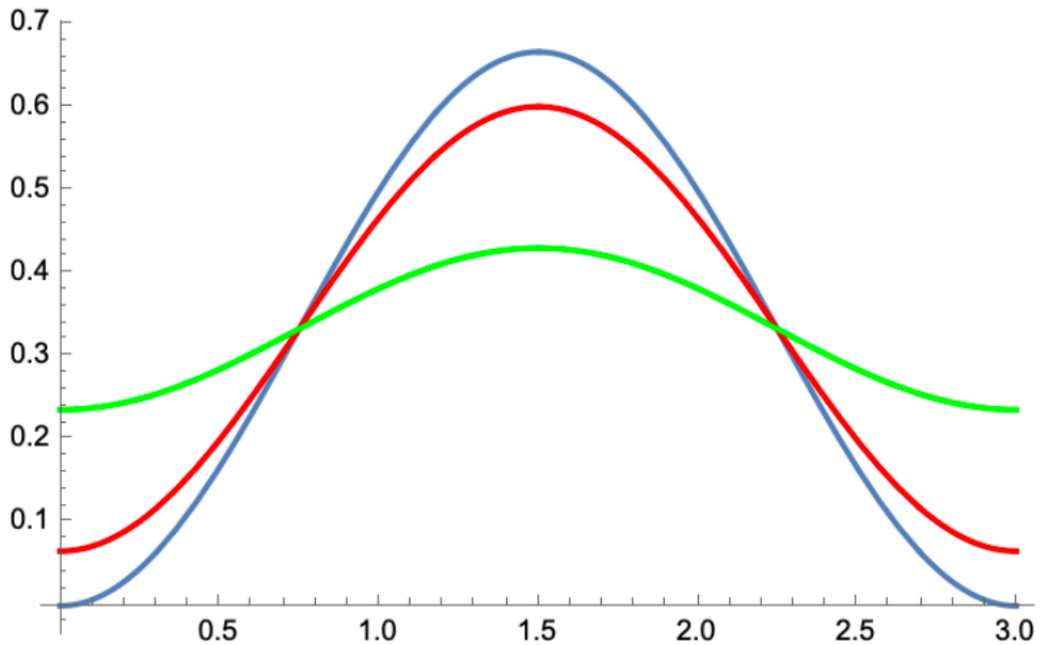
Figure 1: Corrected probability density of the harmonic oscillator from Eqn. (18), where the states are modified using the effective mass from Eqn. (26). Here, $m = \omega = 1$, for $a = 0$ (blue), $a = 0.1$ (red), $a = 0.5$ (green).

For an infinite well we find

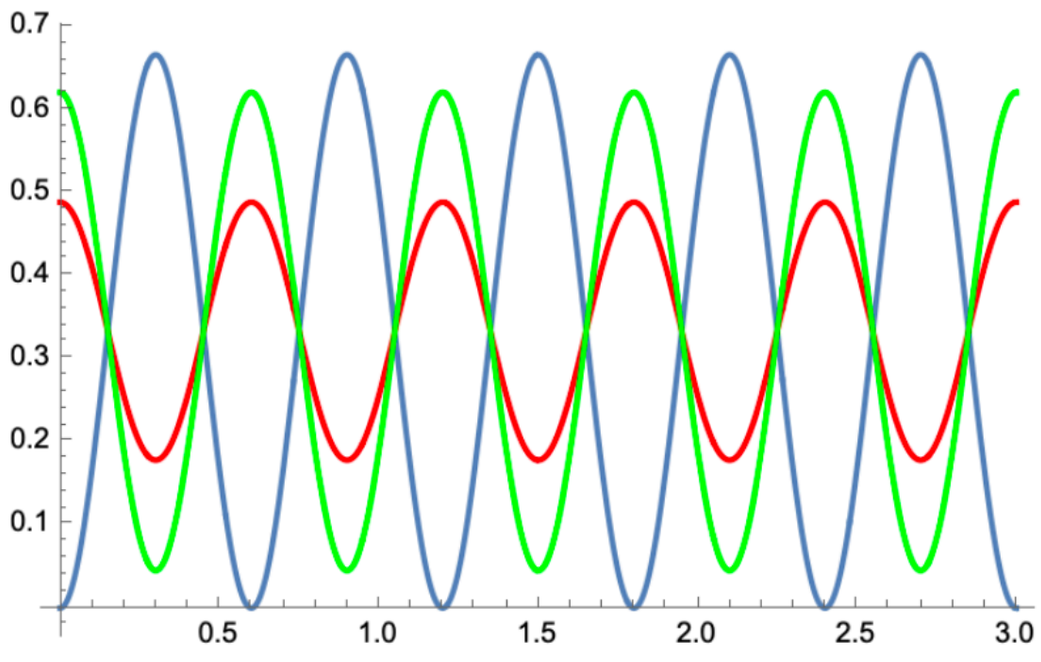
$$E_n = \frac{\epsilon_n}{1 + 2am\epsilon_n}.$$

$$\epsilon_n = \frac{n^2\pi^2}{2mL^2}$$

Again we have the limiting energy $(2am)^{-1}$. But now there is no possibility for ionization; the energy is simply bounded above!



(a) Ground state



(b) Fifth excited state

Figure 2: Corrected probability density of the infinite well, from Eqn. (18) with $L = 3$, for $a = 0$ (blue), $a = 0.1$ (red), $a = 0.5$ (green).

For a free particle we have the dispersion relation

$$\omega(1 + ak^2) = \frac{k^2}{2m}$$

leading to phase and group velocities

$$\frac{\omega}{k} = \frac{k}{2m}\frac{1}{1 + ak^2}$$

$$\frac{d\omega}{dk} = \frac{k}{m}\frac{1}{(1 + ak^2)^2}.$$

Thus, the highly excited waves slow down!

As we'll see shortly, the energy associated with the wave $e^{i(kx-\omega t)}$ is ω while the momentum is $k(1+ak^2)$.

Again we encounter the limiting energy $(2am)^{-1}$.

(4a) Addendum

Step Potential / Klein Paradox

The Klein paradox is a classic of quantum field theory. It concerns the behavior of the Dirac equation in the presence of a high potential step.

When $\Delta\phi > 2m$ the wave-function oscillates rather than dies in the classically forbidden region.

In the context of quantum field theory, this gets interpreted quite differently from barrier penetration.

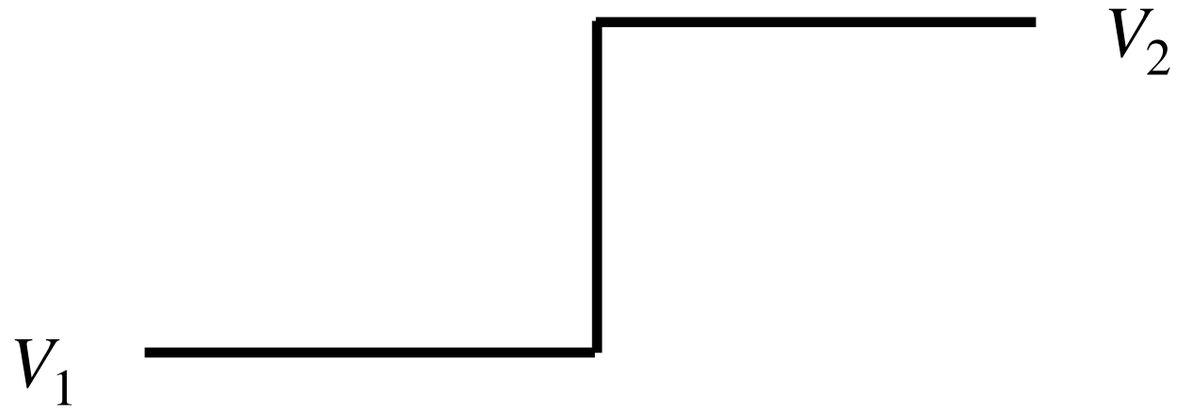
The particle is totally reflected, but induces pair creation.

In our examples we don’t have negative energies, or pairs, so the interpretation must be self-contained.

Though it seems strange on first encounter, I don’t see anything wrong with an effective mass going negative at high energy.

For a direct comparison, following Klein, let's look at the step problem.

First, with the $V\psi^*\psi$ interaction:



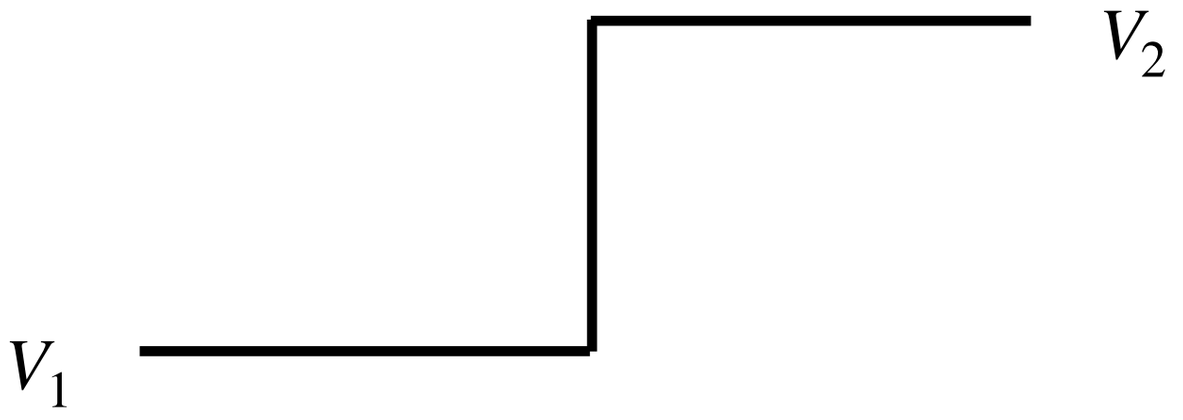
$$k^2 = \frac{(E - V_j)2m}{1 - 2maE}$$

If $E < (2ma)^{-1}$, all is normal: allowed region allowed, forbidden region forbidden, quantitative changes in transmission and reflection.

If $E > (2ma)^{-1}$, this is reversed: “allowed” region forbidden, “forbidden” region allowed. The anomalous allowed region only occurs if $V_j > E > (2ma)^{-1}$ (i.e., large, “Klein-ish” potentials).

Second, with the $V = A_0$ minimal coupling interaction:

$$\left((i\partial_t - V) - a\partial_x(i\partial_t - V)\partial_x\right)\psi = -\frac{1}{2m}\partial_x^2\psi$$



$$E - V_j = \frac{k_j^2}{2m(1 + ak_j^2)}$$

Here the a term (with $a > 0$) introduces quantitive changes, but the qualitative behavior is basically “normal”.

(There is also a singular interaction at the jump.)

(5) Local Energy and Momentum Currents

Derived from Lagrangian Dynamics

We can derive other conservation laws too, as Noether's theorem assures us.

It is instructive, and reassuring, to get them directly from the Lagrangian equations.

Here I will indicate the logic and the results, foregoing the algebra:

To get energy conservation, multiply the equation of motion for ψ with $\partial_t \psi^*$, add the complex conjugate, and re-organize.

One finds $\partial_t \varepsilon + \nabla j_\varepsilon = 0$, with

$$\varepsilon = \psi^* V \psi + \frac{1}{2m} \nabla \psi^* \cdot \nabla \psi$$

Same, same but different.

$$j_\varepsilon = ia(\partial_t \psi^* \partial_t \nabla \psi - \partial_t \nabla \psi^* \partial_t \psi) - \frac{1}{2m}(\partial_t \psi^* \nabla \psi + \nabla \psi^* \partial_t \psi)$$

To get momentum conservation - and to identify stresses - multiply the equation of motion for ψ by $\partial_k \psi^*$, add the complex conjugate, and re-organize.

One finds $\partial_t \pi_k + \partial_l \tau_{lk} = -\psi^* \partial_k V \psi$, with

$$\pi_k = -2\,\mathrm{Im}\,(\partial_k \psi^* \psi + a\,\nabla\psi^* \partial_k \nabla\psi)$$

$$\tau_{lk} = \frac{1}{m}\,\mathrm{Re}\,(\psi^* \partial_k \partial_l \psi - \partial_l \psi \partial_k \psi^*) - 2a\,\mathrm{Im}\,(\partial_k \psi^* \partial_t \partial_l \psi + \psi \partial_k \partial_t \partial_l \psi^*)$$

(6) Hamiltonian Formulation

Closing the Loop

Time-energy duality is embodied in the equation

$$i\partial_t \psi \;=\; H\psi$$

In our context, this identifies

$$H \;=\; (1 - a\nabla^2)^{-1}\,\left(-\frac{1}{2m}\nabla^2 + V\right)$$

Note that $1 - a\,\nabla^2$ is invertible for $a \geq 0$. The inverse is non-local, but can be expressed as a simple convolution in space.

How is this result consistent with the unmodified expression for energy density?

The point is that when we take expectation values the ket vector has an extra factor, stemming from

$$|\psi\rangle = \int \psi(x)\,|x\rangle \Rightarrow \langle\psi| = \int \psi^*(y)\langle y|$$

with the non-standard overlap we saw earlier. This factor can also be regarded as a non-standard measure in spatial integrals.

Putting it in, we find

$$\langle \psi | H | \psi \rangle = \int \psi^* (1 - a\nabla^2) H \psi = \int \psi^* \epsilon \psi$$

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Going back to the Lagrangian: it tells us that the canonical conjugate to ψ is $(1 - a\nabla^2)\,\psi^*$. Thus, expressions that are simple and local in terms of ψ and ψ^* will be non-local and generally awkward in terms of canonical variables. Presumably, in the end they lead to the same results.

(7) Extensions

Things Worthy of Further Exploration

1. For two-component spinor fields, we could also include $\Delta L \propto \mathrm{Re}\ \psi^* \sigma \cdot \nabla \partial_t \psi$, which has even lower dimension. It violates parity, however, and it involves a conserved charge density that is not necessarily positive.

Positivity can be restored by combining this with the sort of term we've been discussing, in the form $\Delta L \propto \mathrm{Re}\ \psi^* (1 + ib\sigma \cdot \nabla)^2 \partial_t \psi$.

2. One could also explore, at a formal level, the use of general kernels, in the form

$$\Delta \int L = \int dx\, dy\, \psi^*(x)\, K(x,y)\, i\partial_t \psi(y)$$

with suitable reality and positivity properties.

3. There is no difficulty in extending the preceding discussions to many-body wave functions and to models with more complex conventional interactions. Thus we can infer modified equations of state for quantum ideal gases, modified densities of states, and so forth.

4. Since the a term and its relatives improve ultraviolet behavior, one might consider their use as regulators in field theory. They are free of the "ghosts" that plague covariant higher-derivative regulators.