

Harmonic oscillators in relativistic quantum mechanics

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Abstract Relativistic generalisations of the harmonic oscillator are analysed. Lévy–Leblond, Dirac and Klein–Gordon equations which in the limit of a non-relativistic and spinless particle transform into Schrödinger equation for the harmonic oscillator are constructed. Properties of their solutions, in particular the structure of their spectra, are analysed. Applications to modelling phenomena relevant in quantum chemistry are briefly discussed.

Keywords Harmonic oscillator · Schrödinger equation · Klein–Gordon equation · Dirac equation · Lévy–Leblond equation

1 Introduction

Harmonic oscillators belong to the most important and most commonly used physical models. Due to the formal simplicity, they are used as most basic pedagogical examples of exactly solvable quantum mechanical problems. The Hooke force is used to model a wide variety of phenomena ranging from molecular vibrations to the behaviour of quantised fields. The Schrödinger equation for an electron in a uniform magnetic field confined by a harmonic oscillator type potential was solved in 1928 by Fock [1] and 2 years later again by Darwin [2]. Though the non-relativistic harmonic oscillator seems to be well understood, there are many recent studies dealing with this subject. Among them one should mention

a paper on symplectic models of n -particle systems confined in a harmonic oscillator potential [3] and another one on rotation–vibration spectra of diatomic molecules [4]. Harmonic oscillator potentials may be used to describe spatial confinement of quantum objects, as for example the effects of the embedding of particles in nano-cavities, in fullerenes, in liquid helium. A discussion of these issues and more references to the literature may be found in [5, 6].

A relativistic generalisation of harmonic oscillator is far from being trivial and is certainly not unique. In particular, the mode of a generalisation depends upon the definition of the relativistic oscillator. Already in early 1930s Nikolsky [7] and Postępska [8] were concerned with a Dirac equation for an electron in the field of a quadratic potential. The resulting eigenvalue problem reduces to a quartic equation with no bound solutions. The non-relativistic discrete energy levels correspond in this oscillator to resonances. Relativistic systems which have an infinite number of bound states whose energy levels are all equally spaced have recently been discussed by Toyama and Nogami [9]. Such a system has been constructed using the inverse scattering method [9, 10]. Another approach, leading to the so-called Dirac oscillator, is based on a construction of the Dirac equation which is exactly solvable and in the non-relativistic limit gives the Schrödinger harmonic oscillator equation [11–15].

The Schrödinger equation for two unconfined interacting particles may always be reduced to a system of two one-particle equations: one for the relative motion of the particles and another for the motion of the centre of mass. Among textbook examples the best known are the hydrogen atom and the nuclear motion in the diatomic molecule. In general, this separation is impossible if the motion of the particles is confined by an external potential (e.g., two interacting electrons confined by a Coulomb potential modelling a helium-like atom). The only confinement which does not

Dedicated to Serafin Fraga, in memoriam.

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obstruct the separability is the one by a parabolic potential. The best known system of this kind is referred to as the Hook atom or harmonium. Probably the first studies on this system, aimed at an exact description of the wavefunction near the electron correlation cusp, were due to Kestner and Sinanoğlu [16] and to Santos [17], who found the analytical solutions to the problem. During the next decades harmonium [18–21] and related systems [22, 23] were studied in a variety of contexts including very interesting and non-trivial generalisations to the case of three confined particles [24].

Two simple properties of the quadratic forms: (1) a linear combination of quadratic forms is a quadratic form, and (2) a linear transformation of the variables transforms a positive definite quadratic form to the diagonal form with positive coefficients, imply that a Hookean molecule can be reduced to a problem similar to harmonium. An ingenious implementation of these properties resulted in exactly solvable models of molecules [24–28], giving a possibility of a precise analysis of the Born–Oppenheimer approximation.

In this paper we are concerned with relativistic generalisations of harmonic oscillator and with the influence of spin on the spectrum of a particle confined by a harmonic oscillator potential. The non-relativistic harmonic oscillator is the only quantum system which is invariant with respect to a canonical transformation interchanging coordinates and momenta, i.e., its eigenvalue problem looks the same in the coordinate and in the momentum representation. We take this feature as the definition of harmonic oscillator. Thus, we are looking for relativistic oscillators which are described by the same Hamiltonian in both coordinate and momentum representations. We discuss a spin 0 particle described by the Klein–Gordon equation and, in the non-relativistic limit, by the Schrödinger equation as well as a spin 1/2 particle described by the Dirac equation and, in the non-relativistic limit by the Lévy–Leblond equation [29].

This paper has been dedicated to the memory of Professor Serafín Fraga. Between 1972 and 1976 JK spent more than 2 years in his group in Edmonton. First as a Postdoctoral Fellow and then as a Research Associate. I am most grateful to my Teacher and Friend, for passing to me his appreciation for simplicity in mathematical modelling of science. Also in this paper I try to follow his advice and retain simplicity of the formulation.

Atomic units are used in this paper, however, the mass μ of the particle is explicitly given in all equations.

2 Formulation of the problem

Let us assume that a particle moves in an external field described by a stationary model potential $\mathbf{A}^\nu = \{\mathbf{V}, \mathbf{A}\}$. Its first component, $A^0 \equiv V$, not quite correctly but customarily, is referred to in this paper as the *scalar potential* (this

cannot bring any confusion since we shall not be concerned with a potential which is scalar under the Lorentz transformation). The remaining three components of \mathbf{A}^ν form a three-dimensional vector \mathbf{A} , which we shall refer to as the *vector potential*. The model potential has to be of neither electromagnetic origin nor Hermitian, though the resulting Hamiltonian has to be Hermitian.

If the particle is spinless, it is described by the Klein–Gordon equation

$$\left[H_S - \frac{1}{2\mu c^2} (\mathbf{V} - E)^2 \right] \psi_K = E \psi_K, \quad (1)$$

where

$$H_S = \frac{1}{2\mu} (\mathbf{p} - \mathbf{A})^\dagger (\mathbf{p} - \mathbf{A}) + V, \quad (2)$$

$c \approx 137$ is the velocity of light, E is the energy relative to μc^2 and other symbols have their usual meaning. In the nonrelativistic limit the Klein–Gordon equation transforms to the Schrödinger equation

$$H_S \psi_S = E \psi_S. \quad (3)$$

A spin- $\frac{1}{2}$ particle is described by the Dirac equation which, in the standard (Dirac–Pauli) representation, reads

$$\begin{pmatrix} (\mathbf{V} - E)l, & (\mathbf{p} - \mathbf{A})^\dagger \boldsymbol{\sigma} \\ \boldsymbol{\sigma} (\mathbf{p} - \mathbf{A}), & [(\mathbf{V} - E)/c^2 - 2\mu] l \end{pmatrix} \begin{pmatrix} \psi_D^l \\ c \psi_D^s \end{pmatrix} = 0, \quad (4)$$

where l is a 2×2 unit matrix, $\boldsymbol{\sigma}$ are the Pauli spin matrices and ψ_D^l/ψ_D^s are traditionally called the large/small components of the wavefunction. The non-relativistic limit of Eq. (4)

$$\begin{pmatrix} (\mathbf{V} - E)l, & (\mathbf{p} - \mathbf{A})^\dagger \boldsymbol{\sigma} \\ \boldsymbol{\sigma} (\mathbf{p} - \mathbf{A}), & -2\mu l \end{pmatrix} \begin{pmatrix} \psi_L^l \\ \psi_L^s \end{pmatrix} = 0 \quad (5)$$

is known as the Lévy–Leblond equation [29]. The elimination of ψ_L^s from Eq. (5) gives

$$\left[H_S l - \frac{\boldsymbol{\sigma}}{2\mu} [(\nabla \times \mathbf{A}) + \mathbf{M}] \right] \psi_L^l = E \psi_L^l, \quad (6)$$

where

$$\mathbf{M} = (\mathbf{A}^\dagger - \mathbf{A}) \times \nabla - i (\mathbf{A}^\dagger \times \mathbf{A}) \quad (7)$$

and ψ_L^l is the two-component Pauli spinor. If \mathbf{A} is Hermitian then $\mathbf{M} = 0$ and Eq. (6) takes the standard form of the nonrelativistic Schrödinger–Pauli equation. Let us note that Eq. (6) rather than Eq. (3) should be interpreted as the non-relativistic limit of the Dirac equation.

In this paper we are concerned with a comparative study on solutions of Eqs. (1)–(6) in which the model potentials \mathbf{V} and \mathbf{A} are selected in such a way that in the non-relativistic limit they describe harmonic oscillators. In particular we compare spectra of bosonic (i.e., either Schrödinger or Klein–Gordon) and fermionic (i.e., either Lévy–Leblond or

Dirac) oscillators and point out the differences which already appear in the case of a single particle.

3 Harmonic oscillator

The Schrödinger equation describing a spinless particle confined by a harmonic oscillator potential is usually written in the form

$$\left(\frac{\mathbf{p}^2}{2\mu} + \frac{\mu\omega^2}{2}\mathbf{r}^2\right)\psi_S = E\psi_S. \quad (8)$$

Equation (8) corresponds to two different sets of potentials defining the Hamiltonian (2):

$$\mathbf{V} = \frac{\mu\omega^2}{2}\mathbf{r}^2, \quad \mathbf{A} = 0, \quad (9)$$

and

$$\mathbf{V} = \frac{3\omega}{2}, \quad \mathbf{A} = i\mu\omega\mathbf{r}. \quad (10)$$

Though the first option is more intuitive (explicitly describes a Hooke system), the second one has many formal advantages and allows for a deeper understanding of not only harmonic oscillator itself, but also the structure of the quantum theory.¹

In the second option (10), by introducing operators

$$\begin{aligned} \mathbf{a} &= \frac{i}{\sqrt{2\mu\omega}}(\mathbf{p} - \mathbf{A}) = \frac{1}{\sqrt{2\mu\omega}}(\mu\omega\mathbf{r} + i\mathbf{p}), \\ \mathbf{a}^\dagger &= -\frac{i}{\sqrt{2\mu\omega}}(\mathbf{p} - \mathbf{A})^\dagger = \frac{1}{\sqrt{2\mu\omega}}(\mu\omega\mathbf{r} - i\mathbf{p}) \end{aligned} \quad (11)$$

we get

$$[\mathbf{a}_j, \mathbf{a}_k^\dagger] = \delta_{jk}, \quad (12)$$

and Eq. (8) may be rewritten as

$$\left(\mathbf{a}^\dagger\mathbf{a} + \frac{3}{2}\right)\psi_S = \frac{E}{\omega}\psi_S. \quad (13)$$

The next step is the observation that \mathbf{a}^\dagger and \mathbf{a} act as ladder operators and may be used to generate the Hamiltonian spectrum in a simple algebraic way. The products of $\mathbf{a}_j^\dagger\mathbf{a}_k$ form $SU(3)$ algebra and the Hamiltonian is its element. The further development leads to the construction of the number representation, second quantisation and quantum electrodynamics.

¹ It may be tempting to expect that the potentials (9) and (10) are related by a gauge transformation. This is not the case. More than that, none of them corresponds to a realistic external electromagnetic field. However, it is easy to see that the option given by (10) defines the superpotential corresponding to (9) [30].

4 Relativistic oscillators

The substitutions (9) and (10) are equivalent as long as we are concerned with the Schrödinger Hamiltonian (2). As one can easily see they are by far non-equivalent in the context of relativistic generalisations of the harmonic oscillator.

The relativistic counterpart of the Schrödinger equation, i.e., the Klein–Gordon equation (1), upon the substitution (9), becomes

$$\left(\frac{\mathbf{p}^2}{2\mu} + \frac{\mu\bar{\omega}^2}{2}r^2 - \lambda r^4\right)\psi_K = \bar{\varepsilon}\psi_K = 0, \quad (14)$$

where $\bar{\varepsilon} = E(1 + E/2\mu c^2)$, $\bar{\omega} = \omega\sqrt{1 + E/\mu c^2}$, and $\lambda = \mu\omega^4/8c^2$. The effective radial potential in Eq. (14)

$$V_K(r) = \frac{\mu\bar{\omega}^2}{2}r^2 - \lambda r^4 \quad (15)$$

has nodes at $r = 0$ and at $r = \sqrt{2}r_{\max}$, a maximum equal to $V_{\max} = \mu^2\bar{\omega}^4/16\lambda$ at $r_{\max} = \pm\bar{\omega}\sqrt{\mu}/2\sqrt{\lambda}$ and a minimum $V_{\min} = 0$ at $r_{\min} = 0$. The potential is energy dependent. Its maximum grows up with increasing energy in such a way that there are no continuum eigenstates (no energies higher than the maximum of the potential). However, there are no stationary, square-integrable, states either. All states are metastable and the particle may dissociate to the continuum tunnelling through the finite potential barrier. Three effective potentials $V_K(r)$ corresponding to $E = q\mu c^2$ with $q = 0, \frac{1}{4}, \frac{1}{2}$ are displayed in Fig. 1. For comparison the corresponding energy levels and the parabolic approximations are also shown. In a similar way one may also obtain the Dirac equation. It also

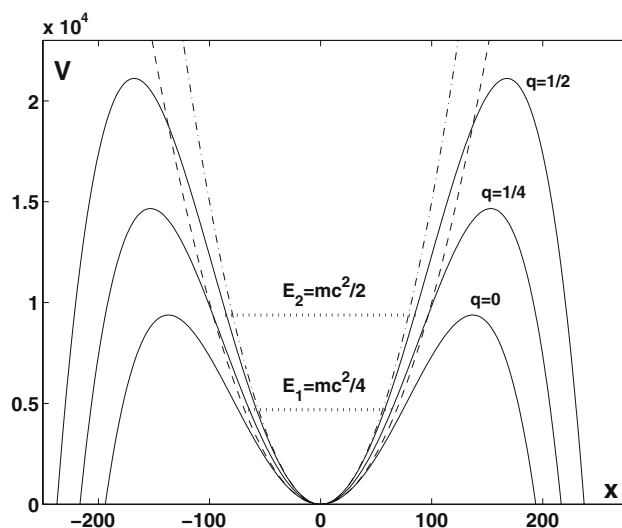


Fig. 1 Effective quartic oscillator potentials (solid lines) appearing in the Klein–Gordon equation with the Hooke-law electrostatic potentials V (broken lines) corresponding to $E = q\mu c^2$ for $q = 0, 1/4, 1/2$. For comparison the corresponding energy levels and the parabolic approximations for $q = 1/4$ and $q = 1/2$ are also given

may be expressed as a rather complicated quartic oscillator equation with no square-integrable solutions. We conclude that the properties of the model obtained as a result of this mode of relativistic generalisation does not meet our expectations.

By an inspection of the Klein–Gordon (1), Dirac (4) and Lévy–Leblond (5) equations we can see that in all cases the substitution given by Eq. (10) results in equations which are invariant under the transformation

$$\mathbf{p} \leftrightarrow a\mathbf{r} \quad (16)$$

where a is a constant. The invariance is obvious in the case of Eq. (1). Equations (4) and (5) are also invariant because $\nabla \times \mathbf{A} = 0$ and

$$\mathbf{M} = 2i\mu\omega[\mathbf{a}^\dagger \times \mathbf{a}] = 2\mu\omega\mathbf{L}, \quad (17)$$

where $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the orbital angular momentum.

It is very important that all operators appearing in the equations resulting from the substitution (10) are expressible in terms of linear combinations of $\mathbf{a}_j^\dagger \mathbf{a}_k$. Then, they belong to $SU(3)$ algebra and, consequently, the corresponding eigenvalue problems are exactly solvable and the spectra may be generated using appropriate ladder operators.

Another option leading to equations invariant with respect to the transformation (16) and, thus, exactly solvable is

$$\mathbf{V} = 0, \quad \mathbf{A} = \frac{1}{2}[\mathbf{B} \times \mathbf{r}], \quad (18)$$

where $\mathbf{B} = \nabla \times \mathbf{A}$ may be interpreted as the external magnetic field. This option is valid for two-dimensional problems only. In this case $\mathbf{M} = 0$ and, assuming $\mathbf{B} = \{0, 0, B\}$,

$$(\mathbf{p} - \mathbf{A})^2 = p^2 + \frac{1}{4}B^2\rho^2 - (\mathbf{B}\mathbf{L}), \quad (19)$$

where $\rho^2 = x_1^2 + x_2^2$.

By solving a simple inverse problem one can find an effective potential which introduced to either Klein–Gordon or Dirac equation results in an equation invariant with respect to the transformation (16) also for \mathbf{V} not equal to a constant. Regrettably, such an effective potential has to be energy dependent. In the case of the Klein–Gordon equation it reads:

$$V_E = V_0 \left[\left(1 + \sqrt{1 - \frac{2V_0}{\mu c^2(1+\delta)^2}} \right) (1+\delta)/2 \right]^{-1}, \quad (20)$$

where $V_0 = \mu\omega^2 r^2/2$ and $\delta = E/2\mu c^2$. The potential is real in a finite range of r [for $\omega r \leq c(1+\delta)$]. In the non-relativistic limit $V_E = V_0$ and in the first-order approximation

$$V_E = V_0 \left(1 + \frac{V_0 - 2E}{2\mu c^2} \right) + O(\alpha^4), \quad (21)$$

where $\alpha \approx 1/137$ is the fine-structure constant. It seems, however, that this mode of the relativistic generalisation is of some rather limited interest.

4.1 Spin 0

In the case described by Eq. (10) both Schrödinger and Klein–Gordon equations may be written as

$$\left(\frac{\mathbf{p}^2}{2\mu} + \frac{\mu\omega^2}{2} r^2 \right) \Psi = \varepsilon_{nl} \Psi, \quad (22)$$

where

$$\varepsilon_{nl}^0 = \begin{cases} E_{nl}, & \text{(Schrödinger),} \\ E_{nl}(1 + E_{nl}/2\mu c^2), & \text{(Klein–Gordon).} \end{cases} \quad (23)$$

As it is well known, $\varepsilon_{nl}^0 = (2n + \ell + \frac{3}{2})\omega$. Then, in the Schrödinger case

$$E_{nl} \equiv E_{nl}^S = (2n + \ell + \frac{3}{2})\omega, \quad (24)$$

and in the Klein–Gordon one

$$E_{nl} \equiv E_{nl}^K = \mu c^2 \left[-1 \pm \sqrt{1 + \frac{2E_{nl}^S}{\mu c^2}} \right] \quad (25)$$

$$= \begin{cases} E_{nl}^S - E_{nl}^{S^2}/(2\mu c^2) + O(\alpha^4), \\ -2\mu c^2 - E_{nl}^S + E_{nl}^{S^2}/(2\mu c^2) + O(\alpha^4). \end{cases}$$

Hence, the Klein–Gordon spectrum is composed of two sequences of discrete energy levels separated by the $2\mu c^2$ gap. The negative energy part of the spectrum is the mirror image of the positive one. Contrary to the non-relativistic case the energy levels are not equally spaced (though the eigenvalues ε are). The distance between two consecutive levels is equal to

$$E_{N+1}^K - E_N^K = \omega - 2(N+2) \frac{\omega^2}{2\mu c^2} + O(\alpha^4), \quad (26)$$

where $N = 2n + \ell$. Then, it is always smaller than in the Schrödinger case and decreases with increasing energy.

Also in the case of axial oscillators corresponding to the potential defined in Eq. (18) both Schrödinger and Klein–Gordon equation reads

$$\left[\frac{\mathbf{p}^2}{2\mu} + \frac{\mu\omega^2}{2} \rho^2 - \xi L_z \right] \Psi = \varepsilon_{nm} \Psi, \quad (27)$$

where $z \equiv x_3$, $\xi = B/2\mu$ and ε_{nm} is related to the Schrödinger and to the Klein–Gordon energies in the same way as in Eq. (23). The Hamiltonian in Eq. (27) commutes with L_z . Therefore its eigenfunctions may be expressed as

$$\Psi(\rho, \phi) = \psi_{nm}(\rho) \Phi_m(\phi) \quad (28)$$

with $L_z \Phi_m = m \Phi_m$ and

$$\varepsilon_{nm} = (2n + |m| + 1)\omega + m\xi. \quad (29)$$

4.2 Spin 1/2

A spin 1/2 particle is described by the Dirac equation and, in the non-relativistic limit, by the Lévy–Leblond equation. Upon the substitution (10) both equations may be separated to the large- and small-component equations. The equation for the large component of the wavefunction reads

$$\left[\left(\frac{\mathbf{p}^2}{2\mu} + \frac{\mu\omega^2}{2} r^2 \right) I - \omega (\boldsymbol{\sigma}\mathbf{L}) \right] \Psi^1 = \varepsilon_{n\ell j}^{1/2} \Psi^1. \quad (30)$$

The relation between the eigenvalue $\varepsilon_{n\ell j}^{1/2}$ and the energy is the same as in Eq. (23) except that “Schrödinger” has to be replaced by “Lévy–Leblond” and “Klein–Gordon” by “Dirac”. The angular and spinor parts of the large component may easily be obtained from the requirement that it is an eigenfunction of the angular momentum operators \mathbf{J}^2 , \mathbf{L}^2 and \mathbf{S}^2 . Since

$$(\boldsymbol{\sigma}\mathbf{L}) = 2(\mathbf{S}\mathbf{L}) = \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2, \quad (31)$$

where $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$ is the spin operator, and $\mathbf{J} = \mathbf{L} + \mathbf{S}$, the scalar product $(\boldsymbol{\sigma}\mathbf{L})$ in the radial equation may be replaced by the corresponding eigenvalue $[j(j+1) - \ell(\ell+1) - 3/4]$ matrix. Consequently, the radial part of the spinor describing the large component of the wavefunction is equal to the appropriate eigenfunction of the spherical harmonic oscillator. The small components of the Dirac bi-spinor may easily be obtained from the original Dirac equation.

The eigenvalues are equal to

$$\varepsilon_{n\ell j}^{1/2} = \begin{cases} \varepsilon_{n\ell+}^{1/2} = (2n + \frac{3}{2})\omega, & \text{if } j = \ell + \frac{1}{2}, \\ \varepsilon_{n\ell-}^{1/2} = (2n + 2\ell + \frac{5}{2})\omega, & \text{if } j = \ell - \frac{1}{2}. \end{cases} \quad (32)$$

The spectrum is highly degenerate. If $j = \ell + \frac{1}{2}$ then the energies are ℓ -independent, i.e., each energy level is infinitely degenerate. The second branch of the spectrum corresponding to $j = \ell - \frac{1}{2}$ is structurally similar to $S = 0$ case. Several simple relations between $S = 0$ and $S = 1/2$ eigenvalues are worth noticing: $\varepsilon_{n\ell+}^{1/2} = \varepsilon_{n\ell}^0 - \ell$, $\varepsilon_{n\ell-}^{1/2} = \varepsilon_{n\ell}^0 + \ell + 1$ and

$$\varepsilon_{n\ell}^0 = \frac{(\ell + 1)\varepsilon_{n\ell+}^{1/2} + \ell\varepsilon_{n\ell-}^{1/2}}{2\ell + 1}. \quad (33)$$

It is interesting to note that each degenerate multiplet ε_N^0 , where $N = 2n + \ell$, due to the spin-orbit splitting, contributes one eigenvalue to the infinitely degenerate ground state $\varepsilon_{0\ell+}^{1/2}$; each but the lowest two degenerate multiplets ε_N^0 contribute one eigenvalue to $\varepsilon_{1\ell+}^{1/2}$, etc.

5 Spin-orbit interaction in non-relativistic oscillators

In the cases of non-relativistic oscillators (Schrödinger and Lévy–Leblond) the equations which are invariant with respect

to the transformation (16) may also be obtained if

$$V = k_v r^2 + \frac{3k_a}{2\mu}, \quad \mathbf{A} = ik_a \mathbf{r}, \quad (34)$$

where k_a and k_v are positive constants. In the case of $S = 0$, Eq. (22) remains valid with

$$\omega = \frac{1}{\mu} \sqrt{k_a^2 + 2\mu k_v}. \quad (35)$$

In the case of $S = 1/2$, the corresponding Lévy–Leblond equation reads

$$\left(\frac{\mathbf{p}^2}{2\mu} + \frac{\mu\omega^2}{2} r^2 - \xi \boldsymbol{\sigma}\mathbf{L} \right) \Psi_L^1 = E_{n\ell j}^L \Psi_L^1, \quad (36)$$

where $\xi = k_a/\mu$ and ω is given by Eq. (35). The energies of a particle described by Eq. (36) are equal to

$$E_{n\ell j}^L = (2n + \ell + \frac{3}{2})\omega + \begin{cases} -(\ell + \frac{3}{2})\xi, & \text{if } j = \ell + \frac{1}{2}, \\ +(\ell - \frac{1}{2})\xi, & \text{if } j = \ell - \frac{1}{2}. \end{cases} \quad (37)$$

If $\xi \ll \omega$, the last equation describes the spectrum of the Schrödinger spherical harmonic oscillator perturbed by the spin-orbit splitting with the spin-orbit parameter equal to ξ . The spectrum may be viewed as a set of towers of equally spaced energy levels. Several lowest energies are shown in Table 1. As one can see, the degeneracy of the energy levels related to the symmetries of the spherical oscillator for a spinless particle has been removed (unless there are some specific relations between ω and ξ). A diagram representing the lowest energy levels in the spectrum of the spherical Lévy–Leblond harmonic oscillator is shown in Table 2. A comparison of the boson and fermion harmonic oscillator spectra is given in Fig. 2.

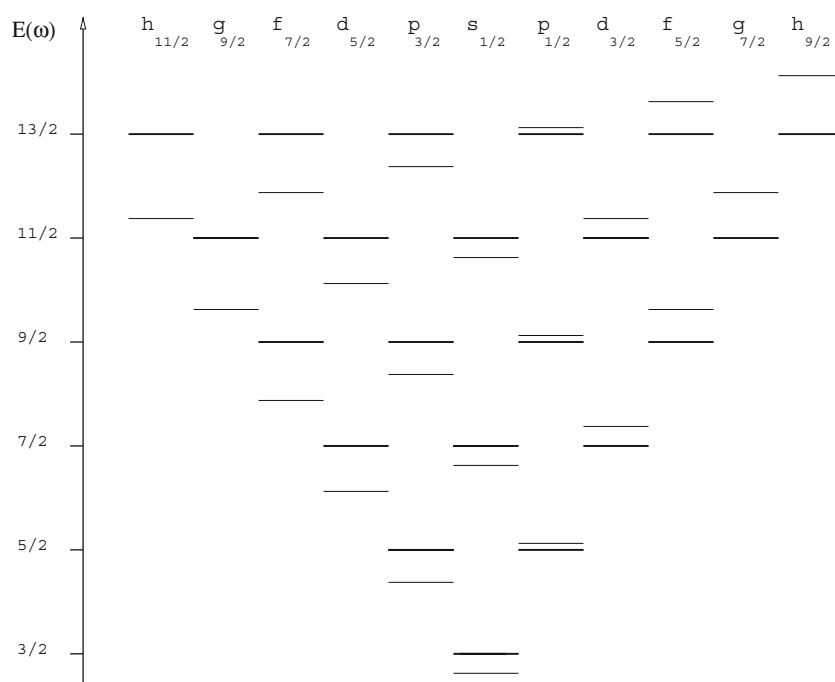
Table 1 Expression $2E_{n\ell j}^L = (N_\omega\omega + N_\xi\xi)/2$ for the energy levels of the Lévy–Leblond harmonic oscillator

n	$s_{1/2}$	$p_{3/2}$	$d_{5/2}$	$p_{1/2}$	$d_{3/2}$	$f_{5/2}$
0	$3\omega - 3\xi$	$5\omega - 5\xi$	$7\omega - 7\xi$	$5\omega + \xi$	$7\omega + 3\xi$	$9\omega + 5\xi$
1	$7\omega - 3\xi$	$9\omega - 5\xi$	$11\omega - 7\xi$	$9\omega + \xi$	$11\omega + 3\xi$	$13\omega + 5\xi$
2	$11\omega - 3\xi$	$13\omega - 5\xi$	$15\omega - 7\xi$	$13\omega + \xi$	$15\omega + 3\xi$	$17\omega + 5\xi$

Table 2 Lowest energy levels $E_{n\ell j}^L = (\omega N_\omega + \xi N_\xi)/2$ in the spectrum of the Lévy–Leblond harmonic oscillator

N_ω	N_ξ	-11	-9	-7	-5	-3	+1	+3	+5	+7
3								$1s_{1/2}$		
5					$1p_{3/2}$			$1p_{1/2}$		
7				$1d_{5/2}$		$2s_{1/2}$		$1d_{3/2}$		
9			$1f_{7/2}$		$2p_{3/2}$		$2p_{1/2}$		$1f_{5/2}$	
11		$1g_{9/2}$		$2d_{5/2}$		$3s_{1/2}$		$2d_{3/2}$		$1g_{7/2}$

Fig. 2 A comparison between spectra of non-relativistic spherical harmonic oscillator for spin 0 (*thick lines*) and for spin 1/2 (*thin lines*)



A general Schrödinger harmonic oscillator in which $\mathbf{V} = k_v^\rho \rho^2 + k_v^z z^2$ and $\mathbf{A} = \frac{1}{2}[\mathbf{B} \times \mathbf{r}]$, is described by a cylindrically symmetric Schrödinger equation

$$\left[\frac{\mathbf{p}^2}{2\mu} + \frac{\mu}{2} (\omega_\rho^2 \rho^2 + \omega_z^2 z^2) - \xi L_z \right] \Psi^S = E_{n_1 n_2 m}^S \Psi^S \quad (38)$$

where

$$\omega_\rho = \frac{1}{\mu} \sqrt{k_a^2 + 2\mu k_v^\rho}, \quad (39)$$

$\xi = k_a/\mu = B/(2\mu)$ and

$$\omega_z = \sqrt{\frac{2k_v^z}{\mu}}. \quad (40)$$

Equation (38) may be separated to two harmonic oscillator equations (a two-dimensional one with frequency ω_ρ and a one-dimensional one with frequency ω_z). The resulting energy is equal to

$$E_{n_1 n_2 m}^S = (2n_1 + |m| + 1) \omega_\rho + (n_2 + \frac{1}{2}) \omega_z + m \xi, \quad (41)$$

$n_1, n_2 = 0, 1, 2, \dots; m = 0, \pm 1, \pm 2, \dots$

Two special cases are of a particular interest. The first one, described by the Hamiltonian of a spherically symmetric oscillator with an additional term proportional to L_z , is obtained by taking $k_v^z = k_v^\rho + k_a^2/(2\mu)$. The energy in this case is equal to $(2n + \ell + \frac{3}{2})\omega_\rho + m\xi$. The second one corresponds to the case of $\mathbf{V} = 0$. Then the movement of the particle along z axis is unconstrained, and in the energy expression (41) $(n_2 + \frac{1}{2})\omega_z$ is replaced by $p_z^2/(2\mu)$, i.e.,

$$E_{n_1 p_z m}^S = (2n_1 + |m| + 1) \omega_\rho + p_z^2/2\mu + m \xi. \quad (42)$$

The axial Lévy–Leblond equation reads

$$\left[\frac{\mathbf{p}^2}{2\mu} + \frac{\mu}{2} (\omega_\rho^2 \rho^2 + \omega_z^2 z^2) - \xi (L_z + \sigma_z) \right] \Psi_L = E^L \Psi_L. \quad (43)$$

Now the energy depends upon the projection of the spin on the z axis:

$$E^L \equiv E_{n_1 n_2 m m_s}^L = E_{n_1 n_2 m}^S + 2m_s \xi, \quad (44)$$

where $m_s = \pm \frac{1}{2}$. Spectra of the axial oscillators are displayed in Fig. 3.

6 Final remarks

In the case of the Schrödinger equation the external Hooke law interactions may be derived from both vector and scalar potentials. Using these potentials in equations which describe non-relativistic fermions leads to a variety of exactly solvable harmonic-oscillator-type equations with spectra entirely different to the ones given by the Schrödinger equation. Relativistic generalisations produce exactly solvable equations only if $\mathbf{V} = \text{const}$ and the external fields are described by properly defined vector potentials. The results of this paper may be relevant not only in modelling quantum chemical phenomena related to the Hooke law interactions in which relativistic effects are important but also, probably first of all, the phenomena in which the oscillating particles possess spin. A description of the relativistic effects associated with the spatial confinement is another area of physical utility

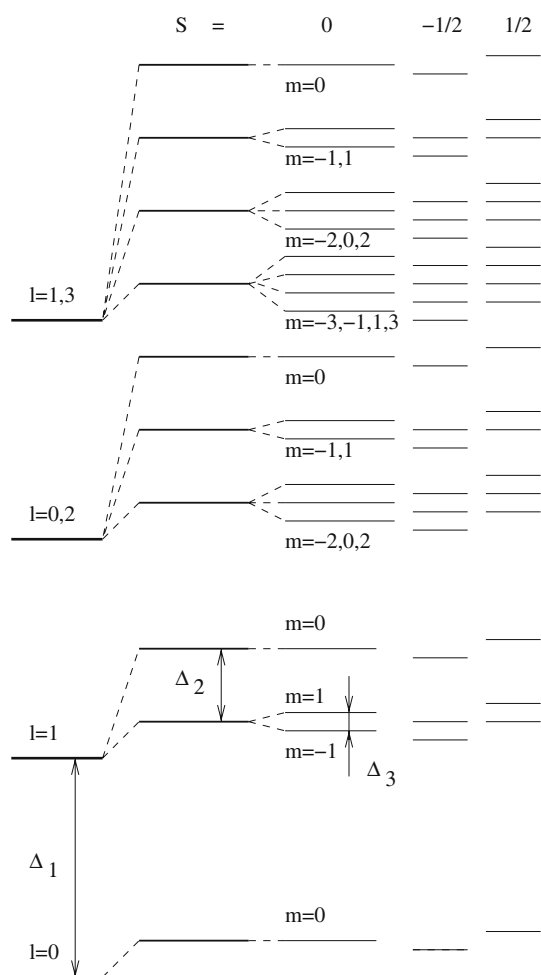


Fig. 3 Spectra of Schrödinger ($S = 0$) and Lévy–Leblond ($S = \pm 1/2$) axial oscillators. The values of splittings are equal to $\Delta_1 = \omega_\rho$, $\Delta_2 = \omega_z - \omega_\rho$ and $\Delta_3 = 2\xi$

of this formalism. In particular, a relativistic generalisation of the model of two spinless particles interacting by an instantaneous Coulomb potential and confined by the harmonic oscillator potential, based on Eqs. (22) and (1) seems to be straightforward.

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