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Minimal relativity and Hulthén potentials

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Abstract

A particular discretization of the nonrelativistic Schrödinger equation is interpreted as a non-perturbative introduction of a certain kinematical relativistic $O(c^{-2})$ correction. We show that both the nonrelativistic (continuous) and semi-relativistic (discrete) partner equations may remain exactly solvable for a class of potentials.

1 Kinetic energy as a difference operator

Numerically, the radial differential Schrödinger equations or their systems, in the matrix notation,

$$-\frac{\hbar^2}{2m}\Psi''(r) + W(r,E)\Psi(r) = 0 \quad (1)$$

are currently solved via their discretization [1]. Basically, one may start from the Taylor-series identity

$$\Psi''(r) = \frac{\Psi(r+h) - 2\Psi(r) + \Psi(r-h)}{h^2} + O(h^2) \quad (2)$$

and replace the continuous Schrödinger equation (1) by its discrete, numerically – recurrently – tractable approximation

$$\Psi^{(h)}(r+h) + \Psi^{(h)}(r-h) = \{2 + \frac{2mh^2}{\hbar^2}W(r,E^{(h)})\}\Psi^{(h)}(r). \quad (3)$$

Thus, one generates the exact numerical solutions of the original Schrödinger equation (1) in the vanishing-error limit $h \to 0$.

In computational practice, the numerical $h \to 0$ convergence may easily be accelerated. Usually, one simply introduces the explicit higher-order corrections, e.g.,

$$\Psi(r+h) + \Psi(r-h) = 2\Psi(r) + h^2\Psi''(r) + +\frac{h^4}{12}\Psi''''(r) + O(h^6) \quad (4)$$

and eliminates them algebraically via a suitable re-arrangement of the original difference equation (3),

$$\Psi^{(h)''}(r) + +\frac{h^2}{12}\Psi^{(h)''''}(r) + O(h^4) = \{2 + \frac{2mh^2}{\hbar^2}W(r,E^{(h)})\}\Psi^{(h)}(r). \quad (5)$$

The further – here, irrelevant – details may be found elsewhere [2].

In the present letter, equation (5) will be given an alternative interpretation. In a preparatory step, let us return to the continuous equation (1) and try to replace its original non-relativistic kinetic energy operator $T_0 = p^2/2m,\ p^2 = -\hbar\,\triangle$ by a relativistic definition

$$T_\infty = (m^2c^4 + p^2c^2)^{1/2} - m\,c^2 = m\,c^2\left[(1+p^2/m^2c^2)^{1/2} - 1\right] =$$

$$= m\,c^2\left[\frac{p^2}{2\,m^2c^2} - \frac{p^4}{8\,m^4c^4} + \dots\right]. \tag{6}$$

In terms of operators (and under standard assumptions concerning the boundedness of the higher derivatives) we get

$$T_\infty = -\frac{\hbar^2}{2m}\triangle - \frac{\hbar^4}{8m^3c^2}\triangle^2 + O(\hbar^6c^{-4})$$

which leads to a semi-relativistic differential Schrödinger equation

$$-\frac{\hbar^2}{2m}\Psi^{[s]\prime\prime}(r) - \frac{\hbar^4}{8\,m^3c^2}\Psi^{[s]\prime\prime\prime\prime}(r) + W(r,E)\Psi^{[s]}(r) = 0 \tag{7}$$

after the omission of all the higher-order $O(\hbar^6c^{-4})$ relativistic corrections. Now, our main idea may be formulated as an observation that, due to the same sign at the second-order corrections, the semi-relativistic differential equation (7) may become reproduced, within its associated error bars $O(c^{-4})$, just by a difference Schrödinger equation of the same type as above. Thus, we are able to guarantee the rigorous coincidence of the second-order *numerical* corrections (cf. (4) and (6)) in our original discrete Schrödinger equation (in its re-arranged form (5)) with the second-order corrections generated by the *kinematical* considerations in the semirelativistic (and continuous) new equation (7).

The comparison requires and implies an explicit specification of the particular "relativistic" size of the numerical step,

$$h = h^{\{c\}} = \sqrt{3}\frac{\hbar}{m\,c} \ll \hbar. \tag{8}$$

Retreating now, for simplicity, to the standard quantum (non-relativistic) units $\hbar = 2\,m = 1$ with $c \gg 1$, we are led to the conclusion that the semi-relativistic wavefunctions may efficiently be determined via the approximative form of the discrete (or recurrent) relationship

$$\Psi^{[s]}(r+\frac{2\sqrt{3}}{c}) + \Psi^{[s]}(r-\frac{2\sqrt{3}}{c}) = \{2+\frac{12}{c^2}W(r,E^{[s]}) + O(c^{-6})\}\Psi^{[s]}(r) \tag{9}$$

similar to the one employed in the preceding purely non-relativistic case.

A pair of remarks is due. Firstly, the smallness of the $O(c^{-6})$ error term is necessary. Then, in a way paralleling the non-relativistic interpretation of eq. (3), we may visualize the whole difference equation (9) as a particular representation of the possible differential equations which all describe the underlying physics within the given and sufficiently small uncertainty.

Secondly, with the axis of coordinates divided into very small steps of a constant size, $h^2 \equiv 12/c^2$, the intrinsic physical ambiguities of the one-particle picture make the present $O(c^{-6})$ precision also more than sufficient. Indeed, corrections of the same order would also result from an account of the other relativistic effects (e.g., from the truly many-body $O(c^{-3}\log c)$ Lamb-shift corrections, etc. [3]). Hence, all the tentative one-body equations of the form

$$T_\infty\Psi + W(r,E)\Psi = 0 \tag{10}$$

and their present approximate $c \gg 1$ realization

$$\Psi^{[s]}(r+h) + \Psi^{[s]}(r-h) = [2 + h^2 W(r, E^{[s]})]\Psi^{[s]}(r), \quad h = \frac{2\sqrt{3}}{c} \tag{11}$$

may be considered equivalent from the point of view of their applications in physics.

Of course, the "relativity-simulating" value of h is fixed and unique. Nevertheless, in the purely numerical perspective, this only means that any further improvement of the "measure of smallness" of errors is already counterproductive and makes in fact the "further improved" solutions less realistic.

2 An exactly solvable example

The one-body relativistic equations of the type (10) are most often considered in their Klein-Gordon and/or Dirac realization [3]. In spite of certain (and well known – cf. our above remark) inconsistencies of these one-body models, they prove attractive due to their simplicity. One even often returns to the non-relativistic concept of the potential in some applications.

In accord with our paper [4] devoted to the problem of simultaneous solvability of the relativistic and non-relativistic equations, one of the most suitable illustrations may be provided by the s-wave interaction

$$W(r, E) = \frac{A(E) + B(E)\,\exp(-\,\gamma(E)\,r)}{1 + D(E)\,\exp(-\,\gamma(E)\,r)}. \tag{12}$$

With the special choice of $W(r, E) = V(r) - E$ and $D = -1$, the force $V(r)$ is well known as the so called Hulthén potential. In accord with ref. [4], it leaves both the Schrödinger (non-relativistic) and Klein-Gordon (relativistic) differential equations exactly solvable in terms of the Gauss hypergeometric special functions ${}_2F_1$.

An alternative choice of the slightly simpler (exponential) forces with $D = 0$ makes both the non-relativistic and relativistic constructions expressible in terms of the Bessel special functions [5].

In the present context, the simultaneous solvability of the non-relativistic differential eq. (1) and its present semi-relativistic difference-equation counterpart (11) represents a more difficult mathematical problem. A guide to its solution is provided by the recent paper by Kvitsinsky [6] where equation (11) is shown exactly solvable for the whole Hulthén class of potentials (12).

For the present purposes, we just have to modify the notation in our eq. (11) and introduce the new variable $z = q^{r/h}$ and wavefunction $\Phi(z) = \Psi^{[s]}(r)$. This enables us to re-write our difference equation with the Hulthén potentials (12) in the form given by Kvitsinsky,

$$\Phi(qz) + \Phi(z/q) + (\omega(z) - E)\Phi(z) = 0, \quad \omega(z) = \frac{a + bz}{1 + dz}. \tag{13}$$

Indeed, the insertion of $z = \exp[r\,(\ln\, q)/h]$ shows the equivalence of both the equations.

In order to be able to confirm our final conclusion that both the bound-state and/or scattering problems with $c = \infty$ and $c < \infty$ are solvable exactly (i.e., in terms of special functions), we have to pay attention to the discrete problem only – it is not necessary to remind the reader about the details of the well known non-relativistic solutions. In the discrete case, fortunately, the main steps of the Kvitsinsky's construction of the two independent power series

$$\Phi^{(\sigma)}(z) = \sum_{n=0}^{\infty} f_n \, z^{n+\sigma}, \sigma = \sigma_1, \ \sigma_2 \tag{14}$$

remain applicable here. In the first step, one determines the (pair of the) admissible parameters $\sigma_{1,2}$ from the small-z limit condition

$$q^{\sigma} + q^{-\sigma} = a + E. \tag{15}$$

Then, the insertion of the Ansatz (14) in equation (13) leads to the two-term recurrences solvable in terms of the standard q-shifted factorials

$$(x;q)_n = \begin{cases} 1 & \text{for } n = 0 \\ (1-x)(1-xq)\dots(1-xq^{n-1}) & \text{for } n > 0. \end{cases} \tag{16}$$

One also notices that a different quadratic equation re-parametrization

$$E + \frac{b}{d} \equiv q^{\tau} + q^{-\tau}, \quad d \neq 0 \tag{17}$$

simplifies the notation and we may, finally, write the general solution as a superposition

$$\Psi^{[s]}(r) = c_{(+)}\Psi^{(+)[s]}(r) + c_{(-)}\Psi^{(-)[s]}(r) \tag{18}$$

of the two so called q-hypergeometric functions [7]. At $d \neq 0$ and with $\varepsilon = \sigma/|\sigma|$ and $h = h^{\{c\}} = \frac{2\sqrt{3}}{c}$, our final formula reads

$$\Psi^{(\varepsilon)[s]}(r) = q^{\sigma r/h} \, {}_2\varphi_1\left(q^{\sigma+\tau}, q^{\sigma-\tau}; q^{2\sigma+1}; q; -dq^{1+r/h}\right). \tag{19}$$

In principle, even the above $d \neq 0$ (purely technical) constraint may be removed: At $d = 0$, the confluent solutions

$$\Psi^{(\varepsilon)[s]}(r) = q^{\sigma r/h} \, {}_1\varphi_1\left(0; q^{2\sigma+1}; q; -bq^{1+\sigma+r/h}\right). \tag{20}$$

may also be written in terms of the so called Hahn-Exton q-Bessel functions – cf. ref. [6] where also the other relevant details, generalizations and references have been discussed.

References

[1] F. Acton, Numerical Methods That Work (Harper and Row, New York, 1970).

[2] D. E. Manolopoulos, M. J. Jamieson and A. D. Pradhan, J. Comp. Phys. 105 (1993) 169 and references contained therein.

[3] J. D. Bjorken and S. D. Drell, Relativistic Quantum Mechanics (McGraw-Hill, New York, 1964).

[4] M. Znojil, J. Phys. A: Math. Gen. 14 (1981) 383.

[5] M. Znojil, J. Math. Phys. 21 (1980) 1629.

[6] A. A. Kvitsinsky, J. Phys. A: Math. Gen. 27 (1994) 215 and references given therein.

[7] G. Gasper and M. Rahman, Basic Hypergeometric Series (Cambridge University Press, New York, 1990).