A notable quasi-relativistic wave equation and its relation to the Schrödinger, Klein-Gordon, and Dirac equations

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{(\gamma_V + 1)m} \frac{\partial^2}{\partial x^2} \psi(x,t)$$

Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi_{Sch}(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{Sch}(x,t)$$

$$\gamma_V = \frac{1}{\sqrt{1 - \frac{V^2}{c^2}}} \approx 1 \ \text{ when } V^2 << c^2$$

References

6. "A notable quasi-relativistic wave equation and its relation to the Schrödinger, Klein-Gordon, and Dirac equations," L. Grave de Peralta, *Canadian Journal of Physics* (under review, 2020).

5. "Exact quasi-relativistic wave functions for Hydrogen-like atoms," L. Grave de Peralta, *Scientific Reports* **10**, 14925 (2020).

4. "Quasi-relativistic description of a quantum particle moving through one-dimensional piecewise constant potentials," L. Grave de Peralta, *Results in Physics,* **18**, 103318 (2020).

3. "Did Schrödinger have other options?" L. Grave de Peralta, *European Journal of Physics*, https://doi.org/10.1088/1361-6404/aba7dc (in press, 2020).

2. "Quasi-relativistic description of Hydrogen-like atoms," L. Grave de Peralta, *Journal of Modern Physics* **11**, 788-802 (2020).

1. "Natural extension of the Schrödinger equation to quasi-relativistic speeds," L. Grave de Peralta, *Journal of Modern Physics* **11**, 196-213 (2020).

Acknowledgments

Prof. Bill Poirier

Dr. Ankit Pandey

$$\widehat{H} = \cfrac{\hat{p}^2}{2m + \cfrac{\hat{p}^2}{2m + \cfrac{\hat{p}^2}{2m + ...}}}$$

A. Pandey, B. Poirier, and L. Grave de Peralta, "Drawing a photon trajectory: An unorthodox study of bidirectional light-like waves,", *Foundations of Physics*, (under review, 2020).

Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi_{Sch}(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{Sch}(x,t)$$

Quantum description of a free particle with mass m and spin-0

Quasi-relativistic wave equation

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{(\gamma_V + 1)m} \frac{\partial^2}{\partial x^2} \psi(x,t)$$

$$\hat{E} = \hat{K} = i\hbar \frac{\partial}{\partial t}, \qquad \hat{p} = -i\hbar \frac{\partial}{\partial x} \qquad (1)$$

Non-relativistic relation between K and p:

$$K = \frac{p^2}{2m} \qquad (2)$$

Substituting (1) into (2):

$$i\hbar \frac{\partial}{\partial t} \psi_{Sch}(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{Sch}(x,t)$$

Relativistic relation between K and p:

$$K = \frac{p^2}{(\gamma_V + 1)m} \qquad (3)$$

Substituting (1) into (3):

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{(\gamma_V + 1)m} \frac{\partial^2}{\partial x^2} \psi(x,t)$$

Some results: 1D piecewise constant potentials

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi(x,t) + U(x)\psi(x,t) \quad (1)$$

Looking for a solution of the form:

$$\psi(x,t) = X_K(x)e^{-\frac{i}{\hbar}E't}, \quad E' = K + U \quad (2)$$

Then:

$$\frac{d^2}{dx^2}X_K(x) + \kappa^2 X_K(x) = 0 \quad (3)$$

$$\kappa = \frac{p}{\hbar} = \frac{1}{\hbar}\sqrt{(\gamma_V+1)mK} = \frac{1}{\hbar}\sqrt{(\gamma_V+1)m(E'-U)} \quad (4)$$

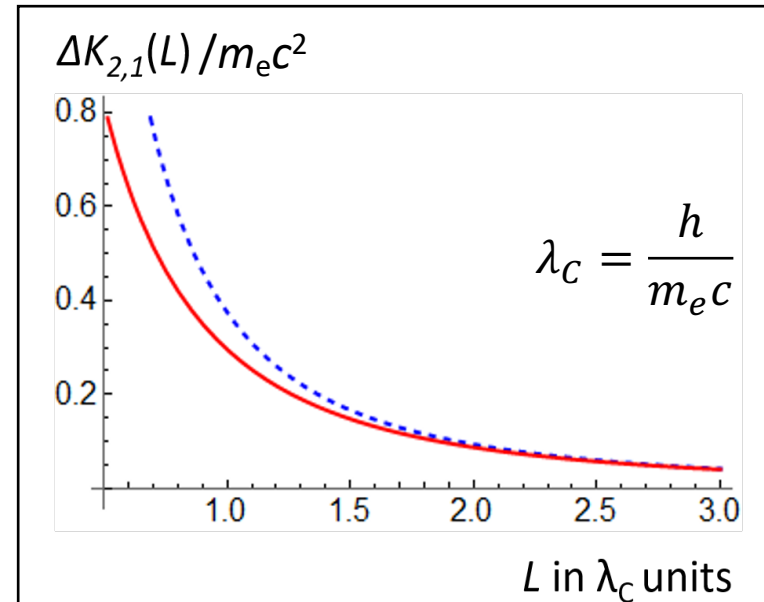The values of κ are determined by the boundary conditions and $K = E' - U$:

$$K = \frac{\hbar^2\kappa^2}{(\gamma_V+1)m} \quad (5) \quad \text{But:} \quad K = (\gamma_V-1)mc^2 \quad (6)$$

Then:

$$\gamma_V{}^2 = 1 + \left(\frac{\hbar k}{mc}\right)^2 \Rightarrow \quad K = \frac{\hbar^2\kappa^2}{\left[1+\sqrt{1+\left(\frac{\hbar k}{mc}\right)^2}\right]m} \quad (7)$$

Infinite rectangular well

From Eq. (3): $X_n(x) = \sqrt{\frac{2}{L}}\,Sin\left(\frac{n\pi}{L}x\right), \kappa_n = \frac{n\pi}{L}, n = 1,2,\dots$

$\Delta K_{2,1}(L)/m_e c^2$

$\lambda_C = \dfrac{h}{m_e c}$

L in λ_C units

$\Delta K_{2,1}$ calculated for $m = m_e$ using (**continuous**) quasi-relativistic wave and (**dashed**) Schrödinger equations.

It is impossible to confine a single particle with mass in a point, this should be true for an electron, a quark, and probably may also be true for a black hole and the whole universe at the beginning of the Big Bang.

Some results: Hydrogen-like atoms

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{[\gamma_V(r)+1]m}\nabla^2\psi(\vec{r},t) + U(r)\psi(\vec{r},t) \quad (1)$$

In Eq. (1):

$$U(r) = U_C(r) = -\frac{e^2}{4\pi\varepsilon_o}\frac{Z}{r} \quad (2)$$

Proceeding as it is done for solving the same problem when using the Schrödinger equation, it can be obtained the following results :

$$E_{QR} = -\frac{\mu c^2}{\beta}\left[\beta - (2n+\Delta)\sqrt{\beta}\right] \quad (3)$$

In Eq. (3), n = 1, 2, ... is the principal quantum number and:
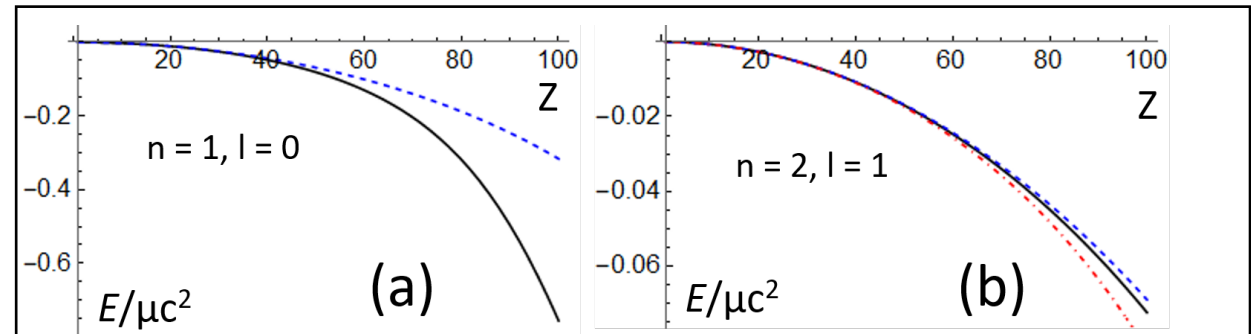
$$\beta = 4n^2 + 4\alpha^2 Z^2 + 4n\Delta + \Delta^2,$$

$$\Delta = \left[\left(1 + \sqrt{(1+2l)^2 - 4\alpha^2 Z^2}\right) - 2(l+1)\right] \quad (4)$$

In Eq. (4), l = 0, 1, ... (n-1) is the orbital quantum number, and α is the fine-structure constant. The following approximated formula is obtained by expressing Eq. (3) in powers of α (up to α^4) :

$$E_{QR} \approx E_{Sch}Z^2\left\{1 - \frac{\alpha^2}{n^2}\left[\frac{3}{4} - \frac{n}{l+\frac{1}{2}}\right]\right\} \quad (5)$$

$$E_{Sch} = -\left[\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_o}\right)^2\right]\frac{Z^2}{n^2} = -\frac{\mu c^2}{4}\frac{\alpha^2 Z^2}{n^2} \quad (6)$$

Comparison of the dependence on Z of the calculated energies for (a) n = 1 and l = 0, (b) n = 2 and l = 1. E was evaluated using (**black continuous**) Eq. (3), and the exact Dirac energies (**blue dashed**) with j = l + ½, and (**red dot-dashed**) with j = l - ½.

Some results: Hydrogen-like atoms

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{[\gamma_V(r)+1]m}\nabla^2\psi(\vec{r},t) + U(r)\psi(\vec{r},t) \quad (1)$$

In Eq. (1):

$$U(r) = U_C(r) = -\frac{e^2}{4\pi\varepsilon_o}\frac{Z}{r} \quad (2)$$

Proceeding as it is done for solving the same problem when using the Schrödinger equation, it was obtained for the ground state of Hydrogen-like atoms :
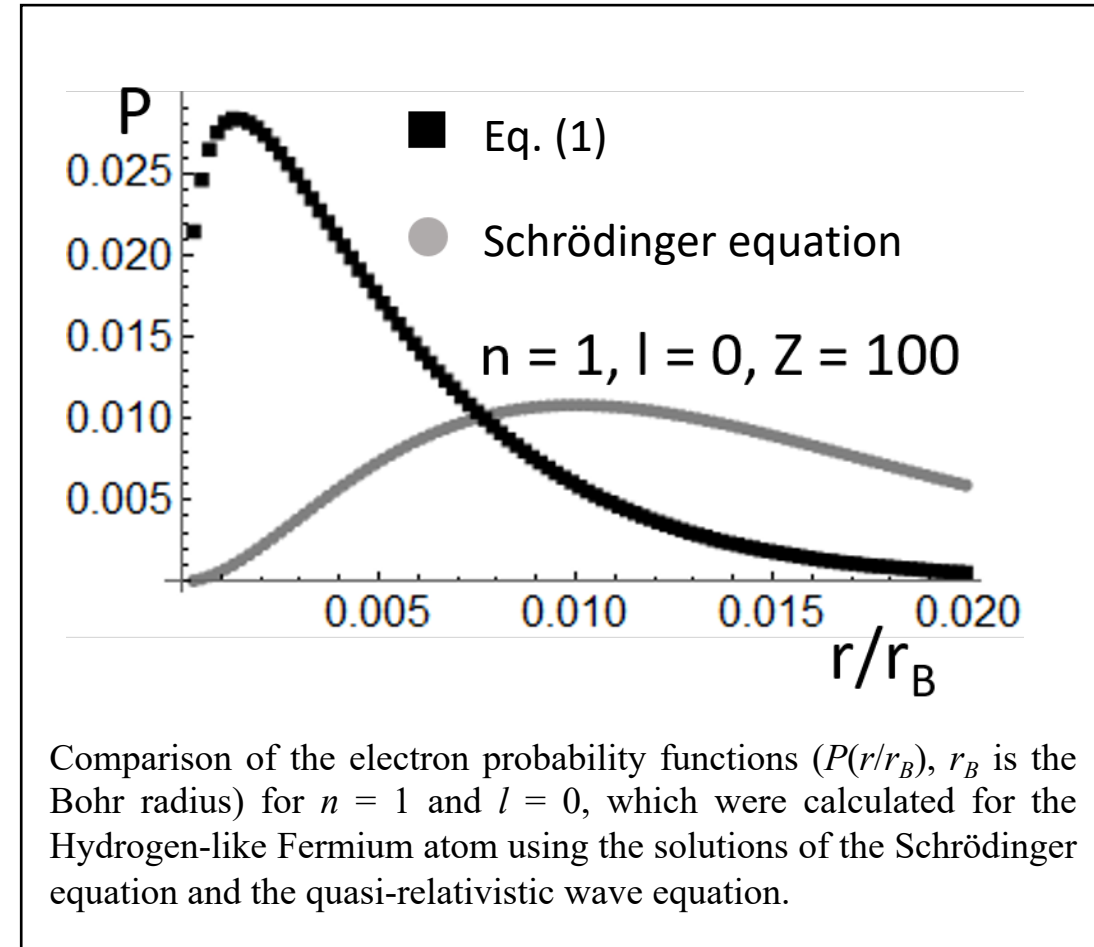
$$Я_{1,0}(r) \propto \frac{\left(C_{1,0}\frac{\mu cr}{\hbar}\right)^{B_{1,0}}}{r}e^{-A_{1,0}\frac{\mu cr}{\hbar}} \quad (3)$$

In Eq. (3), μ is the electron reduced mass, and:

$$A_{1,0} = \frac{\sqrt{2-2\Delta}}{2}, \qquad B_{1,0} = \frac{1+\Delta}{2}, \qquad C_{1,0} = \sqrt{2-\sqrt{2+2\Delta}}$$

When $\alpha^2 Z^2 << 1$: $\quad A_{1,0} \sim \alpha Z, \qquad B_{1,0} \sim 1, \qquad C_{1,0} \sim \alpha Z, \qquad$ thus:

$$Я_{1,0}(r) \approx Я_{1,0,Sch}(r) \propto \frac{Z}{r_B}e^{-\frac{Zr}{r_B}} \quad (4)$$

In Eq. (4), $r_B = \hbar/(\alpha\mu c)$ is the Bohr radius. Therefore, for the Hydrogen atom ($Z = 1$) the solution of Eq. (1) coincides with the solution of the Schrödinger equation. But for $Z = 100$, the Schrödinger equation strongly underestimate the confinement of the electron in the ground state.

Comparison of the electron probability functions ($P(r/r_B)$, r_B is the Bohr radius) for $n = 1$ and $l = 0$, which were calculated for the Hydrogen-like Fermium atom using the solutions of the Schrödinger equation and the quasi-relativistic wave equation.

$$P(r) = \int_{r-\Delta r/2}^{r+\Delta r/2} R_{n,l}^2(\varepsilon)\varepsilon^2 d\varepsilon$$

$$R_{n,l}(r) = \frac{1}{\beta}Я_{n,l}(r), \quad \beta^2 = \int_0^{+\infty} Я^2(\varepsilon)\varepsilon^2 d\varepsilon$$

Klein-Gordon equation

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_{KG}(x,t) = \frac{\partial^2}{\partial x^2}\psi_{KG}(x,t) - \frac{m^2 c^2}{\hbar^2}\psi_{KG}(x,t)$$

$$\hat{E} = i\hbar\frac{\partial}{\partial t}, \qquad \hat{p} = -i\hbar\frac{\partial}{\partial x} \qquad (1)$$

Relativistic relation between $E = K + mc^2$ and p:

$$E^2 - m^2 c^4 = p^2 c^2 \qquad (2)$$

Substituting (1) into (2):

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_{KG}(x,t) = \frac{\partial^2}{\partial x^2}\psi_{KG}(x,t) - \frac{m^2 c^2}{\hbar^2}\psi_{KG}(x,t)$$

Quantum description of a free particle with mass m and spin-0 moving at relativistic speeds

Quasi-relativistic wave equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_V + 1)m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

For E > 0, Eq. (2) is equivalent to:

$$(E + mc^2)(E - mc^2) = p^2 c^2 \Rightarrow (E - mc^2) = \frac{p^2}{(\gamma_V+1)m} \qquad (3)$$

Substituting (1) into (3):

$$i\hbar\frac{\partial}{\partial t}\psi_{KG+}(x,t) = -\frac{\hbar^2}{(\gamma_V + 1)m}\frac{\partial^2}{\partial x^2}\psi_{KG+}(x,t) + mc^2\psi_{KG+}(x,t)$$

Looking for a solution of Eq. (4) in the following form: $\qquad (4)$

$$\psi_{KG+}(x,t) = \psi(x,t)e^{-\frac{i}{\hbar}mc^2} \Rightarrow i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{(\gamma_V+1)m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

When $V^2 \ll c^2$: $\quad i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$

Dirac equation

$$i\hbar \frac{\partial}{\partial t}\psi_D(\vec{r},t) = c\left[\overrightarrow{(\hat{\alpha})}.\overrightarrow{(\hat{p})}\right]\psi_D(\vec{r},t) + mc^2\hat{\beta} \quad (1)$$

Each of the three components of the vector $\overrightarrow{(\hat{\alpha})}$ and and $\hat{\beta}$ are 4 × 4 Dirac's matrices. Each of the tree components of the vector $\overrightarrow{(\hat{p})}$ is the differential operator:

$$\hat{p}_i = -i\hbar\frac{\partial}{\partial i}, \qquad i = x, y, z$$

The bispinor ψ_D has four components; therefore, it can be represented using two spinors in the following way:

$$\psi_D(\vec{r},t) = \begin{pmatrix}\varphi(\vec{r},t) \\ \chi(\vec{r},t)\end{pmatrix} \quad (2)$$

Proposing a solution of Eq. (1) of the following form:

$$\psi_D(\vec{r},t) = \begin{pmatrix}\varphi(\vec{r}) \\ \chi(\vec{r})\end{pmatrix}e^{-\frac{i}{\hbar}Et} \quad (3)$$

Produces the following system of two time-independent spinor equations [Eqs. (4) and (5)]:

$$c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\chi = (E - mc^2)\varphi = K\varphi \quad (4)$$

$$c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]\varphi = (E + mc^2)\chi \quad (5)$$

Each of the three components of the vector $\overrightarrow{(\sigma)}$ is a 2 × 2 Pauli's matrix. E + mc^2 > 0 when E > 0, thus when E > 0, the bottom equation of Eq. (5) can be rewritten in the following way:

$$\chi = \frac{c\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]}{(E+mc^2)}\varphi = \frac{\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]}{(\gamma_V+1)mc}\varphi \quad (6)$$

The two-component (spinor) time-independent quasi-relativistic wave equation for a free-particle particle with mass *m* and spin-1/2 can be obtained substituting Eq. (6) in Eq. (4):

$$\frac{\left[\overrightarrow{(\hat{\sigma})}.\overrightarrow{(\hat{p})}\right]^2}{(\gamma_V + 1)m}\varphi = -\frac{\hbar^2}{(\gamma_V + 1)m}\nabla^2\varphi = K\varphi \quad (7)$$

Therefore, when E > 0, each one of the two components of φ exactly satisfices the same time-independent quasi-relativistic wave equation, which corresponds to a free spin-0 particle with kinetic energy K. Consequently, when V^2 << c^2, each one of the two components of φ exactly satisfices the same time-independent Schrödinger equation :

$$-\frac{\hbar^2}{2m}\nabla^2\psi_{Sch} = K\psi_{Sch} \quad (8)$$

The two-component (spinor), time-independent, Pauli-like quasi-relativistic wave equation

(For a free electron moving through a constant magnetic field with magnitude B_{ext} pointing in the z direction)
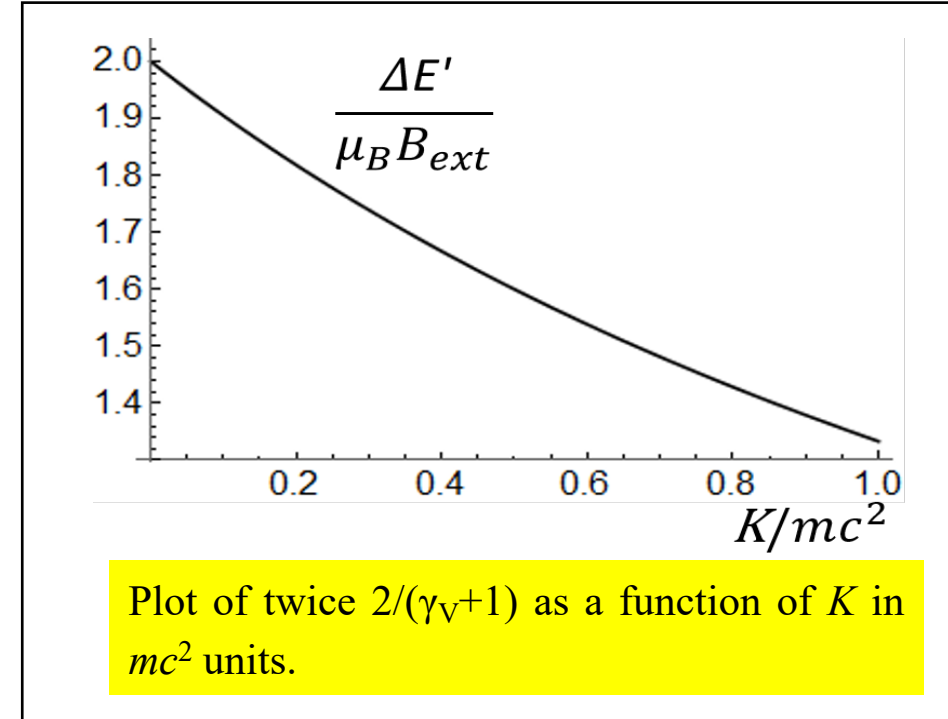
$$-\frac{\hbar^2}{(\gamma_V+1)m}\nabla^2\varphi_P(\vec{r}) - \frac{2\mu_B}{(\gamma_V+1)}B_{ext}\,\sigma_z\varphi_P(\vec{r}) = E'\varphi \quad (1)$$

In Eq. (1) $\mu_B = e\hbar/(2mc)$ is the Bohr magneton, and the spinor φ_P is given by:

$$\varphi_P(\vec{r}) = \begin{pmatrix} \varphi_{P+}(\vec{r}) \\ \varphi_{P-}(\vec{r}) \end{pmatrix}$$

Eq. (1) reduces to the corresponding time-independent Pauli equation when $V^2 \ll c^2$:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi_P(\vec{r}) - \mu_B B_{ext}\,\sigma_z\varphi_P(\vec{r}) = E'\varphi \quad (2)$$

Plot of twice $2/(\gamma_V+1)$ as a function of K in mc^2 units.

Equation (1) is the quasi-relativistic version of Eq. (2). When the electron moves slowly, $\gamma_V \sim 1$, thus Eq. (1) coincides the non-relativistic Pauli equation. Eq. (1) includes two corrections to Eq. (2). First, includes the correct relativistic relation between K and p. **Second, as shown in in the above figure, the energy difference corresponding to the two components of φ_P is not independent of K, as suggested by Eq. (2), but decreases by a factor of twice $2/(\gamma_V+1)$ at quasi-relativistic energies. This relevant result could be easily tested experimentally.**

Some results: Hydrogen-like atoms

Energies of the electron bound states in Hydrogen-like atoms using a perturbative approach based on the Schrödinger equation:

$$E' = E_{Sch}\left(1 + \Delta E_{K,Sch} + \Delta E_{D,Sch} + \Delta E_{SO,Sch}\right) \quad (1)$$

In Eq. (1), there are three relativistic corrections. The first one is the relativistic correction to K, the second one is the Darwin correction, and the third is the spin-orbit correction. However, when using a perturbative approach based in the quasi-relativistic wave equation:
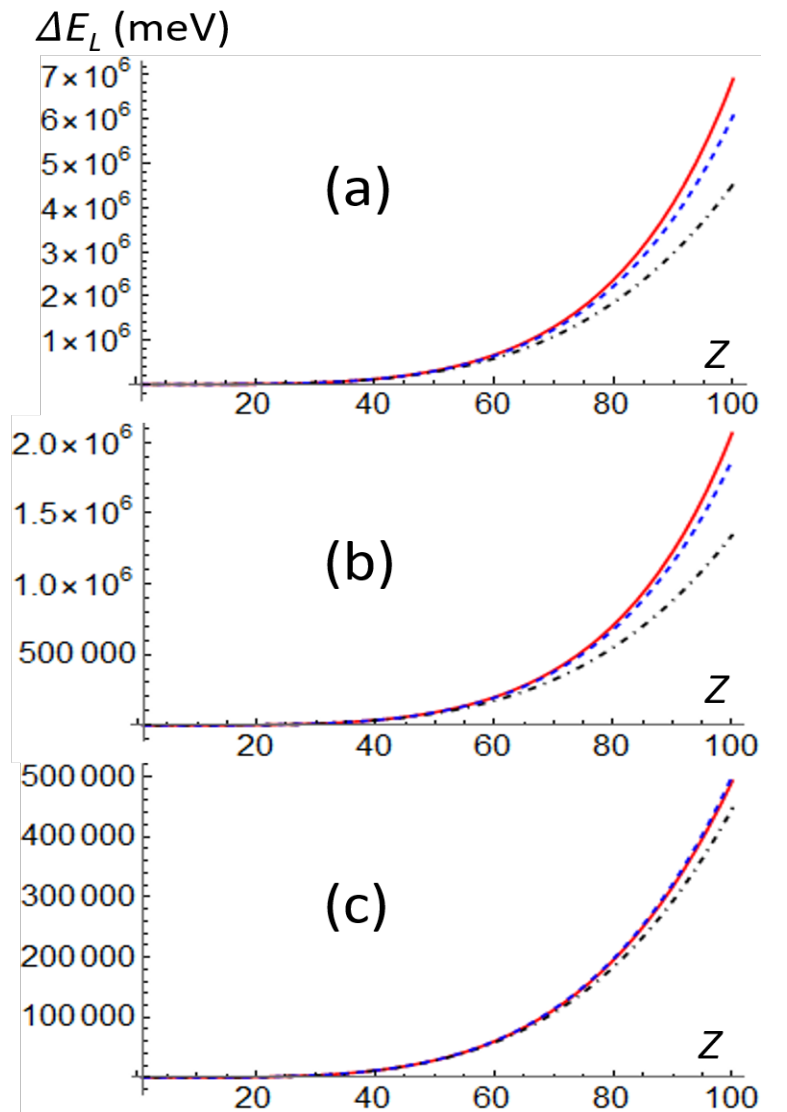
$$E' = E_{QR}\left(1 + \Delta E_{D,QR} + \Delta E_{SO,QR}\right) \quad (2)$$

In Eq. (2), there only are two relativistic corrections. The Darwin and spin-orbit corrections are given now by the following equations:

$$\Delta E_{D,QR} = -k_D E_{QR}\frac{\alpha^2 Z^2}{n}, \quad k_D = (\gamma_V + 1)^{\frac{n}{n+1}} \quad (3)$$

$$\Delta E_{D,Sch} = -k_{SO}E_{QR}\frac{\alpha^2 Z^2}{2n}\frac{j(j+1) - l(l+1) + \frac{3}{4}}{l\left(l+\frac{1}{2}\right)(l+1)}, k_{SO} = \left(\frac{\gamma_V+1}{2}\right)^{-(n-l+1)^{\frac{5}{2}}} \quad (4)$$

In Eq. (4), $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$. Therefore; the energies corresponding to the spectral lines are $\Delta E_L = E'_{n2,l2,j2} - E'_{n1,l1,j1}$
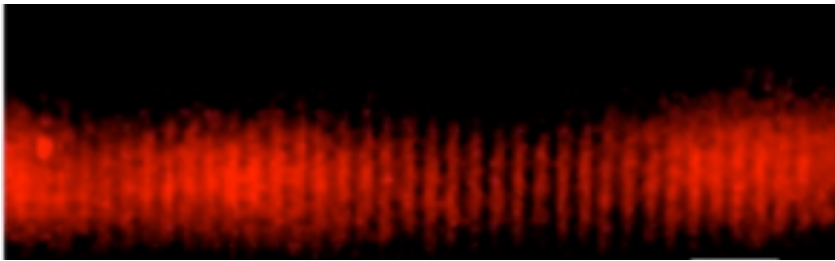

Dependence on Z of ΔE_L (in meV) calculated using (**red, continuous**) the exact values of the Dirac's energies, (**black, dot-dashed**) Eq. (1), and (**blue, dashed**) Eq. (2) for (a) α-Lyman doublet, (b) α-Balmer doublet, (c) another example corresponding to corresponding to the energy difference between two others emission lines involving a state with $l \neq 0$.

About the relativistic invariance of luminal standing waves

Dr. Ankit Pandey

A. Pandey, B. Poirier, and L. Grave de Peralta, "Drawing a photon trajectory: An unorthodox study of bidirectional light-like waves,", *Foundations of Physics*, (under review, 2020).

A luminal standing wave is formed by the superposition of two coherent beams of light traveling in the vacuum in opposite directions. The optical disturbance (ψ') of a luminal standing wave is described by the following equation :

$$\Psi'(x',t') = \sin(kx')\cos(wt'), \quad k = 2\pi/\lambda, \quad w = 2\pi v, \quad \lambda v = c. \qquad (1)$$

However, due to the Doppler effect for light, one should expect that the optical disturbance (ψ) seen by an observer moving respect to the interference pattern should not be described by the above equation. This is because an observer moving parallel to the beams with speed V_o respect to the stationary interference fringes will see the superposition of two light beams with different frequencies. Therefore, the observer moving respect to the interference pattern would describe the optical disturbance resulting from the superposition of the light beams as the superposition of two plane waves with different frequencies traveling in opposite directions. It can be shown that the optical disturbance seen by the moving observer is described by the following expression:

$$\Psi(x,t) = Sin[k_{sb}(x - V_o t)] \, Cos[k_{sp}x - w_{sp}t] \, . \qquad (2)$$

We found that the "cosine" factor in Eq. (2) have a superluminal phase velocity, which is not a "likable" feature. We also found that **this "cosine" factor is a solution of the Klein-Gordon equation**. I get curious about this, and I looked for a way to get rid of this unlikable feature. I found that the following wavefunction has a subluminal phase velocity:

$$\varphi(x,t) = Cos[k_{sp}x - w_{sp}t]e^{\frac{i}{\hbar}mc^2} \qquad (3)$$

Are there particles with mass and spin-0, which are formed from a superposition of two coherent beams of light?

Moreover, I found that $\varphi(x, t)$ satisfies the following equation:

$$i\hbar\frac{\partial}{\partial t}\varphi(x,t) = -\frac{\hbar^2}{(\gamma_V + 1)m}\frac{\partial^2}{\partial x^2}\varphi(x,t)$$

The rest is just curiosity + Chinese flu + good luck + more curiosity + Bill Poirier!

Prof. Bill Poirier

$$K = \sqrt{m^2 c^4 + p^2 c^2} - mc^2 \quad \rightarrow \quad \frac{K}{c^2} = \frac{p^2}{2m + K/c^2} \qquad \text{(see deduction below)}$$

In units where $c = 1$: $\quad K = \dfrac{p^2}{2m + K}$

Poirier introduced the following recursive definition of the operator K:

$$\widehat{K}_{Poirier} = \frac{\widehat{p}^2}{2m + \widehat{K}} = \frac{\widehat{p}^2}{2m + \dfrac{\widehat{p}^2}{2m + \widehat{K}}} = \frac{\widehat{p}^2}{2m + \dfrac{\widehat{p}^2}{2m + \dfrac{\widehat{p}^2}{2m + \dfrac{\widehat{p}^2}{2m + \widehat{K}}}}} = \cdots$$

$$K = \frac{p^2}{(\gamma_V+1)m} = \frac{p^2 c^2}{(\gamma_V+1)mc^2} = \frac{p^2 c^2}{\gamma_V mc^2 + mc^2} = \frac{p^2 c^2}{2mc^2 + (\gamma_V-1)mc^2} = \frac{p^2 c^2}{2mc^2 + K} \Rightarrow K(2mc^2 + K) = p^2 c^2 \Rightarrow K^2 + 2mc^2 K - p^2 c^2 = 0$$

Consequently: $\qquad K = \dfrac{-2mc^2 + \sqrt{4m^2 c^4 + 4p^2 c^2}}{2} = \sqrt{m^2 c^4 + p^2 c^2} - mc^2 = \text{E} - mc^2$