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Quantization of the charge in Coulomb plus harmonic potential

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We consider two models where the wave equation can be reduced to the effective Schrödinger equation whose potential contains both harmonic and the Coulomb terms, $\omega^2 r^2 - a/r$. The equation reduces to the biconfluent Heun's equation, and we find that the charge as well as the energy must be quantized and state-dependent. We also find that two quantum numbers are necessary to count radial degrees of freedom and suggest that this is a general feature of differential equation with higher singularity like the Heun's equation.

Subject Index E01, E02, E31, E38

1. Introduction

Since Schrödinger established the equation in his name, it has been believed that for any confining potential there exists discrete energy levels, although we may not write the analytic solution explicitly. However, recent experience [1,2] tells us that this may not be the case. When the potential has higher singularity, we need a higher regularity condition. As a consequence, there is no normalizable solution unless the potential itself is quantized.

In this paper, we consider two models where the wave equation can be reduced to the effective Schrödinger equation whose potential contains both a harmonic term $\omega^2 r^2$ and the Coulomb term $-a/r$. The equation of motion reduces to the biconfluent Heun's equation, and we find that the charge as well as the energy must be quantized. That is, both energy and charge must depends on the states.

We also find that, due to the higher singularity, a new quantum number appears. For example, in a spherically symmetric case, apart from the radial quantum number N and two angular ones L, m, one more quantum number, K, appears. It turns out that only when we combine the two quantum numbers N, K can the full radial degree of freedom be counted. We suggest that the presence of extra quantum numbers to count correct radial degrees of freedom is a general feature of differential equations with higher singularity like the Heun's equation.

2. A quark model with Coulomb and linear scalar potential

Lichtenberg et al. [3] found a semi-relativistic Hamiltonian which leads to a Krolikowski-type second-order differential equation [4–6] in order to calculate meson and baryon masses. In the center-of-mass system, the total energy H of two free particles of masses m_1, m_2, is

$$H = \sqrt{\boldsymbol{p}^2 c^2 + m_1^2 c^4} + \sqrt{\boldsymbol{p}^2 c^2 + m_2^2 c^4}. \tag{1}$$

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Let S be the Lorentz scalar interaction and V be the interaction which is a time-component of a 4-vector. It is then natural to incorporate the V and S terms into Eq. (1) by making the replacements

$$H \to H + V, \qquad m_i \to m_i + \frac{1}{2}S, \qquad i = 1, 2\,. \tag{2}$$

We set $m_1 = m_2 = 0$ and introduce $V = -a/r$ and study its effect on the spin-free Hamiltonian which was proposed for the meson ($q\bar{q}$) system in Refs. [7–10]. Then we have

$$\left(E + \frac{a}{r}\right)^2 \psi(r) = 4\left\{c^4\left(\frac{1}{2}br\right)^2 + c^2\left[P_r^2 + \frac{\hbar^2 L(L+1)}{r^2}\right]\right\}\psi(r), \tag{3}$$

where b is a real positive constant and we used $\boldsymbol{p}^2 = P_r^2 + [\hbar^2 L(L+1)]/r^2$ with $P_r^2 = -\hbar^2\{(\partial^2/\partial r^2) + [(2/r)(\partial/\partial r)]\}$. The linear scalar potential is for the confinement of the quarks bound by a QCD flux string with constant string tension b. Previously, we investigated the model in the case $V = 0$ [1] and concluded that for the consistency of the spectrum the current quark should have zero mass. Here we want to introduce $V = -a/r$ and understand its effect in the presence of the confining potential.

Factoring out the behavior near $r = 0$ by $\psi(r) = r^{\tilde{L}} f(r)$, the above equation becomes

$$\frac{d^2 f(r)}{dr^2} + \frac{2(\tilde{L}+1)}{r}\frac{df(r)}{dr} + \left(\frac{\mathcal{E}^2}{4} - \frac{b_0^2}{4}r^2 + \frac{\mathcal{E}a_0}{2r}\right)f(r) = 0, \tag{4}$$

where $a_0 = a/\hbar c$, $b_0 = bc/\hbar$, $\mathcal{E} = E/\hbar c$ and $\tilde{L} = -1/2 + \sqrt{(L+1/2)^2 - a_0^2/4}$. If we further factor out the near-∞ behavior by $f(r) = \exp\left[-(b_0/4)r^2\right] y(r)$ and introduce $\rho = \sqrt{b_0/2}\,r$, we get

$$\rho\frac{d^2 y}{d\rho^2} + \left(\mu\rho^2 + \varepsilon\rho + \nu\right)\frac{dy}{d\rho} + (\Omega\rho + \beta)\,y = 0, \tag{5}$$

with $\mu = -2$, $\varepsilon = 0$, $\nu = 2(\tilde{L}+1)$, $\beta = \epsilon a_0$ and

$$\Omega = \epsilon^2 - (2\tilde{L} + 3), \text{with } \epsilon = \mathcal{E}/\sqrt{2b_0}. \tag{6}$$

This equation is a biconfluent Heun's equation which has a regular singularity at the origin and an irregular singularity of rank two at the infinity [11,12].

Substituting $y(\rho) = \sum_{n=0}^{\infty} d_n \rho^n$ into (5), we obtain the recurrence relation:

$$d_{n+1} = A_n\, d_n + B_n\, d_{n-1} \qquad \text{for } n \geq 1, \text{with} \tag{7}$$

$$A_n = -\frac{\varepsilon n + \beta}{(n+1)(n+\nu)}, \quad B_n = -\frac{\Omega + \mu(n-1)}{(n+1)(n+\nu)}. \tag{8}$$

For the $n = 0$ term, only d_1, d_0 appear and give $d_1 = A_0 d_0$.

Notice that when $a_0 = 0$, we have

$$A_n = \frac{\beta}{(n+1)(n+\nu)} = \frac{\epsilon a_0}{(n+1)[n + 2(\tilde{L}+1)]} = 0, \tag{9}$$

so that the three-term recurrence relation given in Eq. (7) is reduced to a two-term recurrence relation between d_{n+1} and d_{n-1} and the Heun's equation is reduced to a hypergeometric one. That is, in this scaling, the Coulomb parameter is precisely the term increasing the singularity order. Similarly, if

Table 1. Roots of a_0^2 for $N = 8$.

	a_{00}^2	a_{01}^2	a_{02}^2	a_{03}^2	a_{04}^2
$L = 0$	0	None	None	None	None
$L = 1$	0	2.35525	7.90698	None	None
$L = 2$	0	2.97179	11.2403	21.9815	None
$L = 3$	0	3.43735	13.3617	28.3483	44.4635
$L = 4$	0	3.81341	14.9937	32.6448	54.7228
$L = 5$	0	4.12728	16.3243	35.9753	61.791

$b_0 = 0$, the system can also be mapped to a hypergeometric type. The problem arises only when both potential terms are present.

Now, unless $y(\rho)$ is a polynomial, $\psi(r)$ is divergent as $\rho \to \infty$. Therefore, we need to impose regularity conditions by which the solution is normalizable. If we impose the two conditions [11,12]

$$B_{N+1} = d_{N+1} = 0 \qquad \text{where } N \in \mathbb{N}_0, \tag{10}$$

the series expansion becomes a polynomial of degree N: as one can see from Eq. (7), Eq. (10) is sufficient to give $d_{N+2} = d_{N+3} = \cdots = 0$ recursively. Then the solution is a polynomial of the order of N, $y_N(\rho) = \sum_{i=0}^{N} d_i \rho^i$. The question whether imposing both equations in Eq. (10) is really necessary for the finite solution was studied numerically and was concluded affirmatively in our earlier work [1].

In general, $d_{N+1} = 0$ will define a $(N+1)$th-order polynomial $\mathcal{P}_{N+1}$ in a_0, so that Eq. (10) gives

$$\epsilon_{N,L} = \sqrt{2N + 2\tilde{L} + 3}, \quad \mathcal{P}_{N+1}(a_0) = 0, \tag{11}$$

where the first equation comes from $B_{N+1} = 0$, and it is nothing but the usual energy quantization condition. Below we will examine the meaning of the second condition by constructing explicitly the expressions of a few low-order polynomial $\mathcal{P}_{N+1}$, which are given in the appendix.

One surprising fact is that for a given N, L there are many solutions which we can index by an integer K which is smaller than N. Depending on whether N is even or odd, the distribution of solutions of $\mathcal{P}_{N+1}(a_0) = 0$ is different. For low-lying L, the number of roots increases with L but not regularly. However, for $L \geq [N/2] - 1$ the number of roots is given by $[N/2] + 2$. Here, $[x]$ is the integer part of $x > 0$. The presence of an extra quantum number is natural from the algebraic point of view. We postpone the dynamics of associated K to the next section, where we discuss the problem with a simpler model.

Table 1 shows some real roots of a_0^2 values for each L with fixed $N = 8$; here, a_{0i}^2 is the ith root of a_0^2 with given N, L. Similarly, Table 2 shows real roots of a_0^2 values for each L when $N = 9$.

For lower values of K, we can find an approximate fitting function. For example, for $K = 0$ and for odd N, it is given by

$$a_{0,NL0}^2 \approx 1.22 \tan^{-1}\left[\frac{(L+1)^{0.6} - 0.5}{0.55N^{0.7} + 0.5}\right] + 0.18. \tag{12}$$

We calculated 338 different values of a_0^2 at various (N, L) and the results are shown by the dots in Fig. 1. These data are fitted well by the above formula. Notice also that for even values of N, $a_0 = 0$ is always a solution for any L.

Table 2. Roots of a_0^2 for $N = 9$.

	a_{00}^2	a_{01}^2	a_{02}^2	a_{03}^2	a_{04}^2
$L = 0$	0.374151	None	None	None	None
$L = 1$	0.580422	4.80626	None	None	None
$L = 2$	0.71935	6.26714	16.0299	24.9066	None
$L = 3$	0.828203	7.32404	19.5432	35.397	48.5634
$L = 4$	0.917807	8.17078	22.1613	41.6303	63.7813
$L = 5$	0.993589	8.87727	24.2768	46.338	73.3714

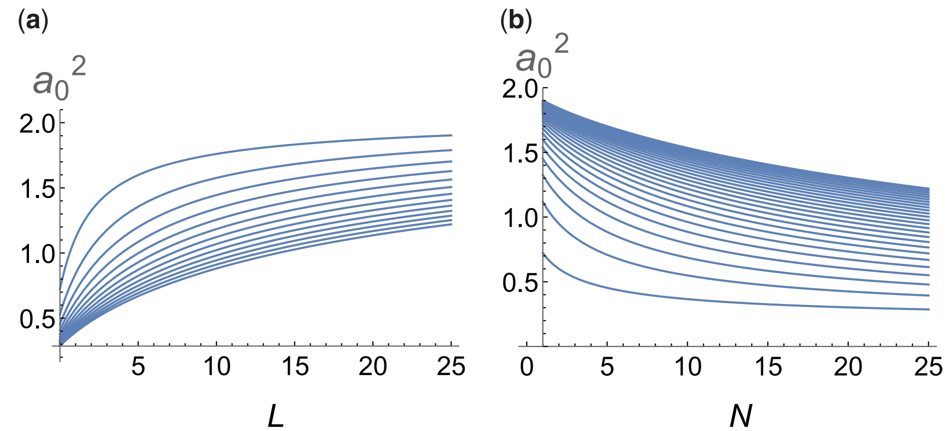

Fig. 1. (a) Fitting of a_0^2 data by Eq. (12), as functions of L. The lowest line is for $N = 1$, the top line is for $N = 25$. (b) Fitting of a_0^2 data by Eq. (12) as functions of odd N with L. The lowest line is for $L = 0$, the top one is for $L = 25$. In both figures (a) and (b), N is odd.

By substituting Eq. (12) into Eq. (11), we can fit the experimental data of E, which is the hadron mass.

$$E_{N,L} \simeq \sqrt{2\hbar c \cdot bc^2 \left[2N + 2 + \sqrt{(2L+1)^2 - a_{0,NLK}^2}\right]}, \tag{13}$$

where $a_0 = a/\hbar c$. What is surprising is the fact that the charge parameter a should be quantized as values approximately given in Eq. (12) if the charge is coming in the presence of the linear scalar potential which gives the confinement. Our treatment gives the analytic results in the presence of both the linear potential and the Coulomb potential. However, we must also comment that in the presence of the quark mass our method breaks down.

3. Quantum dot with Coulomb and harmonic potential

Here we consider a non-relativistic Schrödinger equation with Coulomb potential and external harmonic oscillator potential for a system of two electrons in a three-dimensional Euclidean space [13–16]. The Schrödinger equation is given by

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + V_{\text{eff}}(r)\right]\psi(r) = E\psi(r), \tag{14}$$

$$\text{with } V_{\text{eff}}(r) = \omega^2 r^2 - \frac{a}{r} + \frac{\hbar^2}{2m}\frac{L(L+1)}{r^2}, \tag{15}$$

Introducing $\rho = r\left[(2m\omega^2)/\hbar^2\right]^{1/4}$, the above equation becomes

$$\rho\frac{d^2\psi}{d\rho^2} + \frac{2}{\rho}\frac{d\psi}{d\rho} + \left[\epsilon - \rho^2 + \frac{a_0}{\rho} - \frac{L(L+1)}{\rho^2}\right]\psi = 0, \tag{16}$$

where

$$\epsilon = \frac{E}{\omega}\sqrt{\frac{2m}{\hbar^2}}, \quad a_0 = \frac{a}{\sqrt{\omega}}\left(\frac{\hbar^2}{2m}\right)^{-3/4}. \tag{17}$$

Factoring out the behavior near $\rho = 0$ by $\psi(\rho) = \rho^L f(\rho)$, it becomes

$$\frac{d^2 f(\rho)}{d\rho^2} + \frac{2(L+1)}{\rho}\frac{df(\rho)}{d\rho} + \left(\epsilon - \rho^2 + \frac{a_0}{\rho}\right)f(\rho) = 0. \tag{18}$$

Factoring out near-∞ behavior by $f(\rho) = e^{-\rho^2/2}y(\rho)$, we get the standard form Eq. (5) with

$$\mu = -2, \varepsilon = 0, \nu = 2(L+1), \beta = a_0, \Omega = \epsilon - (2L+3).$$

Similarly, if we impose Eq. (10), the series expansion becomes a polynomial of degree N. The solution becomes a polynomial $y_N(\rho) = \sum_{i=0}^{N} d_i \rho^i$. In general, $d_{N+1} = 0$ will define a $(N+1)$th order polynomial $\mathcal{P}_{N+1}$ in a_0, so that Eq. (10) gives

$$\epsilon_{N,L} = 2N + 2L + 3, \quad \mathcal{P}_{N+1}(a_0) = 0. \tag{19}$$

where the first comes from $B_{N+1} = 0$, which is the energy quantization condition. Below, we will examine the meaning of the second equation. To do that we need explicit expressions of a few lower-order polynomial $\mathcal{P}_{N+1}$:

$$\begin{aligned}
\mathcal{P}_1(a_0) &= a_0, \\
\mathcal{P}_2(a_0) &= a_0^2 - 4(L+1), \\
\mathcal{P}_3(a_0) &= a_0^3 - 4(4L+5)a_0, \\
\mathcal{P}_4(a_0) &= a_0^4 - 20(2L+3)a_0^2 + 144(L+1)(L+2), \\
\mathcal{P}_5(a_0) &= a_0^5 - 20(4L+7)a_0^3 + 32[89 + 16L(2L+7)]a_0.
\end{aligned} \tag{20}$$

In the appendix, we give a few low-order polynomial $y_N(\rho)$ with $d_0 = 1$.

We have seen that a and ω are related by Eq. (17) and that $\mathcal{P}_{N+1}(a_0) = 0$ does not contain any dimensional parameter. This means that $a/\sqrt{\omega}$ should be a solution of a polynomial equation, which depends on N, L. Such extra quantization is a consequence of the Heun's equation. For the hypergeometric equations, the recurrence relation is reduced to two terms after factoring out the asymptotic behavior. There, we do not have $d_{N+1} = 0$. Hence to have a normalizable polynomial solution, we only need to fine-tune just one parameter; the energy. For the Heun's equation, we have to impose two constraints, which in turn requires the charge quantization of the system. In short, its higher singularity requires a higher regularity condition. This is the origin of the charge quantization.

Notice that a depends on the quantum numbers that parametrize quantum states. This means that when the electron makes a transition from one state to another, the charge parameter must be changed to a new value. This raises the question of how the dynamics of one particle can change the

Table 3. Roots of a_0^2.

	$N=4$				$N=5$		
	a_{00}^2	a_{01}^2	a_{02}^2		a_{00}^2	a_{01}^2	a_{02}^2
$L=0$	0	24.701	115.299	$L=0$	6.38432	64.8131	208.803
$L=1$	0	41.8531	178.147	$L=1$	10.9664	102.965	306.069
$L=2$	0	58.414	241.586	$L=2$	15.2359	140.155	404.609
$L=3$	0	74.7438	305.256	$L=3$	19.3928	176.898	503.709
$L=4$	0	90.9604	369.04	$L=4$	23.4959	213.403	603.101
$L=5$	0	107.114	432.886	$L=5$	27.5688	249.768	702.664

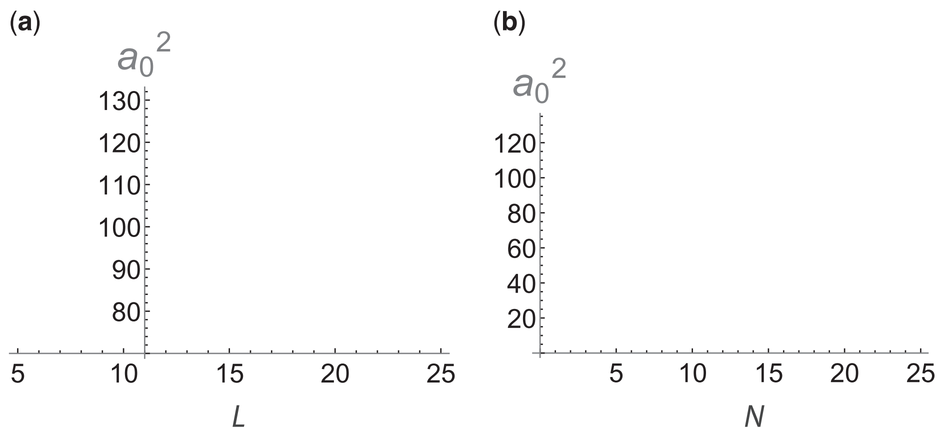

Fig. 2. Roots of the smallest a_0^2, as function of L and N. In (a), the lowest line is for $N = 1$, the top line is for $N = 25$. In (b), the lowest line is for $L = 0$, the top one is for $L = 25$. In both figures (a) and (b), N is odd.

potential energy which is determined by the surrounding system. In fact, V is not the potential but the potential energy. The potential belongs to the surroundings while the potential energy contains both surrounding and particle information. Therefore a should be written as a product of the particle's charge q times the charge Q which makes the potential ϕ_Q, so that $V = q\phi_Q$. When we say that charge is quantized, what we mean is the quantization of q. In short, when the potential energy has higher singularity, the charge as well as the energy should depends on the state. At first, this concept was rather drastic, but it is a consequence of requiring d_{N+1}, the necessity of which was confirmed by numerical investigation; without it, the shooting method did not work.

Notice that in this model the energy ϵ is linear in N, L and does not depend on a quantized value of a_0^2. Table 3 shows all roots of a_0^2 values for each L for $N = 4, 5$.

Since the quantized values of a_0^2 depend on three quantum numbers, we choose the $K = 0$ sector of a_0^2 with given (N, L). Then, Fig. 2 shows us that a_0^2 is roughly linear in N, L for odd N. For even N, the $K = 0$ sector gives $a_0^2 = 0$.

For the figure, we calculated 338 different values of a_0^2 at various (N, L). From the explicit calculation, we find the following pattern: List N+1 a_0^2 in the increasing order such that $a_{0,K}$ is the Kth one, $K = 0, 1, \cdots, [N/2] - 1$; here, $[x]$ means the integer part of the positive real number x. Then, although the total number of nodes is N, some of them are in the negative region of ρ. The polynomial with a_{0K} has $N - \lfloor N/2 \rfloor + K$ nodes in the region $\rho > 0$. Therefore K counts the number of nodes that crossed $\rho = 0$ compared with $K = 0$ in the positive domain. We give several plots of $y5$ in Fig. 3 for better understanding.

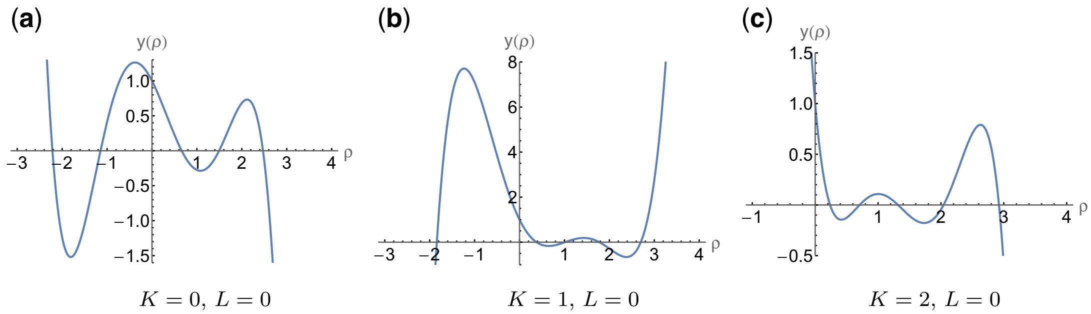

Fig. 3. y_5 for various a_{0K} values with $K = 0, 1, 2$ and $L = 0$. For each a_{0K}, the number of positive roots is given by $N - \lfloor N/2 \rfloor + K = K + 3$.

In three dimensions, a spinless hydrogen atom has three quantum numbers: N, L, m: N for radial and the other two for angular momentum. However, in the presence of the harmonic potential, the charge and energy have discrete values depending on the four quantum numbers N, L, m, K, which shows an apparent mismatch between the number of degrees of freedom and that of the quantum numbers. However, as we have shown above, with $K = 0$, only half of the nodes of the radial wave function are in the positive region. This means that the radial solution for fixed K, say $K = 0$, can not span an arbitrary shape of the radial function in the positive region. In fact, K counts the number of nodes moved from negative to positive region compared with the $K = 0$ case. This means that N together with K counts the full radial degrees of freedom, and without the extra quantum number K the solutions cannot be a basis of the radial wave functions.

We expect that the presence of an extra quantum number to count correct radial degrees of freedom is a general feature of differential equations with higher singularity like the Heun's equation.

4. Discussion

Caruso et al. [13] investigated a non-relativistic two-dimensional radial Schrödinger equation which can be related to ours just by shifting L to $L - 1/2$ in Ref. (15). They obtained part of the result of section 3 of this paper but they interpreted the result as the quantization of ω, the coefficient of the harmonic potential. The quantization of ω would imply that the single-particle dynamics changes the potential's parameter, which does not sound plausible. In our case, a is split into particle charge q and charge Q in the potential, so that Couomb term can be written as $V_{Coulomb} = q\phi_Q(r)$. q is a property of the particle, therefore dependence of the particle charge on the state is natural although the concept is still not familiar so far. In field theory, charge depends on the probe energy scale due to the renormalization. Thus the state-dependence of the charge can be regarded as discrete renormalization of the charge induced by the smoothing-out process of the singularity of the potential.

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Appendix A. $\mathcal{P}_N$ for $N = 0,1,...,5$

We lists expressions of a few-order polynomial $\mathcal{P}_N$+1 of Eq. (11):

$$\begin{aligned}
\mathcal{P}_1(a_0) &= a_0,\\
\mathcal{P}_2(a_0) &= a_0^2\left[4+\sqrt{(2L+1)^2-a_0^2}\right]-2\left[1+\sqrt{(2L+1)^2-a_0^2}\right],\\
\mathcal{P}_3(a_0) &= a_0\left\{-a_0^2\left[6+\sqrt{(2L+1)^2-a_0^2}\right]+12+8\sqrt{(2L+1)^2-a_0^2}\right\},\\
\mathcal{P}_4(a_0) &= -a_0^6+a_0^4\left[85+4L(L+1)+16\sqrt{(2L+1)^2-a_0^2}\right]\\
&\quad-8a_0^2\left[47+10L(L+1)+25\sqrt{(2L+1)^2-a_0^2}\right]\\
&\quad+144\left[L^2+L+1+\sqrt{(2L+1)^2-a_0^2}\right]
\end{aligned} \tag{A1}$$

Appendix B. $y_N(\rho)$ polynomials for $N = 0,1,...,5$

We lists expressions of a few lower-order polynomial $y_N(\rho)$:

$$\begin{aligned}
y_0(\rho) &= 1,\\
y_1(\rho) &= 1-\frac{a_0\rho}{2(1+L)},\\
y_2(\rho) &= 1+\frac{[a_0^2-8(L+1)]\rho^2-2a_0(2L+3)\rho}{4(L+1)(2L+3)}\\
y_3(\rho) &= 1+\frac{a_0(36+28L-a_0^2)\rho^3+6(L+2)[a_0^2-12(L+1)]\rho^2-12(L+2)(2L+3)a_0\rho}{24(L+1)(L+2)(2L+3)}\\
y_4(\rho) &= 1+\frac{1}{96(L+1)(L+2)(2L+3)(2L+5)}\\
&\quad\times\Big\{(384(L+1)(L+2)-4(25+16L)a_0^2+a_0^4)\rho^4+4(2L+5)(52+40L-a_0^2)a_0\rho^3\\
&\quad-24(L+2)(2L+5)(16+16L-a_0^2)\rho^2-48(L+2)(2L+3)(2L+5)a_0\rho\Big\}\\
y_5(\rho) &= 1+\frac{1}{960(L+1)(L+2)(L+3)(2L+3)(2L+5)}\\
&\quad\times\Big\{-a_0(6880+2384L^2+24L(354-5a_0^2)+a_0^2(a_0^2-220))\rho^5\\
&\quad+10(L+3)(720(L+1)(L+2)-4(35+22L)a_0^2+a_0^4)\rho^4\\
&\quad+40a_0(L+3)(2L+5)(68+52L-a_0^2)\rho^3-240(L+2)(L+3)(2L+5)(20+20L-a_0^2)\rho^2\\
&\quad-480a_0(L+2)(L+3)(2L+3)(2L+5)\rho\Big\}
\end{aligned} \tag{B1}$$

In Eq. (19) the roots $\mathcal{P}_{N+1}(a_0) = 0$ are simple and there is the orthogonality relation [11]

$$\int_0^\infty d\rho\ \rho^{2L+1} e^{-\rho^2} y_{N,K}(\rho) y_{N',K'}(\rho) = \mathcal{M}(N,K)\delta_{NN'}\delta_{KK'}. \tag{B2}$$

Here, $a_0 \in \{a_{0,0}, a_{0,1}, a_{0,2}, \cdots, a_{0,K}\}$ for $0 \le K \le [N/2+1]$ for the normalization constant.

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