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Exact solutions of the Schrödinger equation for some quantum-mechanical many-body systems

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We have solved exactly the Schrödinger equation in hyperspherical coordinates for some quantum-mechanical many-body systems. These systems, which interact with Coulomb, inverse-square, harmonic-oscillator, dipole, or Yukawa potentials, etc., can be solved in a similar way. Wave functions are expanded into orthonormal complete basis sets of the hyperspherical harmonics of hyperangles and generalized Laguerre polynomials of the hyperradius. The eigenvalues can be obtained explicitly by solving a simple secular equation. The results of practical calculations of Coulomb potential systems, such as H, He, and H^-, etc., agree well with the reported exact ones.

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I. INTRODUCTION

Since quantum mechanics was introduced, the Schrödinger equation has proved to be very useful for understanding microsystems. But the only exact solutions found for systems in nature are for free-particle motion, the particle in a box, the hydrogen atom, hydrogenlike ions, the hydrogen molecular ion, the rigid rotator, the harmonic oscillator, Morse and modified [1] Morse oscillators, etc. For more complicated systems, however, approximation methods have to be used, for instance, the variation method, the perturbation method, etc., which sometimes give poor results compared with experimental ones, and practical calculations with them are usually very difficult, even with the use of powerful computers.

Concerning the Schrödinger equation for complicated systems, scientists had looked for many possible solutions, but little success was achieved until hyperspherical coordinates [2] were used, with which a very beautiful coupled second-order differential equation with the hyperradius as a variable was obtained by integrating out the hyperangular parts [3,4]. Therefore, the concentration was on solving the hyperradial part of the wave function.

To solve this coupled differential equation of D-dimensional systems, great efforts have been made. The method of directly expanding the hyperradial wave function in terms of powers of the hyperradius r was not efficient here. Fock [5] analyzed the properties of the hyperradial part of the wave function for the helium atom, and expanded it in terms of positive powers of r and $\ln r$. Later, this representation was studied and extended to polyelectron atoms [3,4,6–11]. And exact solutions had been obtained [3,4,10]; however, two of their methods [3,4] were very difficult to use and one [10] met with difficulties in numerical approaches.

We [12] considered this problem in a way entirely different from the approaches mentioned above for the Coulomb interaction system. Instead of following Fock's expansion, we expanded the hyperradial part of the wave function in terms of an orthonormal complete basis set of generalized Laguerre polynomials (GLP's). This led the equation to a simple recurrence relation of expansion coefficients, therefore, the Schrödinger equation became solvable for this system. In this paper, we treat the general complicated systems with potentials described by the distances between the particles, such as Coulomb, inverse square, harmonic-oscillator, and dipole as well as the Yukawa, Gauss, and negative exponential types.

This paper is organized in the following way: In Sec. II, we give the general deduction of solving the coupled differential equation for the potentials mentioned above. In Sec. III we study hydrogenlike systems with the scheme proposed in Sec. II and the discussion on the wave function near $r=0$. The fourth section includes detailed calculations of several heliumlike systems, numerical results, discussion on the convergent speed, and the possibility of the usage of this scheme for complicated systems. In the final section is our conclusions.

II. SOLVING THE COUPLED SECOND-ORDER DIFFERENTIAL EQUATIONS

For a nonrelativistic many-body system, the Schrödinger equation is (in atomic units)

$$\left\{-\frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}\nabla_{\mathbf{r}_i}^2+\sum_{i<j}\hat{V}(r_{ij})\right\}\phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=E\phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)\;, \tag{1}$$

where N is the number of particles in the system, m_i is the mass of ith particle, E is the energy of the system, ϕ is the wave function corresponding to the energy, $\sum_{i<j}\hat{V}(r_{ij})$ is the potential of the system, and r_{ij} represents the distance between the i and the j particles.

To give the deduction for general potentials, we first start with the well-known Coulomb potential, of which the potential is

$$\sum_{i<j}\hat{V}(r_{ij})=\sum_{i<j}\frac{z_iz_j}{r_{ij}}\;, \tag{2}$$

where z_i is the number of charges (including sign) carried by the ith particle.

Using the coordinate transformation,

$$\begin{aligned}
\rho_1 &= \mathbf{r}_2 - \mathbf{r}_1 \,, \\
\rho_2 &= \mathbf{r}_3 - (m_1\mathbf{r}_1 + m_2\mathbf{r}_2)/(m_1+m_2) \,, \\
&\vdots \\
\rho_{N-1} &= \mathbf{r}_N - \left[\sum_{i=1}^{N-1} m_i\mathbf{r}_i\right] \Big/ \sum_{i=1}^{N-1} m_i \,, \\
\mathbf{R}_c &= \left[\sum_{i=1}^{N} m_i\mathbf{r}_i\right] \Big/ \sum_{i=1}^{N} m_i \,,
\end{aligned} \tag{3}$$

to nullify the motion of center of mass and make mass scaling, we come to the following equation,

$$\left\{ -\frac{1}{2}\sum_{i=1}^{N-1} \nabla^2_{\rho_i} + \sum_{i<j} \hat{V}(r_{ij}) \right\} \Psi(\rho_1,\rho_2,\ldots,\rho_{N-1}) = E\Psi(\rho_1,\rho_2,\ldots,\rho_{N-1}) \,. \tag{4}$$

There are different representations [2–4,13,14] of the hyperspherical coordinates. Calculations with them give the same results (we have tested it by using the method in this paper). Therefore, any of them can be chosen in practical calculations. The coordinates used in the calculations of Sec. IV are the same as those of Klar and Klar [13]. Whichever representation we take, the Schrödinger equation can be transformed into the same form as [3,4,13,14]

$$\left\{ -\frac{1}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{D-1}{r}\frac{\partial}{\partial r} - \frac{\hat{\Lambda}^2(\Omega)}{r^2} \right] - \frac{\hat{Z}(\Omega)}{r} - E \right\} \Psi(r,\Omega) = 0 \,, \tag{5}$$

where r is the hyperradius, $\hat{\Lambda}^2(\Omega)$ is the generalized angular momentum operator, Ω stands for the collective hyperspherical angles, and D, being equal to $3(N-1)$, represents the dimension.

Expanding the wave function into hyperspherical harmonics (HH), which are the simultaneous eigenfunctions of the generalized angular momentum operator, the squared total orbital angular momentum operator, its space-fixed component operator, the parity operator, and the electron exchange operator [3,7,13]

$$\Psi(r,\Omega) = \sum_{\lambda,\mu} \phi_{\lambda\mu}(r) Y_{\lambda\mu}(\Omega) \,, \tag{6}$$

and integrating out the hyperangular part, a set of coupled second-order differential equations can be obtained,

$$\left\{ -\frac{1}{2}\left[\frac{d^2}{dr^2} + \frac{D-1}{r}\frac{d}{dr} - \frac{\lambda(\lambda+D-2)}{r^2} \right] - E \right\} \phi_{\lambda\mu}(r) - \frac{1}{r}\sum_{\lambda',\mu'} Z_{\lambda\mu\lambda'\mu'}\phi_{\lambda'\mu'}(r) = 0 \,, \tag{7}$$

where λ is the quantum number of generalized angular momentum operator, μ stands for a set of quantum numbers belonging to λ, $\phi_{\lambda\mu}(r)$ and $Y_{\lambda\mu}(\Omega)$ are the hyperradial wave function and HH belonging to $\lambda\mu$, respectively, and $Z_{\lambda\mu\lambda'\mu'}$ are the coupling constants of the generalized angular momentum,

$$Z_{\lambda\mu\lambda'\mu'} = \int d\Omega \, Y^*_{\lambda\mu}(\Omega)\hat{Z}(\Omega)Y_{\lambda'\mu'}(\Omega) \,, \tag{8}$$

the matrix of which is symmetric.

In matrix notation, Eq. (7) is written in a familiar form

$$\left\{ -\frac{1}{2}\left[\frac{d^2}{dr^2} + \frac{D-1}{r}\frac{d}{dr} - \frac{\underline{\Lambda}(\underline{\Lambda}+D-2)}{r^2} \right] - \frac{\underline{Z}}{r} - E \right\} \underline{\phi}(r) = 0 \,, \tag{9}$$

where $\underline{\Lambda}$ is an $M \times M$ diagonal matrix with elements $\lambda\delta_{\lambda\lambda'}\delta_{\mu\mu'}$, $\underline{Z}$ is an $M \times M$ matrix with elements $Z_{\lambda\mu\lambda'\mu'}$, M being the number of orthonormal basis functions of HH taken, and $\underline{\phi}(r)$ is a one column matrix $\underline{\phi}(r) = \{\phi_{\lambda\mu}(r)\}$.

The general potential of a system is

$$\sum_{i<j} \hat{V}(r_{ij}) = \sum_{i<j}\sum_{k=-2}^{K} Z_k^{ij} r_{ij}^k \,, \tag{10}$$

where Z_k^{ij} is a constant factor and K is an integer. We write the potential part in this complicated form only because we want to include not only the potentials of Coulomb, inverse square, harmonic-oscillator, and dipole types, but also the Yukawa potential $\alpha r_{ij}^{-1} e^{-\beta r_{ij}}$, the Gauss potential $\alpha e^{-\beta r_{ij}^2}$, the negative exponential potential $\alpha e^{-\beta r_{ij}}$, and so on. The latter terms should be expanded into $\sum_{k=0}^{\infty} Z_k^{ij} r_{ij}^k$, and we have to truncate this expansion at some value $k = K$.

With a treatment similar to the above-mentioned Coulomb interaction system, we get the matrix form of a general coupled second-order differential equation with the hyperradius as a variable,

$$\left\{ -\frac{1}{2}\left[\frac{d^2}{dr^2} + \frac{D-1}{r}\frac{d}{dr} - \frac{\underline{\Lambda}(\underline{\Lambda}+D-2)}{r^2} \right] + \sum_{k=-2}^{K} \underline{Z}_k r^k - E \right\} \underline{\phi}(r) = 0 \,, \tag{11}$$

where $\sum_{k=-2}^{K} \underline{Z}_k r^k$ corresponds to the general matrix potentials, in which $\underline{Z}_k$ is the general coupling matrix of the generalized angular momentum.

For bound states, we present the following deduction.

First we examine the behavior of wave function as $r \to \infty$. For potentials expressed in negative powers of r_{ij}, or the Yukawa, Gauss, and negative exponential types of potentials, which are equal to zero as $r \to \infty$, we obtain

$$\phi_{\lambda\mu}(r) \overset{r\to\infty}{\longrightarrow} e^{-\xi r}$$

where $\xi^2 = -2E$. Thus, we make the substitution

$$\underline{\phi}(r) = e^{-\xi r}\underline{\psi}(r) \tag{12}$$

and get

$$\frac{d^2\underline{\psi}}{dr^2}+\left[\frac{D-1}{r}-2\xi\right]\frac{d\underline{\psi}}{dr}-\frac{D-1}{r}\xi\underline{\psi}-\sum_{k=-2}^{K}2\bar{\underline{Z}}_k r^k\underline{\psi}=0 \ , \tag{13}$$

where

$$\bar{\underline{Z}}_k=\begin{cases}\underline{Z}_{-2}+\underline{\Lambda}(\underline{\Lambda}+D-2)/2 & \text{for } k=-2 \ ,\\ \underline{Z}_k & \text{otherwise} \ .\end{cases} \tag{14}$$

Let $\rho=2\xi r$; we have

$$\frac{d^2\underline{\psi}(\rho)}{d\rho^2}+\left[\frac{D-1}{\rho}-1\right]\frac{d\underline{\psi}(\rho)}{d\rho}-\frac{D-1}{2\rho}\underline{\psi}(\rho)-\sum_{k=-2}^{K}\tilde{\underline{Z}}_k(\xi)\rho^k\underline{\psi}(\rho)=0 \ , \tag{15}$$

where $\tilde{\underline{Z}}_k(\xi)=2\bar{\underline{Z}}_k/(2\xi)^{k+2}$.

By expanding $\underline{\psi}(\rho)$ according to

$$\underline{\psi}(\rho)=\sum_{n=0}^{\infty}\underline{C}_n L_n^{\nu}(\rho) \ , \tag{16}$$

where $\underline{C}_n$ is the column matrix of expansion coefficients, and $L_n^{\nu}(\rho)$ are generalized Laguerre polynomials [15], which form a complete set of orthonormal basis functions that satisfy the equation

$$\frac{d^2}{d\rho^2}L_n^{\nu}(\rho)+\left[\frac{\nu+1}{\rho}-1\right]\frac{d}{d\rho}L_n^{\nu}(\rho)+\frac{n}{\rho}L_n^{\nu}(\rho)=0 \tag{17}$$

and have the properties

$$\rho L_n^{\nu}=-(\nu+n)L_{n-1}^{\nu}+(\nu+2n+1)L_n^{\nu}-(n+1)L_{n+1}^{\nu} \ , \tag{18}$$

$$\rho\frac{d}{d\rho}L_n^{\nu}=nL_n^{\nu}-(\nu+n)L_{n-1}^{\nu} \ , \tag{19}$$

$$\int_0^{\infty}\rho^{\nu}e^{-\rho}L_n^{\nu}(\rho)L_{n'}^{\nu}(\rho)d\rho=\delta nn'\Gamma(\nu+n+1)/n! \ . \tag{20}$$

Substituting Eq. (16) into Eq.(15) with $\nu=D-2$, we arrive at the equation

$$\sum_{n=0}^{\infty}\left\{\underline{C}_n\left[\frac{d^2}{d\rho^2}L_n^{\nu}+\left[\frac{D-1}{\rho}-1\right]\frac{d}{d\rho}L_n^{\nu}+\frac{n}{\rho}L_n^{\nu}\right]-\left[\frac{2n+D-1}{2}\frac{1}{\rho}+\sum_{k=-2}^{K}\tilde{\underline{Z}}_k(\xi)\rho^k\right]\underline{C}_nL_n^{\nu}\right\}=0 \ . \tag{21}$$

By considering Eq. (17), we have

$$\sum_{n=0}^{\infty}\left[\frac{2n+D-1}{2}\frac{1}{\rho}+\sum_{k=-2}^{K}\tilde{\underline{Z}}_k(\xi)\rho^k\right]\underline{C}_nL_n^{\nu}=0 \tag{22}$$

or

$$\sum_{n=0}^{\infty}\sum_{k=-2}^{K}\underline{W}_k(n,E)\rho^k\underline{C}_nL_n^{\nu}(\rho)=0 \ , \tag{23}$$

where

$$\underline{W}_k(n,E)=\begin{cases}\tilde{\underline{Z}}_{-1}(\xi)+[(2n+D-1)/2]\underline{1} & \text{for } k=-1 \ ,\\ \tilde{\underline{Z}}_k(\xi) & \text{otherwise} \ .\end{cases} \tag{24}$$

and $E=-\xi^2/2$.

Returning to Eq. (11), for the general potentials which are not equal to zero at $r\rightarrow\infty$ (for instance, the harmonic oscillator type), we choose

$$Z^0=\max\{(Z_k)_{\lambda\mu\lambda\mu}\} \ , \tag{25}$$

where we assume that the largest power of r_{ij} in the potential parts is K. So the behavior of the wave function at $r\rightarrow\infty$ is described by

$$-\frac{1}{2}\frac{d^2}{dr^2}\phi_{\lambda\mu}(r)+Z^0r^k\phi_{\lambda\mu}(r)=0 \tag{26}$$

for which the acceptable solution as $r\rightarrow\infty$ is

$$\phi_{\lambda\mu}(r)\xrightarrow{r\rightarrow\infty}e^{-Ar^B} \ , \tag{27}$$

where $A=2(2Z^0)^{1/2}/(K+2)$ and $B=(K+2)/2$. Therefore, we make the substitution

$$\underline{\phi}(r)=e^{-Ar^B}\underline{\psi}(r) \ . \tag{28}$$

Substituting Eq. (28) into Eq. (11), we get

$$\frac{d^2}{dr^2}\underline{\psi}(r)+\left[\frac{D-1}{r}-1\right]\frac{d}{dr}\underline{\psi}(r)-[2(2Z^0)^{1/2}r^{K/2}-1]\frac{d}{dr}\underline{\psi}(r)-(2Z^0)^{1/2}(D-1+K/2)r^{(K-2)/2}\underline{\psi}(r)-\sum_{k=-2}^{K}2\bar{\underline{Z}}_k(E)r^k\bar{\underline{\psi}}(r)=0 \ , \tag{29}$$

where

$$\bar{\underline{Z}}_k(E)=\begin{cases}\underline{Z}_k-Z^0\underline{1} & \text{for } k=K \ ,\\ \underline{Z}_0-E\underline{1} & \text{for } k=0,\\ \underline{Z}_{-2}+\underline{\Lambda}(\underline{\Lambda}+D-2)/2 & \text{for } k=-2,\\ \underline{Z}_k & \text{otherwise.}\end{cases} \tag{30}$$

Expanding $\underline{\psi}(r)$ according to Eq. (16), and substituting it into Eq. (29) (changing the variable from ρ to r), we come to

$$\sum_{n=0}^{\infty}\left\{[2(2Z^0)^{1/2}r^{K/2}-1]\frac{d}{dr}L_n^\nu(r)+(2Z^0)^{1/2}(D-1+K/2)r^{(K-2)/2}L_n^\nu(r)+\frac{n}{r}L_n^\nu(r)+\sum_{k=-2}^{K}2\underline{\bar{Z}}_k(E)r^kL_n^\nu(r)\right\}\underline{C}_n=0\ , \tag{31}$$

with the help of Eq. (17). Considering Eq. (19), Eq. (31) is transformed into

$$\sum_{n=0}^{\infty}\left\{[2(2Z^0)^{1/2}r^{K/2}-1]\frac{1}{r}[nL_n^\nu-(\nu+n)L_{n-1}^\nu]+(2Z^0)^{1/2}(D-1+K/2)r^{(K-2)/2}L_n^\nu(r)\right.$$
$$\left.+\frac{n}{r}L_n^\nu(r)+\sum_{k=-2}^{K}2\underline{\bar{Z}}_k(E)r^kL_n^\nu(r)\right\}\underline{C}_n=0\ . \tag{32}$$

For even K, the above equation can be expressed as

$$\sum_{n=0}^{\infty}\sum_{k=-2}^{K}\underline{\overline{W}}_k(n,E)r^kL_n^\nu(r)\underline{C}_n=0\ . \tag{33}$$

This is similar to Eq. (23).

By repeatedly using Eq. (18) in Eq. (33), the power of r in the equation is reduced to zero. Then equating the coefficients of $L_n^\nu(r)$ to zero, we get a recurrence equation of the coefficient column matrix $\underline{C}_n$ [this treatment is performed on Eq. (23) similarly]. All of the equations satisfied by $\underline{C}_n$ form a set of homogeneous linear equations. If we require that $\underline{C}$, which is a large column matrix formed by all of $\underline{C}_n$, have a nontrivial solution, the determinate of its coefficient matrix must be equal to zero. From this we get a secular equation of E, and the energies finally.

The determinate has a band structure. A more appropriate basis set to the hyperradial wave function can be chosen in practical application; then a thinner band structure is obtained, with which the convergence of calculation will be faster.

In calculations, if we want every eigenvalue to be exact, we should construct a determinant with an infinite size. In fact, what we usually need to know is the first several lower states of the system, thus we only need to solve an equation with a finite size of determinate, the size of which should be determined by the practical needs and the types of potentials. We believe that, no matter how complicated the potential of the system is, the convergence of the calculations with GLP is much faster than that with HH. The calculations of Coulomb systems in Sec. IV will make this conclusion evident, where only several GLP's are needed to get a convergent result of the ground state, in comparison with the need of hundreds of the HH.

It is easy to see that the determination of the eigenvalues in the present method is different from that in the conventional power-series-expansion method. In the conventional one, the eigenvalues result from the truncating power series to satisfy the requirement of the wave function being convergent at infinity. But here, we demand that the column matrix of expansion coefficient $\underline{C}$ have a solution. It forces the eigenvalues to come from a secular equation. The eigenfunctions obtained from this treatment satisfy the boundary conditions near $r=0$ and $r\rightarrow\infty$ automatically, or we cannot get a nontrivial $\underline{C}$. Therefore, this method avoids the difficulties in the description of the wave function near $r=0$ and in the usual complicated treatment to the wave function at $r\rightarrow\infty$. This is an advantage of this method. It is obvious that the wave functions are absolutely convergent and satisfy the boundary conditions.

III. CALCULATIONS OF HYDROGENLIKE SYSTEMS AND THE WAVE FUNCTION NEAR $r=0$

To show how easily this scheme can be handled, and how the wave function satisfies the behavior near $r=0$, we give the calculations of hydrogenlike systems.

Because the radial differential equation is uncoupled in these special cases, we can solve Eq. (7) with $Z_{\lambda\mu\lambda'\mu'}=z\delta_{\lambda\lambda'}\delta_{\mu\mu'}$, z being the number of nuclear charges, and $\lambda=l$, $l=0,1,2,\ldots$, being the angular momentum quantum number. Therefore, the problem becomes easier to handle.

By the following expansion to the radial wave function of this system

$$\phi_l(r)=e^{-\xi r}\sum_n C_n(l)L_n^\nu(2\xi r),\quad \nu=1\ , \tag{34}$$

where $\xi=\sqrt{-2E}$, we get a recurrence relation of expansion coefficients with the help of the theory mentioned in the above section,

$$n(z-n\xi)C_{n-1}+\{[l(l+1)+2(n+1)^2]\xi-2(n+1)z\}C_n+(n+2)[z-(n+2)\xi]C_{n+1}=0\ . \tag{35}$$

The matrix equation satisfied by the column matrix $\underline{C}$ is formed by

$$\begin{bmatrix} (\bar{\Lambda}+2)\xi-2z-4\xi+2z & -4\xi+2z & 0 & 0 & \cdots \\ -\xi+z & (\bar{\Lambda}+8)\xi-4z & -9\xi+3z & 0 & \cdots \\ 0 & -4\xi+2z & (\bar{\Lambda}+18)\xi-6z & -16\xi+4z & \cdots \\ 0 & 0 & -9\xi+3z & (\bar{\Lambda}+32)\xi-8z & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ \vdots \end{bmatrix} = 0 , \tag{36}$$

where $\bar{\Lambda}=l(l+1)$. With this equation, we get eigenvalues of the hydrogen atom ($z=1$) listed in Table I. This result can be obtained even with a pen and paper.

We are familiar with the conventional solution of this atom, whereas here is another exact one. The calculated eigenvalues are entirely the same as that of experiments. But we must point out that it is not easy to determine the main quantum number here except for the special case of $l=0$. In this example, convergence is no problem.

The expansions in Eqs. (16) and (34) can include the behavior of wave functions near $r=0$, but it is not obvious. The point of this paper is to avoid the description of the wave function near $r=0$, which is difficult to express in the power of the hyperradius r for the coupled system. After demanding that the determinate of the coefficient matrix of the expansion coefficient column matrix $\underline{C}$ must be equal to zero, which means we can have a nontrivial solution of $\underline{C}$, the corresponding solution satisfies the behavior near $r=0$ and also at $r\rightarrow\infty$ automatically like that discussed in the above section. To show it more obviously, we make the following expansion instead of Eq. (34) for this system according to the scheme in Ref. [12]

$$\phi_l(r)=e^{-\xi r}r^l\sum_n C_n(l)L_n^{\nu}(2\xi r); \quad \nu=2l+1 . \tag{37}$$

Here, we have considered the behavior of the wave function near $r=0$. With this expansion, we get the relation

$$[z/\xi-(n+l+1)]C_n=0 . \tag{38}$$

If we want $\underline{C}$ not to be equal to zero, the coefficient of one of the C_n must be equal to zero, that is,

$$z/\xi-(n+l+1)=0 . \tag{39}$$

Therefore we get the eigenvalues of $\xi=z/(n+l+1)$, and the eigenenergies

$$E=-\frac{z^2}{2(n+l+1)^2}, \quad n=0,1,2,\ldots . \tag{40}$$

This is just the same result as that given in general textbooks.

By comparing the two routines using the expansions of Eqs. (35) and (37), it can be found that the cost of avoiding the term r^l of Eq. (37) in Eq. (34) is a set of GLP's to describe the wave function. This payment can supply a powerful tool for the complicated coupling systems.

IV. CALCULATIONS OF HELIUMLIKE SYSTEMS OF THE CONVERGENT SPEED OF CALCULATIONS

In the following, after giving the recurrence relation of expansion coefficients for Coulomb interaction systems (the relation in [12] returns to this one for S states of heliumlike systems since λ_0 equals zero), we give more calculated results to show how fast the convergence is in the hyperradial part and discuss the problems still present.

The recurrence relation of this system is

$$n\left[\underline{Z}-\left[n+\frac{D-3}{2}\right]\xi\right]\underline{C}_{n-1}+\{[\underline{\Lambda}+\tfrac{1}{2}(D-1+2n)^2]\xi-(D-1+2n)\underline{Z}\}\underline{C}_n + (D-1+n)\left[\underline{Z}-\left[n+\frac{D+1}{2}\right]\xi\right]\underline{C}_{n+1}=0 \tag{41}$$

TABLE I. Calculated results of hydrogen atom (atomic units). $N_{\rm GLP}$ is the number of generalized Laguerre polynomials.

l	0					1					2				
$N_{\rm GLP}$	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
	1	1	1	1	1	2	2	2	2	2	3	3	3	3	3
		2	2	2	2		3	3	3	3		4	4	4	4
$\xi^{-1}=(-2E)^{-1/2}$			3	3	3			4	4	4			5	5	5
				4	4				5	5				6	6
					5					6					7

where $\xi=\sqrt{-2E}$, and $\overline{\underline{\Lambda}}=\underline{\Lambda}(\underline{\Lambda}+D-2)$. By solving the secular equation formed by the coefficients of column matrix $\underline{C}$, and remembering the relation of $E=-\xi^2/2$, we can get the energies.

We have performed the practical calculations with this scheme to ^1S and ^3S states of helium atom and to ^1S states of heliumlike ions, H^-, Li^+, and Be^{2+}. The results are listed in Tables II and III, respectively. In the following we use N_{HH} to represent the number of HH and N_{GLP} the number of GLP for the convenience of discussion. In calculations, the used N_{HH}'s are 6, 36, 100, 196, and 256, and N_{GLP}'s are 1, 2, 3, 4, 5, and 7. Here, we do not include the calculations with the N_{GLP}'s being larger than 4 when $N_{HH}=196$, and the N_{GLP}'s being larger than 3 when $N_{HH}=256$ because of the cost in calculations. And to ^3S states of the helium atom, we only outlist the calculations with $N_{HH}=100$.

The results listed in Table II are several selected lower states of ^1S and ^3S of the helium atom, and those in Table III are only the ground states of H^-, Li^+, and Be^{2+}. In fact, we can get eigenvalues with the number of $N_{HH}\times N_{GLP}$.

By these calculations, we find that the convergence is very slow, especially slower than that of the adiabatic channel expansion [13,16,17] with Brillouin-Wigner perturbation treatment [18]. It reflects an intrinsic property of the HH which makes the convergence slow [19,20]. Thus, a large N_{HH} is always needed here. But to the ground states, we can get a convergent eigenvalue by taking only a small number of GLP with a fixed N_{HH}. If we need convergent eigenvalues of excited states, we should increase the N_{GLP}. Above all, the results converge much faster with the GLP than with the HH, that is, $N_{GLP} \ll N_{HH}$. To the systems with more complicated potentials, we believe this relation still holds.

Making a simple comparison of the present work with that of Mandelzweig [10], it will be found that our calculated eigenenergies using only several GLP's are very similar to his with the same N_{HH}. It indicates that the exact results are the same no matter which expansion of the hyperspherical wave function is used. What is important here is that the present calculations are easy to do and more analytical, and that it is possible for us to perform the calculations with a huge number of bases to obtain more accurate results. We will report these results in another paper.

We can also use the method of Haftel and Mandelzweig [20] to make the convergence faster. With this treatment, it will be possible for us to get exact results with required precision for complicated systems. We are making this improvement and plan to perform practical calculations of electronic correlation and other interesting topics.

TABLE II. Eigenvalues of S states of He (atomic units). N_{HH}: the number of hyperspherical harmonics; N_{GLP}: the number of generalized Laguerre polynomials.

		N_{GLP}						
	N_{HH}	1	2	3	4	5	7	Ref. [21]
$^1S_1$	6	−2.780 15	−2.785 12	−2.785 02	−2.785 01	−2.785 00	−2.785 00	−2.903 72
	36	−2.855 36	−2.890 75	−2.893 44	−2.893 58	−2.893 59	−2.893 59	
	100	−2.858 85	−2.897 20	−2.900 84	−2.901 15	−2.901 18	−2.901 19	
	196	−2.859 50	−2.898 46	−2.902 34	−2.902 71			
	256	−2.859 63	−2.898 71	−2.902 64				
$^1S_2$	6	−0.515 88	−1.577 64	−1.600 40	−1.600 15	−1.600 13	−1.600 13	−2.145 97
	36	−0.548 91	−1.741 56	−1.920 60	−1.977 55	−1.991 98	−1.994 56	
	100	−0.552 44	−1.753 13	−1.954 74	−2.035 26	−2.067 15	−2.081 93	
	196	−0.553 17	−1.755 47	−1.962 21	−2.049 12			
	256	−0.553 32	−1.755 94	−1.963 75				
$^1S_3$	6	−0.345 52	−0.654 98	−1.063 54	−1.099 76	−1.099 37	−1.099 36	−2.061 27
	36	−0.440 77	−0.762 74	−1.247 67	−1.500 05	−1.618 75	−1.676 87	
	100	−0.445 25	−0.774 55	−1.261 27	−1.539 71	−1.696 13	−1.827 42	
	196	−0.446 12	−0.777 14	−1.264 18	−1.548 53			
	256	−0.446 29	−0.777 67	−1.264 78				
$^1S_4$	6	−0.132 69	−0.494 28	−0.663 10	−0.770 64	−0.812 40	−0.811 92	−2.033 59
	36	−0.140 85	−0.589 18	−0.760 22	−0.930 45	−1.189 86	−1.413 09	
	100	−0.141 11	−0.593 11	−0.771 85	−0.943 04	−1.225 65	−1.534 03	
	196	−0.141 13	−0.593 87	−0.774 57	−0.945 79			
	256	−0.141 13	−0.594 02	−0.775 14				
$^3S_2$	100	−1.419 43	−1.891 23	−2.041 35	−2.096 33	−2.115 63	−2.122 92	−2.175 24
$^3S_3$	100	−0.254 02	−0.859 80	−1.363 17	−1.617 04	−1.753 14	−1.855 87	−2.068 69
$^3S_4$	100	−0.204 94	−0.445 00	−0.578 45	−1.013 99	−1.287 47	−1.571 82	−2.036 51
$^3S_5$	100	−0.076 97	−0.385 93	−0.536 80	−0.570 83	−0.779 19	−1.226 40	−2.02262

TABLE III. Eigenvalues of ^1S ground states of H^-, Li^+, and Be^{2+} (atomic units). N_{HH} is the number of hyperspherical harmonics; N_{GLP} is the number of generalized Laguerre polynomials.

		N_{GLP}						
	N_{HH}	1	2	3	4	5	7	Ref. [21]
H^-	6	−0.479 01	−0.481 32	−0.481 25	−0.481 25	−0.481 25	−0.481 25	−0.527 75
	36	−0.500 91	−0.517 14	−0.520 28	−0.520 79	−0.520 85	−0.520 86	
	100	−0.502 00	−0.519 75	−0.524 04	−0.525 17	−0.525 45	−0.525 52	
	196	−0.502 21	−0.520 27	−0.524 86	−0.526 21			
	256	−0.502 25	−0.520 38	−0.525 03				
Li^+	6	−7.030 89	−7.040 12	−7.039 99	−7.039 98	−7.039 98	−7.039 99	−7.280 08
	36	−7.192 00	−7.257 40	−7.261 10	−7.261 24	−7.261 25	−7.261 25	
	100	−7.199 30	−7.270 01	−7.275 01	−7.275 32	−7.275 34	−7.275 34	
	196	−7.200 66	−7.272 46	−7.277 78	−7.278 14			
	256	−7.200 92	−7.272 94	−7.278 32				
Be^{2+}	6	−13.234 76	−13.249 54	−13.249 40	−13.249 39	−13.249 39	−13.249 39	−13.656 00
	36	−13.514 41	−13.619 85	−13.625 01	−13.625 18	−13.625 18	−13.625 19	
	100	−13.526 94	−13.640 83	−13.647 81	−13.648 19	−13.648 19	−13.648 19	
	196	−13.529 27	−13.644 89	−13.652 30	−13.652 73			
	256	−13.529 72	−13.645 68	−13.653 19				

V. CONCLUSIONS

We have given the exact solutions for some many-body systems. The solutions are certain, and the forms are simple and analytical. It is easy to perform the practical calculations using the method we proposed.

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[1] C. H. (Z.H.) Deng and Y. P. Fan, Bull. Shandong Daxue **1**, 162 (1957).
[2] F. T. Smith, Phys. Rev. **120**, 1058 (1960).
[3] D. L. Knirk, J. Chem. Phys. **60**, 66 (1974); **60**, 760 (1974).
[4] H. Klar, J. Phys. A **18**, 1561 (1985).
[5] V. Fock, K. Norske Vidensk. Selsk. Forh. **31**, 138 (1958).
[6] J. H. Macek, Phys. Rev. **160**, 170 (1967).
[7] J. M. Feagin, J. Macek, and A. F. Starace, Phys. Rev. A **32**, 3219 (1985).
[8] J. D. Morgan III, Theor. Chim. Acta **69**, 181 (1986).
[9] P. C. Abbott and E. N. Maslen, J. Phys. A **20**, 2043 (1987).
[10] V. B. Mandelzweig, Phys. Lett. **78A**, 25 (1980).
[11] C. Deng, R. Q. Zhang, and D. C. Feng (unpublished).
[12] C. Deng, R. Q. Zhang, and D. C. Feng, Inter. J. Quant. Chem. (to be published).
[13] H. Klar and M. Klar, J. Phys. B **13**, 1057 (1980).
[14] J. Avery, *Hyperspherical Harmonics and Their Application in Quantum Theory* (Kluwer Academic, Dordrecht, Netherlands, 1989).
[15] Zhuxi Wang and Dunying Guo, *Introduction to Special Functions* (Science, Beijing, 1979), in Chinese.
[16] J. Macek, J. Phys. B **1**, 831 (1968).
[17] C. D. Lin, Phys. Rev. A **10**, 1986 (1974).
[18] J. G. Frey and B. J. Howard, Chem. Phys. **111**, 33 (1987).
[19] J. L. Ballot and J. Navarro, J. Phys. B **8**, 172 (1975).
[20] M. I. Haftel and V. B. Mandelzweig, Ann. Phys. (N.Y.) **189**, 29 (1989).
[21] C. L. Pekeris, Phys. Rev. **112**, 1649 (1958); **126**, 1470 (1962); **127**, 509 (1962).