Relativistic electron confined by isotropic parabolic potential

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Energies and wave functions for quasibound states of a relativistic particle interacting with the field of a quadratic isotropic potential $V(r) = m\omega^2 r^2/2$ are obtained using a power expansion method. The stabilization of autoionizing resonances is performed by introducing the spherical confinement of finite radius R_b. For comparison, the problem is investigated also in the framework of direct perturbation theory (DPT). It has been shown that the substantial degeneracy of nonrelativistic levels of the isotropic harmonic oscillator is completely removed. The relativistic effects, spin effects, fine-structure splittings, and radial densities of probability for several states are studied.

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I. INTRODUCTION

The relativistic harmonic oscillator has been the subject of many works [1–10]. The relativistic theory of the isotropic harmonic oscillator is essential for a more realistic description of many particle confined systems such as Hookean atom (harmonium), Hookean molecules, confined positronium, or related systems, modeled by nonrelativistic Hamiltonians with parabolic potentials [9]. This subject is of interest also because of its applications in nuclear physics and elementary particle physics. The central potentials in the nuclear shell models and two-body confining quark interactions are modeled by nonrelativistic potentials, quadratic in the radial variable r.

The definition of a relativistic counterpart of the quantum-mechanical harmonic oscillator is not unique. The straightforward generalization by the introduction of a quadratic potential into the Klein-Gordon equation leads to the Schrödinger-type equation, with the energy-dependent *quartic* potential, that has no bound solutions [10]. Relativistic generalizations of a one-dimensional harmonic oscillator, obtained by the insertion of a parabolic potential into Dirac equation, have been considered by Nikolsky [1] and Postępska [2]. The effective potentials appearing in the resulting second-order equations do not create stationary, square-integrable states. The discrete energy levels correspond in these oscillator models to autoionizing resonances. The exactly solvable model, for a spin-$\frac{1}{2}$ particle, is the Dirac oscillator (DO) described by the linear in coordinates and momenta Hamiltonian [5]

$$H_{\mathrm{DO}} = c\boldsymbol{\alpha}\cdot(\mathbf{p} - im\omega\beta\mathbf{r}) + \beta mc^2, \tag{1}$$

where ω is the frequency of the oscillator. The Dirac equation with the Hamiltonian (1) leads to the energy eigenvalues [6,7]

$$\mathcal{E}_{\mathrm{DO}} = mc^2\left(\pm\sqrt{1+\frac{2\epsilon_{nlj}}{mc^2}} - 1\right), \tag{2}$$

where we have subtracted the rest energy of electron and

$$\epsilon_{nlj} = \begin{cases} 2n\omega & \text{if} \quad j = l+\frac{1}{2} \\ 2n+2l+1)\omega & \text{if} \quad j = l-\frac{1}{2}. \end{cases} \tag{3}$$

In the nonrelativistic limit the wave equation for the large spinor component [8]

$$\left(\frac{p^2}{2m} + \frac{m\omega^2}{2}r^2 - \omega\boldsymbol{\sigma}\cdot\mathbf{L}\right)\psi_L = \tilde{\mathcal{E}}_N\psi_L \tag{4}$$

contains the spin-orbit term and leads to energy levels

$$\tilde{\mathcal{E}}_N = \mathcal{E}_N + \begin{cases} -l\omega & \text{if} \quad j = l+\frac{1}{2} \\ l+1)\omega & \text{if} \quad j = l-\frac{1}{2}, \end{cases} \tag{5}$$

where energies

$$\mathcal{E}_N = (2n+l+3/2)\omega \tag{6}$$

correspond to the nonrelativistic isotropic harmonic oscillator. Several properties of the Dirac oscillator, defined by the Hamiltonian (1), have been studied in various contexts [10–13]. Other approaches are based on the inverse scattering method and lead to the models of the relativistic oscillator as a quantum system with an infinite number of bound states and equal-spaced energy levels [14,15].

Since relativistic wave equations produce finite potential barriers as a result of substituting the parabolic potential into them, the problem of confinement in relativistic theory, due to the non zero probability of tunneling to the continuum, cannot be modeled by quadratic potentials in an unlimited space region.

The aim of this paper is the solution of the Dirac and Klein-Gordon equations with a spherically symmetric potential

$$V(r) = \tfrac{1}{2}m\omega^2 r^2 \tag{7}$$

using the power-series expansion method [16–18]. In order to stabilize the autoionizing resonances we have introduced the spherical confinement of a radius R_b, corresponding to the maximum of the effective potential.

Without any loss of generality we set for simplicity $m = 1$. We will use the notation $E_A = \mathcal{E}_A/\omega$, where $\mathcal{E}_A$ is the energy and the superscript $A = (N, K, D, \mathrm{DO})$ refers to a specific model.

II. FORMULATION OF THE PROBLEM

The Hamiltonian describing the motion of an electron confined by the potential (7) in atomic units reads

$$H_D = c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta c^2 + \tfrac{1}{2}\omega^2 r^2. \tag{8}$$

The time-independent Dirac equation with the Hamiltonian (8) can be written in matrix form:

$$\begin{bmatrix} \frac{1}{2}\omega^2 r^2 - \mathcal{E}_D & c\boldsymbol{\sigma}\cdot\mathbf{p} \\ c\boldsymbol{\sigma}\cdot\mathbf{p} & \frac{1}{2}\omega^2 r^2 - \mathcal{E}_D - 2c^2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{9}$$

Note that all quantities in Eq. (9) are dimensionless. One can obtain the length, energy, and frequency by taking the products of $r,\mathcal{E}_D,\omega$ and relevant units. These units are the Bohr radius $r_0 = 5.3\times 10^{-9}$ cm as the unit of length, one hartree $\mathcal{E}_0 = 27.2$ eV as the unit of energy, and the value $\omega_0 = 0.413\times 10^{17}$ Hz as the unit of frequency.

In the nonrelativistic limit, after elimination of the lower spinor component, Eq. (9) leads to the Schrödinger equation corresponding to the isotropic harmonic oscillator

$$\left(\frac{p^2}{2} + \frac{1}{2}\omega^2 r^2\right)\Psi_N = \mathcal{E}_N \Psi_N, \tag{10}$$

of which the energies are given by the formula (6).

In the spherical coordinates, after introducing new variables

$$\rho = r\sqrt{\omega}, \quad \lambda = \omega/c^2, \quad E_D = \mathcal{E}_D/\omega \tag{11}$$

and substituting into Eq. (9) the Dirac spinor in the form

$$\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \frac{1}{\rho}\begin{bmatrix} P(\rho)\Omega_{\kappa\mu}(\vartheta,\phi) \\ i\sqrt{\lambda}Q(\rho)\Omega_{-\kappa\mu}(\vartheta,\phi) \end{bmatrix}, \tag{12}$$

where $\Omega_{\kappa\mu}$ is the spherical spinor and κ and μ stand for the Dirac quantum number and the projection of the total angular momentum, respectively, we obtain the radial Dirac equation:

$$\frac{dP}{d\rho} + \frac{\kappa P}{\rho} + \frac{1}{2}\lambda\rho^2 Q - (2+\lambda E_D)Q = 0, \tag{13}$$

$$\frac{dQ}{d\rho} - \frac{\kappa Q}{\rho} - \frac{1}{2}\rho^2 P + E_D P = 0. \tag{14}$$

Let us find the asymptotic behavior of functions P and Q, for $\rho\to 0$. In the case $\kappa > 0$, the asymptotic form of Eqs. (13) and (14) reads

$$\frac{dP}{d\rho} + \frac{\kappa P}{\rho} - (2+\lambda E_D)Q = 0, \tag{15}$$

$$\frac{dQ}{d\rho} - \frac{\kappa Q}{\rho} = 0. \tag{16}$$

Equation (16) has the solution $Q = \text{const}\times\rho^{\kappa}$ and after substituting it into Eq. (15) we find $P = \text{const}\times\rho^{\kappa+1}$. For $\kappa < 0$ the asymptotic behavior of functions P and Q is governed by equations

$$\frac{dP}{d\rho} + \frac{\kappa P}{\rho} = 0, \tag{17}$$

$$\frac{dQ}{d\rho} - \frac{\kappa Q}{\rho} + E_D P = 0, \tag{18}$$

which have finite solutions $P = \text{const}\times\rho^{-\kappa}$ and $Q = \text{const}\times\rho^{-\kappa+1}$. Finally, both cases may be written together as

$$P(\rho)\sim\rho^{l+1}, \quad Q(\rho)\sim\rho^{\tilde{l}+1}, \tag{19}$$

where we have introduced the orbital quantum number l, given by

$$l = |\kappa| + \frac{\kappa}{2|\kappa|} - \frac{1}{2}, \tag{20}$$

and

$$\tilde{l} = l - \frac{\kappa}{|\kappa|}. \tag{21}$$

In order to determine the asymptotic behavior of functions P and Q, for $\rho\to\infty$, we may rewrite Eqs. (13) and (14) in the asymptotic form

$$\frac{dP}{d\rho} + \frac{1}{2}\lambda\rho^2 Q = 0, \tag{22}$$

$$\frac{dQ}{d\rho} - \frac{1}{2}\rho^2 P = 0. \tag{23}$$

After elimination of Q we obtain the second-order differential equation

$$\frac{d^2P}{d\rho^2} + \frac{1}{4}\lambda\rho^4 P = 0, \tag{24}$$

which has the asymptotic solutions

$$P\sim\exp(\pm i\sqrt{\lambda}\rho^3/6). \tag{25}$$

One can see from Eq. (22) that the radial function Q behaves in the same manner. The asymptotic solutions disclose the oscillating behavior typical for motion in the classically allowed, infinite region. This means that the effective potential acting on the electron creates states that are resonances rather than stationary bound states. Since the presence of the autoionizing states is not caused by the spin of the confined particle, we can start from the Klein-Gordon equation, in order to determine the effective radial potential.

By substituting Eq. (7) into the pertinent Klein-Gordon equation, we get the Schrödinger-like equation [10]

$$\left(\frac{p^2}{2} + U(E_K,\rho)\right)\Psi_K = \epsilon_K\Psi_K, \tag{26}$$

where we have introduced the effective, energy-dependent, radial potential

$$U(E,\rho) = \tfrac{1}{2}(1+\lambda E)\rho^2 - \tfrac{1}{8}\lambda\rho^4 \tag{27}$$

and the eigenvalue

$$\epsilon_K = E_K(2+\lambda E_K)/2. \tag{28}$$

Taking the Klein-Gordon wave function in the form

$$\Psi_K(\rho,\vartheta,\phi) = \frac{F(\rho)}{\rho}Y_{lm}(\vartheta,\phi), \tag{29}$$

we transform Eq. (26) into the radial equation

$$\left(h(E_K,\rho) + \frac{l(l+1)}{2\rho^2}\right)F = \epsilon_K F, \tag{30}$$

where

$$h(E,\rho) = -\frac{1}{2}\frac{d^2}{d\rho^2} + U(E,\rho). \tag{31}$$

We may get the approximate expressions for the effective potentials for a spin-$\frac{1}{2}$ particle after transforming Eqs. (13) and (14) into the second-order equations. Acting on Eqs. (13) and (14) by operators $d/d\rho \mp \kappa/\rho$, respectively, after some simple manipulations, we find

$$\left(h(E_D,\rho) + \frac{\kappa(\kappa+1)}{2\rho^2}\right) P + \frac{1}{2}\lambda\rho Q = \epsilon_D P, \tag{32}$$

$$\left(h(E_D,\rho) + \frac{\kappa(\kappa-1)}{2\rho^2}\right) Q - \frac{1}{2}\rho P = \epsilon_D Q, \tag{33}$$

where

$$\epsilon_D = E_D(2+\lambda E_D)/2. \tag{34}$$

The quartic potential (27) corresponds to the effective interactions of a spin-0 particle with the external field of a parabolic potential. In a case of a spin-$\frac{1}{2}$ particle the effective interactions are described by Eq. (27) approximately. Note that both relativistic wave equations behave asymptotically in the same manner. Thus, the main properties of the spectrum resulting from the shape of the potential and derived for the Klein-Gordon equation can also be referred to the Dirac particle.

The effective potential (27) has the maximum

$$U_m = \frac{\omega}{2c^2}(E + c^2/\omega)^2, \tag{35}$$

corresponding to

$$\rho_m = \sqrt{2(E + c^2/\omega)}. \tag{36}$$

The maximum is energy and ω dependent. It exceeds, for arbitrary energy, the value of E. As a consequence, the positive-continuum eigenstates with energies greater than the maximum of the effective potential do not occur. The radius ρ_m is a monotonically decreasing function of ω. The dependence of the maximum U_m on the oscillator frequency is displayed in Fig. 1. The function U_m has a minimum $U_0 = 2E$, which corresponds to $\omega_m = c^2/E$. The dependence of the effective potential on the frequency of the oscillator is illustrated in Fig. 2.

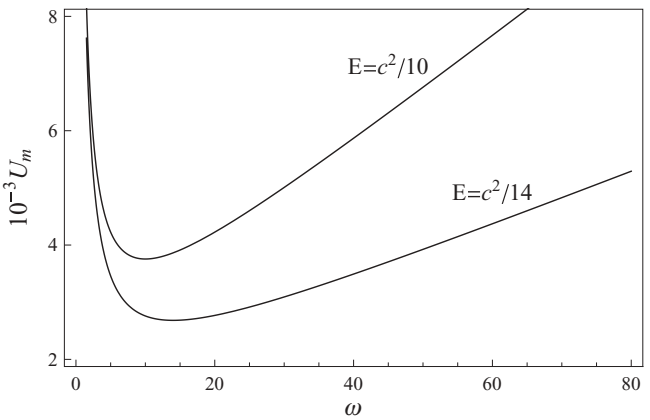

FIG. 1. Dependence of the maximum of effective potential U_m on the oscillator frequency ω, for $E = c^2/10, c^2/14$. The minima $U_0 = 2E$ correspond to $\omega_m = c^2/E$.

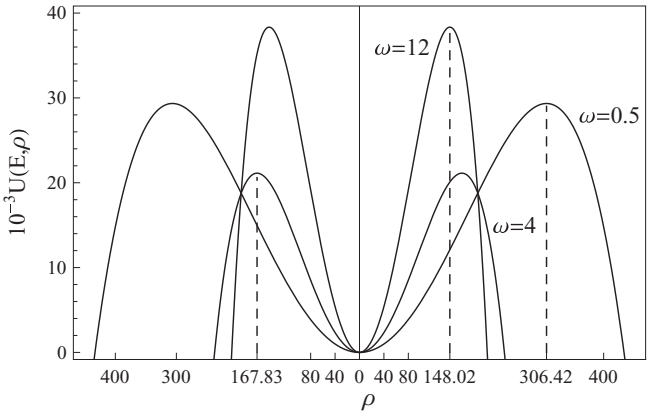

FIG. 2. Effective potentials for $\omega = 0.5, 4, 12$ and the corresponding values of $\rho_m = 306.42, 167.83, 148.02$. The energy is taken as half of the rest energy of the electron. The stationary point $\omega_m = 2$.

Using the rectangular-barrier approximation, we may estimate the magnitude of the probability for the tunneling. The rectangular barrier is characterized by its height G and the length L. From the tunneling effect point of view, only the region lying *over* the level E has a significance. Thus, we define the parameter $G = U_m - E$. The parameter L is determined by the equation $U(E,\rho) = E$. Solving this equation we find two positive roots

$$\rho_{1,2} = [2(E + c^2/\omega) \pm 2\sqrt{E^2 + c^4/\omega^2}]^{1/2} \tag{37}$$

and define $L = |\rho_1 - \rho_2|/2$. The coefficient of the transition through the rectangular barrier reads [19]

$$D \approx 16\frac{E}{U_m}\left(1 - \frac{E}{U_m}\right)\exp(-2\sqrt{2G}L). \tag{38}$$

The energy corresponding to the maximum of D may be found numerically. Since $E \approx 2n + l + 3/2$ we can indicate states with the maximal probability of the decay. One can note that for $\mathcal{E} > 2c^2 \cong 37\,538$, the effects related to the creation of the electron-positron pairs are essential and the one-particle models are not valid anymore. This leads to the upper limit for ω, $\approx 2.5 \times 10^4$. In Table I the coefficients D, for ω running from 10^{-1} to 10^5, are displayed. We can see that the lifetimes ($\sim D^{-1}$) of all autoionizing resonances are extremely large, for a wide range of the oscillator frequency. For this reason we treat, in further calculations, the energy eigenvalues as purely real ones.

III. POWER-SERIES SOLUTIONS

Now we are looking for solutions of the radial equations (13) and (14) in the form of power series,

$$P(\rho) = \rho^{l+1}\sum_{k=0}^{\infty} A_k\rho^k, \quad Q(\rho) = \rho^{\tilde{l}+1}\sum_{k=0}^{\infty} B_k\rho^k. \tag{39}$$

By substituting expansions (39) into Eqs. (13) and (14) and equating coefficients of the equal powers of ρ, we obtain the

TABLE I. Dependence of the maximal transition coefficients D on the oscillator frequency. In the second and fifth columns the approximate values of $\Lambda = 2n + l$ corresponding to states with the maximal probability of the decay are displayed. The numbers in brackets are the powers of 10 by which the entries are to be multiplied.

ω	Λ	D	ω	Λ	D
0.1	56 400	2.20[−123440]	60	94	9.64[−210]
0.4	14 230	2.38[−30863]	100	56	1.86[−127]
0.8	7040	7.57[−15438]	400	14	7.29[−35]
1	5645	1.19[−12347]	1000	5	2.48[−16]
4	1460	2.41[−3090]	4000	0	4.45[−7]
8	720	4.88[−1547]	10 000	0	4.55[−5]
10	560	2.15[−1238]	1 00 000	0	1.58[−5]

recurrent linear relations for the coefficients a_k and b_k, of the form

$$(k+l+\kappa+1)A_k + \tfrac{1}{2}\lambda B_{k-3+\kappa/|\kappa|} - (2+\lambda E_D)B_{k-1+\kappa/|\kappa|} = 0, \tag{40}$$

$$(k+\tilde{l}+\kappa+1)B_k - \tfrac{1}{2}A_{k-3-\kappa/|\kappa|} + E_D A_{k-1-\kappa/|\kappa|} = 0. \tag{41}$$

By solving the linear equations (40) and (41) separately for $\kappa > 0$ and $\kappa < 0$, we can observe that only the coefficients corresponding to the even values of k are nonzero. Therefore, denoting $a_k \equiv A_{2k}$ and $b_k \equiv B_{2k}$, we find for $\kappa > 0$

$$b_0 = \frac{2\kappa+1}{2+\lambda E_D} a_0 \tag{42}$$

and

$$b_k = \left(-E_D a_{k-1} + \tfrac{1}{2}a_{k-2}\right)/(2k), \tag{43}$$

$$a_k = \left((2+\lambda E_D)b_k - \tfrac{1}{2}\lambda b_{k-1}\right)/(2\kappa+2k+1), \tag{44}$$

and for $\kappa < 0$

$$b_0 = \frac{E_D}{2\kappa-1} a_0 \tag{45}$$

and

$$a_k = \left((2+\lambda E_D)b_{k-1} - \tfrac{1}{2}\lambda b_{k-2}\right)/(2k), \tag{46}$$

$$b_k = \left(-E_D a_k + \tfrac{1}{2}a_{k-1}\right)/(2k-2\kappa+1), \tag{47}$$

where a_0 is a nonzero constant. For an arbitrary value of E_D we can generate a set of coefficients a_k and b_k until $k = I$, by starting from $a_0 = 1$ and using relations (42)–(44) for $\kappa > 0$ and relations (45)–(47) for $\kappa < 0$, respectively. The index I determines the number of terms required for the summation of the series on a desired precision level.

The energy eigenvalues and the radial wave functions are determined by the boundary conditions

$$P(\rho_b) = 0, \quad Q(\rho_b) = 0, \tag{48}$$

where ρ_b corresponds to the maximum of the effective potential ($\rho_b = R_b\sqrt{\omega}$). Note that in the nonrelativistic limit, $\rho_b = \infty$. In order to achieve the desired accuracy (10^{-12} hartree) one can terminate the integration process at $\rho < \rho_b$. To this end we extrapolate the boundary conditions to distances $\rho = R$ ($R < \rho_b$) and complete them by the requirement that $dP/d\rho$ and $dQ/d\rho$ decay at $\rho = R$. The calculation of $P(R), Q(R)$ and their derivatives, by the summation of the series at fixed ρ, with energy-dependent coefficients, leads to the energy-dependent functions. Focusing attention on the large component P, we have

$$\Pi(E) = R^{l+1}\sum_{k=0}^{I} a_k(E)R^{2k} \tag{49}$$

and

$$\tilde{\Pi}(E) = \frac{(l+1)\Pi(E)}{R} + 2\sum_{k=0}^{I} k a_k(E)R^{2k+l}, \tag{50}$$

where Π and $\tilde{\Pi}$ denote functions P and $dP/d\rho$, respectively, as functions of energy.

For $E > 0$ functions (49) and (50) oscillate with amplitudes strongly growing for increasing R. They have an infinite number of well-separated zeros lying close to the values $2n + l + 3/2$. For sufficiently large R, zeros of both functions become equal. Moreover, functions (49) and (50) behave in the same manner with the coefficients a_k replaced by b_k. Therefore, we can consider only one equation

$$\Pi(E) = 0 \tag{51}$$

that defines the discrete energy spectrum in a given R approximation. Equation (51) is nonlinear with respect to E and it can be solved by iterative methods. Applying numerical procedures we control the stability of results by comparison of the difference between successive solutions obtained for growing R. The process is terminated if energy differences become $<10^{-12}$ hartree. Figure 3 shows functions $\Pi(E)$ and $\tilde{\Pi}(E)$ for $\omega = 1$ and $\kappa = -1$, calculated for $R = 8$.

The eigenvalues corresponding to the Klein-Gordon equation can be obtained by using the same calculational procedure. By expanding the radial function F in the even powers of ρ

$$F(\rho) = \rho^{l+1}\sum_{k=0}^{\infty} d_k \rho^{2k}, \tag{52}$$

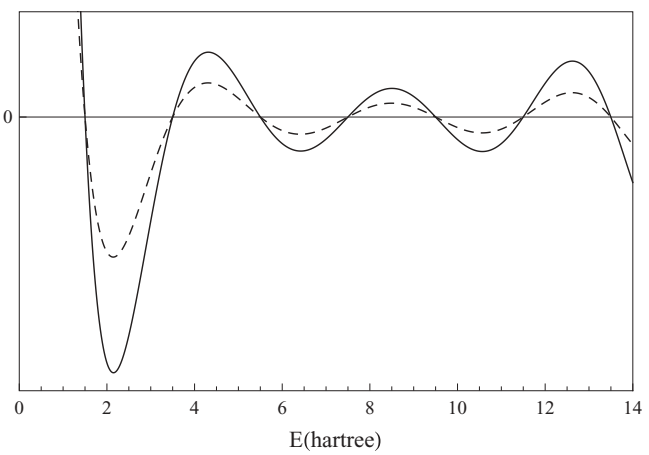

FIG. 3. Functions $\Pi(E)$ (solid line) and $\tilde{\Pi}(E)$ (dashed line) for $\kappa = -1$, $\omega = 1$, and $R = 8$.

with respect to the behavior at small distances described by a factor ρ^{l+1}, we obtain an explicit formula for the expanding coefficients

$$d_k = \left[-E_K(2+\lambda E_K)\, d_{k-1} + (1+\lambda E_K)\, d_{k-2} - \tfrac{1}{4}\lambda\, d_{k-3} \right] / [2k(2k+2l+1)]. \quad (53)$$

Energies are determined by Eq. (51), where the function $\Pi(E)$ is defined by coefficients d_k.

IV. THE PERTURBATION APPROACH

In order to compare the power-series approach with other methods, we investigate the relativistic oscillator problem also in the framework of the first-order perturbation theory. In this theory, relativity is treated as a perturbation with respect to the perturbation parameter $\lambda = \omega/c^2$.

Substituting the perturbation expansions

$$\Psi_K = \sum_{p=0}^{\infty} \Psi_K^{(p)} \lambda^p, \quad E_K = \sum_{q=0}^{\infty} E_K^{(q)} \lambda^q \quad (54)$$

into the Klein-Gordon equation (26) and equating appropriate coefficients we may obtain, in the standard way, a set of the perturbation equations, ordered according to the powers of λ. The first-order equation leads to

$$E_K^{(1)} = -\tfrac{1}{2}E_N^2 + \tfrac{1}{2}E_N \langle \Psi_N | \rho^2 | \Psi_N \rangle - \tfrac{1}{8}\langle \Psi_N | \rho^4 | \Psi_N \rangle. \quad (55)$$

Taking into account the identity [20,21]

$$\langle \Psi_N | \rho^4 | \Psi_N \rangle = \tfrac{3}{2}E_N^2 + \tfrac{1}{8}[3 - 4l(l+1)], \quad (56)$$

and applying the virial theorem, we have

$$E_K^{(1)} = -\tfrac{1}{8}\left(3n(2n+2l+3) + \tfrac{1}{4}(2l+3)(2l+5)\right). \quad (57)$$

For a Dirac particle, the relevant formula resulting from the direct perturbation theory (DPT) [22] has a general form [23]

$$E_D^{(1)} = \tfrac{1}{4}\langle \boldsymbol{\sigma}\cdot\mathbf{p}\Psi_N | V - E_N | \boldsymbol{\sigma}\cdot\mathbf{p}\Psi_N \rangle, \quad (58)$$

where V is a potential appearing in the Schrödinger equation. Taking into account the Hermitian property of $\boldsymbol{\sigma}\cdot\mathbf{p}$ and using the identity [19]

$$(\boldsymbol{\sigma}\cdot\mathbf{p})\rho^2(\boldsymbol{\sigma}\cdot\mathbf{p}) = \rho^2 p^2 - 2\rho\frac{\partial}{\partial\rho} + 2\boldsymbol{\sigma}\cdot\mathbf{L}, \quad (59)$$

we obtain, for the potential (7), the first-order energy correction

$$E_D^{(1)} = E_K^{(1)} - \frac{1}{4}\left\langle \Psi_N \left| \rho\frac{\partial\Psi_N}{\partial\rho} \right\rangle + \frac{1}{4}\langle \Psi_N | \boldsymbol{\sigma}\cdot\mathbf{L} | \Psi_N \rangle. \quad (60)$$

TABLE II. Dirac energies E_D and Klein-Gordon energies E_K in hartrees for states with $l = 0,1,2,3,4$ of the bounded harmonic oscillator with parabolic potential compared with nonrelativistic energies E_N. The radius of spherical bound $\rho_b \approx 194$. The oscillator frequency $\omega = 1$. In the last column the corresponding values of R and I are given. The values of energy are computed with $c = 137.035\,999\,76$ [24].

n	l	κ	State	E_D	κ	State	E_D	E_K	E_N	R,I
0	0	−1	$s_{1/2}$	1.499 995 007 77				1.499 975 039 31	1.5	7,80
1				3.499 895 170 51				3.499 875 203 11	3.5	7,80
2				5.499 715 477 61				5.499 695 511 28	5.5	8,100
3				7.499 455 941 30				7.499 435 976 03	7.5	8,110
4				9.499 116 573 79				9.499 096 609 58	9.5	8,120
5				11.498 697 387 31				11.498 677 424 16	11.5	8,120
0	1	−2	$p_{3/2}$	2.499 975 038 95	1	$p_{1/2}$	2.499 935 104 43	2.499 941 759 52	2.5	7,80
1				4.499 835 270 62			4.499 795 339 28	4.499 801 993 31	4.5	7,90
2				6.499 615 652 76			6.499 575 724 61	6.499 582 377 57	6.5	8,110
3				8.499 316 197 60			8.499 276 272 64	8.499 282 924 54	8.5	8,110
4				10.498 936 917 35			10.498 896 995 57	10.498 903 646 41	10.5	8,120
5				12.498 477 824 23			12.498 437 905 64	12.498 444 555 42	12.5	9,140
0	2	−3	$d_{5/2}$	3.499 941 758 23	2	$d_{3/2}$	3.499 875 203 34	3.499 895 168 88	3.5	7,80
1				5.499 762 061 22			5.499 695 511 64	5.499 715 475 05	5.5	7,90
2				7.499 502 520 79			7.499 435 976 53	7.499 455 937 81	7.5	8,110
3				9.499 163 149 16			9.499 096 610 22	9.499 116 569 38	9.5	8,120
4				11.498 743 958 56			11.498 677 424 93	11.498 697 381 96	11.5	9,140
5				13.498 244 961 19			13.498 178 432 87	13.498 198 387 78	13.5	9,150
0	3	−4	$f_{7/2}$	4.499 895 166 13	3	$f_{5/2}$	4.499 801 993 01	4.499 835 267 93	4.5	7,80
1				6.499 675 542 83			6.499 582 377 14	6.499 615 648 87	6.5	7,90
2				8.499 376 082 22			8.499 282 923 97	8.499 316 192 52	8.5	8,110
3				10.498 996 796 52			10.498 903 645 72	10.498 936 911 07	10.5	8,120
4				12.498 537 697 96			12.498 444 554 59	12.498 477 816 76	12.5	9,140
5				14.497 998 798 73			14.497 905 662 79	14.497 938 921 78	14.5	9,150
0	4	−5	$g_{9/2}$	5.499 835 263 19	4	$g_{7/2}$	5.499 715 473 96	5.499 762 057 20	5.5	7,80
1				7.499 575 715 98			7.499 455 936 32	7.499 502 515 31	7.5	8,110
2				9.499 236 337 59			9.499 116 567 48	9.499 163 142 22	9.5	8,110
3				11.498 817 140 21			11.498 697 379 67	11.498 743 950 16	11.5	8,120
4				13.498 318 136 07			13.499 198 385 09	13.498 244 951 33	13.5	9,140
5				15.497 739 337 38			15.497 619 595 95	15.497 666 157 94	15.5	9,150

Calculating the expectation value appearing in the second term, we have

$$\left\langle \Psi_N \left| \rho \frac{\partial \Psi_N}{\partial \rho} \right\rangle = -\frac{3}{2}. \tag{61}$$

The first-order relativistic correction may be written as

$$E_D^{(1)} = E_K^{(1)} + \frac{1}{8} \times \begin{cases} 2l+3 & \text{if} \quad j = l + \frac{1}{2} \\ -2l+1 & \text{if} \quad j = l - \frac{1}{2}. \end{cases} \tag{62}$$

One can see that $E_K^{(1)}$ is negative for all n and l. This is also true in a case of the Dirac particle. The substitution of Eq. (57) into Eq. (62) leads to the expression

$$E_D^{(1)} = -\frac{1}{8}\left(3n(2n+2l+3) + l^2 + \frac{3}{4}\right) - \frac{1}{4} \times \begin{cases} l & \text{if} \quad j = l + \frac{1}{2} \\ 3l+1 & \text{if} \quad j = l - \frac{1}{2}. \end{cases} \tag{63}$$

V. RESULTS AND DISCUSSION

The algorithm described in the preceding section is based on the expansion into the power series of the radial amplitudes and leads to approximate solutions, corresponding to the bounded system. In a given R approximation, energy eigenvalues correspond to roots of the nonlinear equation (51) and the wave functions are obtained in the compact form as power series, with an explicit given recurrence relation for coefficients. For growing R, energies and wave functions converge to the exact solutions determined by the boundary conditions, imposed at $\rho = \rho_b$.

The power-series method provides a very efficient tool for solving one-particle problems with potentials including rational powers of the radial variable r. More advanced versions of this method have been employed for the solution of the nonseparable wave equations for hydrogenic atoms in an external magnetic field [16–18].

In Table II we list fully relativistic energies E_D and E_K, and compare them with nonrelativistic energies E_N, for the lowest six states with the orbital quantum numbers $l = 0,1,2,3,4$. The maximal absolute error of each value does not exceed ± 1 in the last digits. The minimal values of R and I, which are necessary to obtain this accuracy, are listed in the last column. We can see that all relativistic energies are lower than the corresponding nonrelativistic ones. This property of the relativistic spectra follows directly from perturbation theory. The effect of the *shift down* of the relativistic spectra is caused by the first-order relativistic corrections that give the leading contribution to the energy and for all states are negative. One can find from Eq. (62) that relativistic energy shifts for states

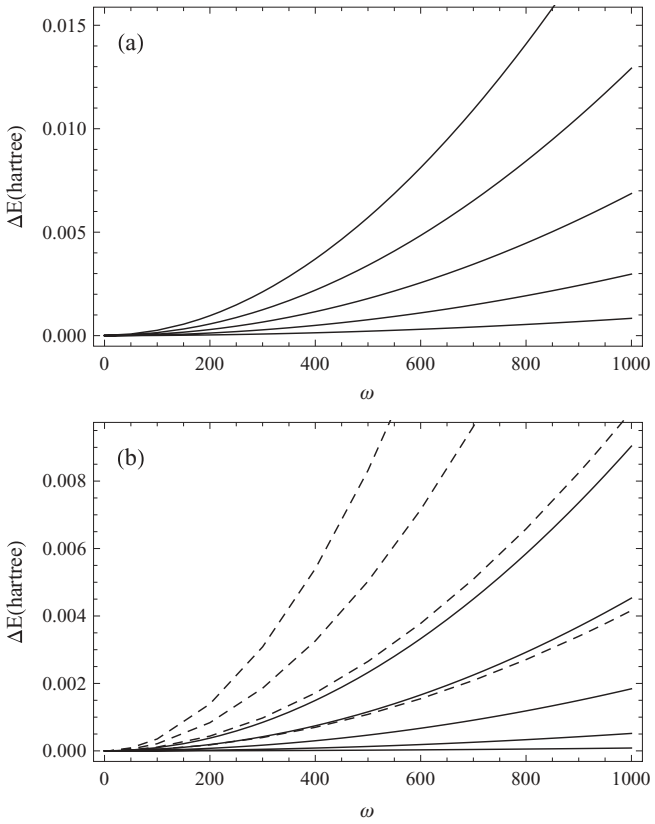

FIG. 4. Dependence on the oscillator frequency of the differences: (a) $\Delta E = E_K - (E_N + \lambda E_K^{(1)})$, for states (from below) $1s,1p,1d,1f,1g$; (b) $\Delta E = E_D - (E_N + \lambda E_D^{(1)})$, for states (from below) $1s_{1/2},1p_{3/2},1d_{5/2},1f_{7/2},1g_{9/2}$ (solid lines) and for states (from below) $1p_{1/2},1d_{3/2},1f_{5/2},1g_{7/2}$ (dashed lines). The ω unit is 0.413×10^{17} Hz.

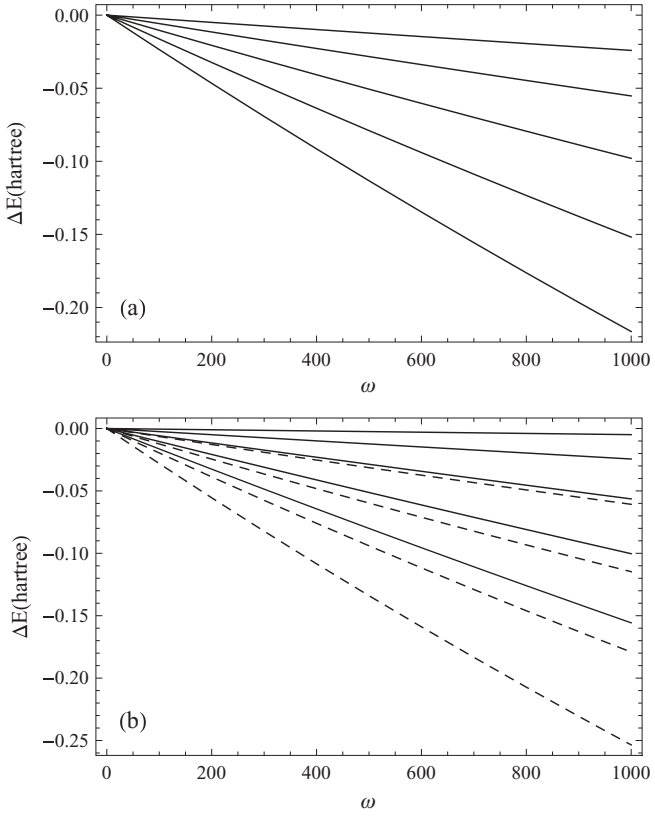

FIG. 5. Dependence on the oscillator frequency of the relativistic effects: (a) $\Delta E = E_K - E_N$ for states (from above) $1s,1p,1d,1f,1g$; (b) $\Delta E = E_D - E_N$ for states (from above) $1s_{1/2},1p_{3/2},1d_{5/2},1f_{7/2},1g_{9/2}$ (solid lines) and for states (from above) $1p_{1/2},1d_{3/2},1f_{5/2},1g_{7/2}$ (dashed lines). The ω unit is 0.413×10^{17} Hz.

TABLE III. Dirac energies E_D and Klein-Gordon energies E_K in hartrees for ground states of bounded harmonic oscillators with parabolic potentials, ordered with growing values of the oscillator frequency. In the second column the corresponding values of ρ_b are displayed. In the last column the modified Dirac oscillator energies $\tilde{E}_{\mathrm{DO}}$ are listed [10]. Power-series energies are obtained with $R \leqslant 7$ and $I \leqslant 200$. The calculations have been performed with $c = 137.035\,999\,76$ [24].

ω	ρ_b	E_D	E_K	$\tilde{E}_{\mathrm{DO}}$
0.001	6128	1.499 999 995 01	1.499 999 975 04	1.499 999 940 09
0.01	1938	1.499 999 950 08	1.499 999 750 38	1.499 999 400 92
0.1	613	1.499 999 500 77	1.499 997 503 85	1.499 994 009 27
0.2	433	1.499 999 001 57	1.499 995 007 72	1.499 988 018 64
0.3	354	1.499 998 502 31	1.499 992 511 61	1.499 982 028 10
0.4	306	1.499 998 003 09	1.499 990 015 51	1.499 976 037 66
0.5	274	1.499 997 503 86	1.499 987 519 43	1.499 970 047 31
0.6	250	1.499 997 004 64	1.499 985 023 37	1.499 964 057 06
0.7	232	1.499 996 505 42	1.499 982 527 33	1.499 958 066 90
0.8	217	1.499 996 006 20	1.499 980 031 31	1.499 952 076 84
0.9	204	1.499 995 506 98	1.499 977 535 30	1.499 946 086 88
1	194	1.499 995 007 77	1.499 975 039 31	1.499 940 097 01
5	87	1.499 975 040 51	1.499 875 214 15	1.499 700 580 71
10	61	1.499 950 065 17	1.499 750 472 29	1.499 401 400 32
50	27	1.499 750 592 16	1.498 754 117 17	1.497 016 515 08
100	19	1.499 501 600 84	1.497 512 602 92	1.494 056 602 72
500	9	1.497 524 809 15	1.487 733 717 91	1.471 185 854 52
1000	6	1.495 092 432 08	1.475 874 843 16	1.444 447 431 79

with $j = l - 1/2$ ($\kappa > 0$) are greater than the shifts related to the spin-0 particle and there is an opposite situation for the states corresponding to $j = l + 1/2$ ($\kappa < 0$). The fully relativistic energies behave in the same manner. By calculating the difference between the total relativistic energy and the perturbation first-order energy, we obtain the contribution of the higher-order relativistic corrections. The dependence on the ω of the differences $E_K - (E_N + \lambda E_K^{(1)})$ and $E_D - (E_N + \lambda E_D^{(1)})$, for the lowest states with $l = 0,1,2,3,4$, are displayed in Fig. 4. We can see that the influence of the higher-order corrections is significant for excited states and for growing ω values. The ω dependence of the relativistic effects is presented in Fig. 5. The spin effects and the fine-structure splittings are displayed in Fig. 6. For comparison, in Fig. 6(b), the first-order perturbation results are shown. We can see that the first-order perturbation theory is relevant only in the low ω limit.

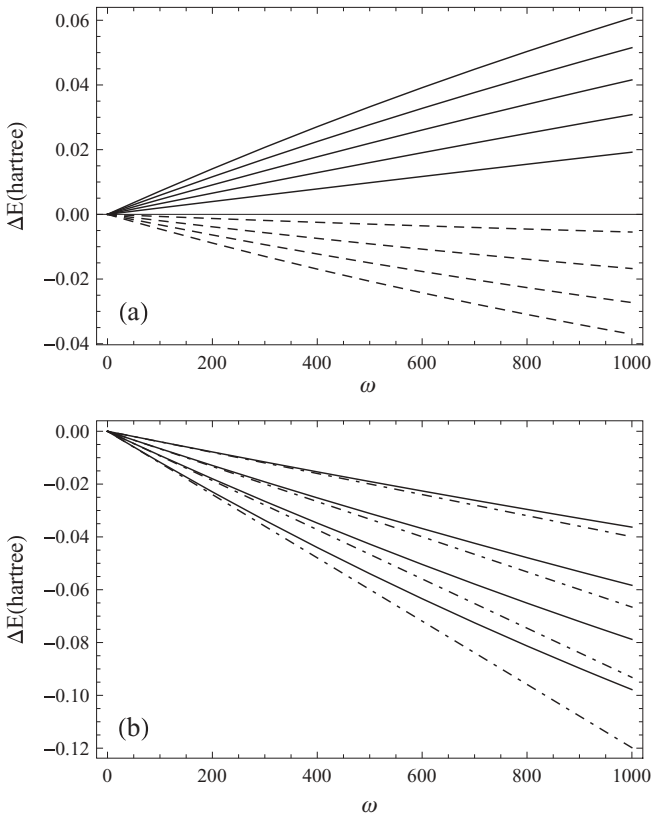

FIG. 6. Dependence on the oscillator frequency: (a) the spin effects $\Delta E = E_D - E_K$ for states (from below) $1s_{1/2}, 1p_{3/2}, 1d_{5/2}, 1f_{7/2}, 1g_{9/2}$ (solid lines) and for states (from above) $1p_{1/2}, 1d_{3/2}, 1f_{5/2}, 1g_{7/2}$ (dashed lines); (b) the fine-structure splitting for states (from above) $1p_{1/2}$-$1p_{3/2}$, $1d_{3/2}$-$1d_{5/2}$, $1f_{5/2}$-$1f_{7/2}$, $1g_{7/2}$-$1g_{9/2}$ (solid lines) and the first-order perturbation results (dot-dashed lines). The ω unit is 0.413×10^{17} Hz.

TABLE IV. First-order relativistic energies $E_{K1} = E_N + \lambda E_K^{(1)}$ and $E_{D1} = E_N + \lambda E_D^{(1)}$ in hartrees for states corresponding to degenerate nonrelativistic states with a given value of $\Lambda = 2n + l$. In the sixth and tenth columns the first-order relativistic corrections are listed. The oscillator frequency $\omega = 1$. The values of energy are computed with $c = 137.035\,999\,76$ [24].

Λ	E_N	States	n	l	$E_K^{(1)}$	E_{K1}	n	κ	$E_D^{(1)}$	E_{D1}
2	3.5	$2s$	1	0	$-75/32$	3.499 875 192 14	1	-1	$-63/32$	3.499 895 161 40
		$1d$	0	2	$-63/32$	3.499 895 161 40	0	-3	$-35/32$	3.499 941 756 33
							0	2	$-75/32$	3.499 875 192 14
3	4.5	$2p$	1	1	$-119/32$	4.499 801 971 53	1	-2	$-99/32$	4.499 835 253 62
							1	1	$-123/32$	4.499 795 315 11
		$1f$	0	3	$-99/32$	4.499 835 253 62	0	-4	$-63/32$	4.499 895 161 40
							0	3	$-119/32$	4.499 801 971 53
4	5.5	$3s$	2	0	$-183/32$	5.499 695 468 82	2	-1	$-171/32$	5.499 715 438 08
		$2d$	1	2	$-171/32$	5.499 715 438 08	1	-3	$-143/32$	5.499 762 033 01
							1	2	$-183/32$	5.499 695 468 82
		$1g$	0	4	$-143/32$	5.499 762 033 01	0	-5	$-99/32$	5.499 835 253 62
							0	4	$-171/32$	5.499 715 438 08

Table III shows the relativistic energies E_D and E_K for ground states of relativistic harmonic oscillators, for growing values of the oscillator frequency. The maximal absolute error of each value does not exceed ± 1 in the last digits. For comparison, the modified Dirac oscillator energies E_{DO} are also displayed [10]. Since in the nonrelativistic limit the Dirac oscillator becomes the isotropic harmonic oscillator with a strong spin-orbit coupling, the spectra may be compared only for the s states.

In Table IV we list the first-order relativistic energies calculated for the nonrelativistic degenerate states with $2n + l = 2,3,4$. One can see that in the first-order perturbation theory, the degeneracy of the nonrelativistic levels corresponding to states with the same value of $\Lambda = 2n + l$ is only partially removed (states $n = 2$, $\kappa = -1$ and $n = 0$, $\kappa = 4$ have the same energy). However, fully relativistic energies are nondegenerate. This is because the dynamical symmetry SU(3), specific for $V \sim r^2$, does not appear in the relativistic models. The degeneracy of the relativistic spectra is caused only by the

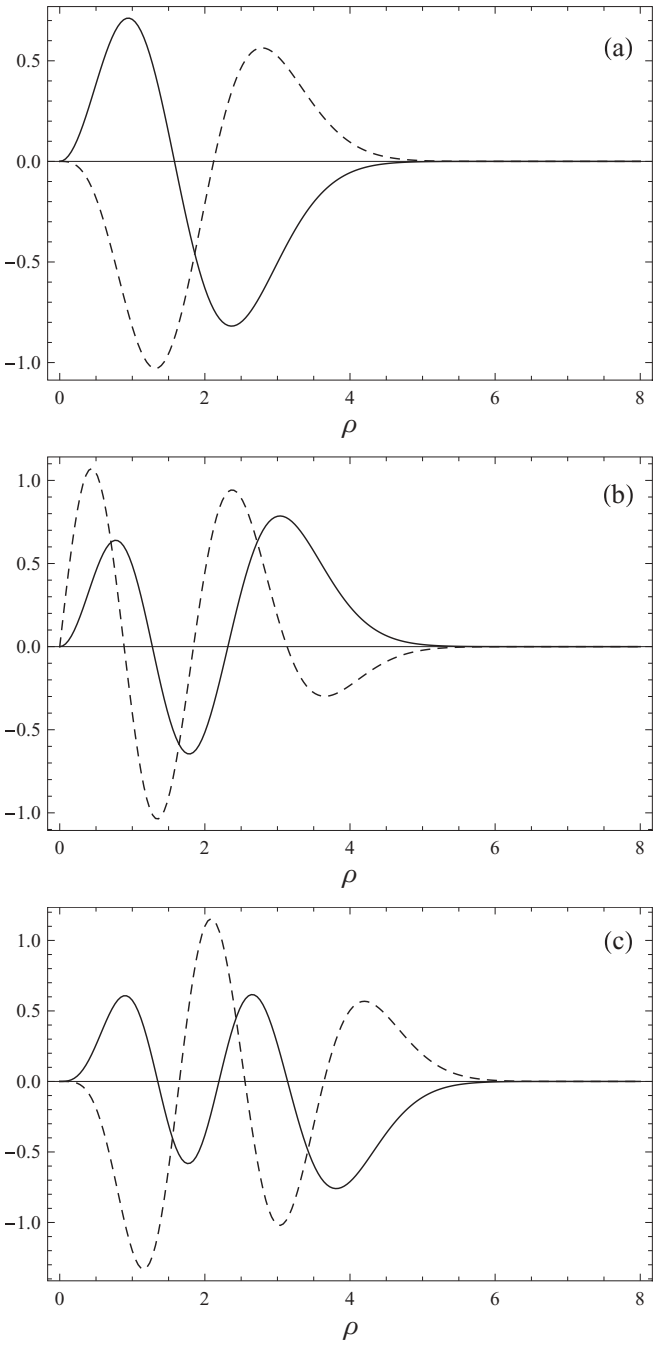

FIG. 7. Normalized radial wave functions $P(\rho)$ (solid line) and $Q(\rho)$ (dashed line) for excited states: (a) $2p_{3/2}$, (b) $3p_{1/2}$, and (c) $4d_{5/2}$, with $\omega = 1$.

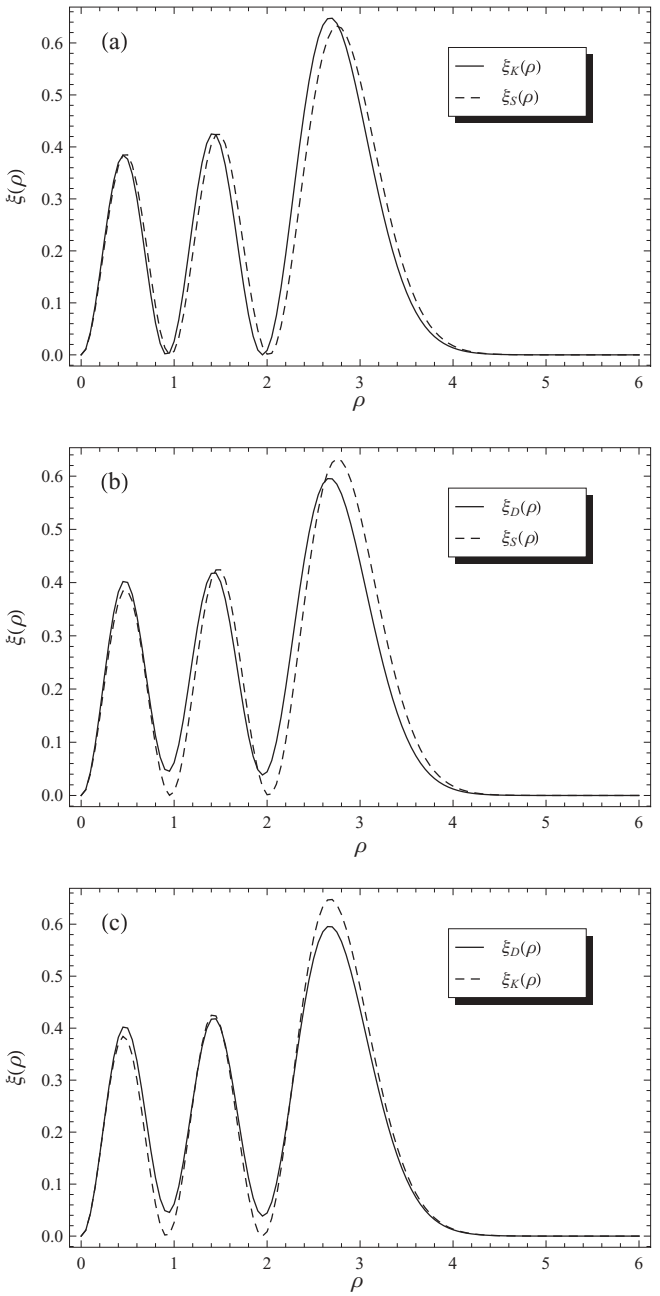

FIG. 8. Radial densities of probability for (a) relativistic spin-0 oscillator ξ_K and nonrelativistic isotropic oscillator ξ_S, (b) relativistic spin-$\frac{1}{2}$ oscillator ξ_D and nonrelativistic isotropic oscillator ξ_S, and (c) relativistic spin-$\frac{1}{2}$ oscillator ξ_D and relativistic spin-0 oscillator ξ_K, for excited states $3s$ and $\omega = 1000$.

symmetry of the Hamiltonian (8) with respect to the rotational group. Since energies are independent of the eigenvalue of the projection of the total angular momentum, the degree of degeneracy of each level is equal to $2j + 1$.

Figure 7 shows the normalized radial amplitudes P and Q for three excited states of a relativistic spin-$\frac{1}{2}$ harmonic oscillator with a parabolic potential, corresponding to $n = 1,2,3$. We can see that the number n corresponds to the number of the nonzero nodes of the radial function P. Thus, the number n can be referred to as the radial quantum number. Note that the radial functions P and Q have different nodes. Consequently, the radial density of probability $\xi_D(\rho)$ does not have any zeros, for $\rho > 0$. The comparison of the radial densities of probability for relativistic spin-0 and spin-$\frac{1}{2}$ oscillators with quadratic potentials and the nonrelativistic isotropic oscillator is made in Fig. 8.

All features of the presented models of the oscillator make them useful for further applications. The generalization to many-particle relativistic problems with harmoniclike interactions may be performed in a similar way as for atomic systems. A relativistic model of the two-body *harmonium* will be investigated in the forthcoming papers.

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