Shifted large-N expansion for a relativistic spin-$\frac{1}{2}$ particle in screened Coulomb potentials

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The difficulties associated with application of the shifted large-N technique to the Dirac equation have been resolved by applying the method to the Klein-Gordon equation in which a spin-orbit interaction term is included analogous to Pauli theory. Explicit analytical expressions for the relativistic screened Coulomb bound-state energies, radial wave functions, and normalizations are given. For the point-Coulomb problem, we restore exact results for the relativistic binding energies and almost exact wave functions. The $1/N$ expansion results are then compared with the exact numerical solutions as well as with those obtained in other analytical methods for a number of screened Coulomb potentials and for a wide range of atomic numbers Z. In general, excellent agreement is found. In contrast to the limited applicability of the usual perturbative methods, our technique is found to be flexible and may be extended to a more general class of relativistic potentials that has applications in atomic and quarkonium physics. Encouraging aspects of the present approach are also briefly discussed.

I. INTRODUCTION

It is well known that analytical study of the relativistic motion of a spin-$\frac{1}{2}$ particle bound in a spherically symmetric potential is extremely difficult. Recently, various perturbative methods[1-9] have been suggested to obtain analytical expressions for Dirac eigenvalues and eigenfunctions. In fact, extremely accurate numerical results for binding energies, normalizations, transition probabilities, etc. for inner-shell electrons in neutral atoms have been obtained. However, these perturbative approaches have limitations, too: first, these methods deal only with Coulomb-like potentials for which the Coulomb potential is treated as the dominant one; second, the algebraic manipulations involved in these perturbative calculations are quite elaborate and time consuming as far as computational work is concerned. It may then be worthwhile to search for an alternative analytical approximation scheme that is applicable to a wider class of potentials and provides results for the screened Coulomb potentials with at least the same order of accuracy. Our objective in this paper is to develop a large-N (N being the number of spatial dimensions) expansion for a relativistic spin-$\frac{1}{2}$ particle moving in a spherically symmetric potential, utilizing the procedure which has been used with great success for nonrelativistic problems.[10-13]

The scope of extension of this method to relativistic problems was initiated by Miramontes and Pajares[14] and Chatterjee.[15] However, these authors used the unshifted $1/N$ expansion which is known to be numerically less accurate than the shifted large-N technique[11] (SLNT) proposed by Sukhatme and co-workers for nonrelativistic bound-state problems. The SLNT has been applied recently by several authors[16-20] to relativistic particles with or without spin moving in a spherically symmetric scalar as well as vector potentials. From careful observations of all these attempts, one finds that the treatment of the Dirac equation within the framework of SLNT suffers from the following limitations: from the work of Atag[18] and Roychoudhury and Varshni[19] it appears that even for the point-Coulomb potential, one merely restores the binding energy correct up to order $1/c^2$. Since the higher-order terms become important for large-Z values, the accuracy of the predicted binding energies for neutral atoms becomes worse with increasing values of Z. It is crucial to emphasize here that whenever a Dirac equation is converted to a Schrödinger-like equation as has been done in Ref. 19, an irregular singular term of the form $(1/r^3)$ arises due to the spin-dependent piece [e.g., Eq. (15) of Ref. 19]. We suspect that perhaps this is the reason for not being able to restore the exact Coulomb results in such an approach. Also correct threshold behavior of the relativistic wave function cannot be achieved.

In a subsequent work, Papp[20] has shown that instead of working with the Dirac equation, the effect of spin can be incorporated in the Klein-Gordon-like equation by redefining the quantum numbers in a suitable fashion. In this way, Papp recovered the exact expression for relativistic Coulomb binding energy. However, since it is well known that the Klein-Gordon (KG) equation does not give the orbital-magnetic splitting of energy levels, he could not obtain the desired contribution due to spin to the energy levels as well as splitting of levels (such as the $2s_{1/2}$-$2p_{1/2}$ splitting) for non-Coulombic potentials.

At this point we address ourselves to the following question: to what extent can spin-orbit interaction be simulated through the use of the KG equation without disturbing the exact Dirac Coulomb result? We demonstrate here that this can be achieved if one follows a

modified approach. Taking the cue from Pauli's work[21] in which spin was introduced in the nonrelativistic theory, we suggest that a manifest spin-orbit interaction term can also be incorporated in the KG equation in such a fashion that exactness of Dirac-Coulomb binding energy will be retained, whereas the spin-orbit splitting for non-Coulombic potential would be obtained as close to that as expected from the Dirac theory. In doing so, we succeed in obtaining not only the exact analytic expressions for the relativistic binding energies and nearly exact eigenfunctions for the Coulomb problem, but also compact and simple analytic expressions for the same for the screened Coulomb potentials. Numerical results can also be predicted without much computational labor and these are found to be quite accurate and comparable to those obtained by other perturbative methods.

The organization of this paper is as follows. In Sec. II we develop the formalism of SLNT for obtaining the binding energies and eigenfunctions of a spin-$\frac{1}{2}$ particle from the KG equation. In Sec. III we apply this method to the point-Coulomb problem. The binding energies, wave functions, and normalizations for an inner-shell electron in a neutral atom are obtained using several screened Coulomb potentials and the results are compared with other calculations in Sec. IV. In the concluding section, we discuss the advantages and usefulness of the present approach in comparison to other perturbative methods for studying relativistic bound-state problems of more general nature. The scope of applicability of our method to other areas of physics is also briefly discussed.

II. RELATIVISTIC BINDING ENERGIES AND WAVE FUNCTIONS IN SLNT

We present here the formulation of the SLNT for the relativistic motion of a spin-$\frac{1}{2}$ particle bound in a radially symmetric potential $V(r)$. As mentioned clearly in the Introduction, treatment of the Dirac equation in the context of the SLNT leads to certain difficulties. On the other hand, we propose here to simulate the effect of spin on the relativistic motion of the particle by including a spin-dependent term in the KG equation in a manner very similar to the way Pauli considered the spin in the Schrödinger equation. We thus begin with the N-dimensional radial KG equation (in atomic units, $\hbar=m=e^2=1$)

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{(K-1)(K-3)}{8r^2}+V(r)+\frac{EV(r)}{c^2}-\frac{[V(r)]^2}{2c^2}\right]\phi(r)=\left[E+\frac{E^2}{2c^2}\right]\phi(r)\ , \tag{1}$$

where $K=N+2l$. Following Ref. 22, we collect the coefficients of $(1/r^2)$ terms in Eq. (1) and redefine K so as to obtain the correct threshold behavior of the relativistic wave function. For this purpose, we decompose the term $[V(r)]^2$ as

$$[V(r)]^2=\frac{\Lambda^2}{r^2}+u(r)\ , \tag{2}$$

where

$$\Lambda=\begin{cases}\text{coupling constant for Coulomb-like potentials}\\ 0 \text{ otherwise}\ .\end{cases}$$

Substituting (2) in Eq. (1) and replacing K by K' given by

$$K'=2+\left[(K-2)^2-\frac{4\Lambda^2}{c^2}\right]^{1/2} \tag{3}$$

one gets

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{(K'-1)(K'-3)}{8r^2}+V(r)+\frac{EV(r)}{c^2}-\frac{u(r)}{2c^2}\right]\phi(r)=\left[E+\frac{E^2}{2c^2}\right]\phi(r)\ . \tag{4}$$

In contrast to the work of Papp,[20] we include at this stage a manifestly spin-dependent term

$$V_s(r)=-\frac{\kappa}{4c^2}H(r) \tag{5}$$

in which $H(r)$ is chosen to be

$$H(r)=\frac{1}{r}\frac{d}{dr}\left[V(r)+\frac{\Lambda}{r}\right] \tag{6}$$

and κ is the conventional eigenvalue of the operator $(\sigma\cdot\mathbf{L}+1)$ and is given by[23,24]

$$\kappa=\begin{cases} l+1, & \kappa>0 \\ -l, & \kappa<0 . \end{cases} \tag{7}$$

The form of $H(r)$ has been taken in such a way that for Coulomb-like potentials, one does not get an irregular singular term of the form $1/r^3$ at the origin. We now introduce a shift parameter a through the relation

$$\bar{K}=K'-a \tag{8}$$

and derive Eq. (4) after including the term in (6) as

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{(\bar{K}+a-1)(\bar{K}+a-3)}{8r^2}+V(r)+\frac{EV(r)}{c^2}-\frac{u(r)}{2c^2}-\frac{\kappa}{4c^2}H(r)\right]\phi(r)=\left[E+\frac{E^2}{2c^2}\right]\phi(r) . \tag{9}$$

This is our starting equation for the systematic $1/\bar{K}$ expansion for the binding energy and wave function. For this purpose, we first rescale the following quantities:

$$\begin{aligned} V(r)&=\bar{K}^2V(r)/Q , \\ u(r)&=\bar{K}^4u(r)/Q^2 , \\ H(r)&=\bar{K}^2H(r)/Q , \\ c^2&=\bar{K}^2c^2/Q , \\ \kappa&=\bar{K}^2\kappa/Q , \\ \Lambda&=\bar{K}^2\Lambda/Q , \end{aligned} \tag{10}$$

and then expand the binding-energy E and the coordinate-dependent terms as

$$E=\bar{K}^2E_0+\bar{K}E_1+E_2+\frac{1}{\bar{K}}E_3+\cdots , \tag{11a}$$

$$V(r)=V(r_0)+\frac{r_0}{\bar{K}^{1/2}}V(r_0)x+\frac{r_0^2}{2\bar{K}}V(r_0)x^2+\cdots , \text{ etc. } , \tag{11b}$$

where $x=[(r-r_0)/r_0]\bar{K}^{1/2}$. The unknown parameter Q in (10) will be set equal to $\bar{K}^2$ later. Using (10) and (11) in Eq. (9) and considering $\bar{k}\to\infty$, the leading-order binding-energy term is obtained to be

$$\bar{K}^2E_0=-\bar{K}^2\frac{c^2}{Q}+\bar{K}^2\frac{V(r_0)}{Q}+\frac{c^2}{4r_0^3V'(r_0)}\left[\bar{K}^2+\frac{4\Lambda^2\bar{K}^2}{c^2Q}+\frac{\bar{K}^2\kappa r_0^3H'(r_0)}{c^2Q}\right] , \tag{12}$$

where r_0 satisfies the equation

$$\frac{r_0^3V'(r_0)}{Q}\left[1+\frac{Q}{4c^2r_0^2}+\frac{\Lambda^2}{r_0^2c^4}-\frac{\kappa H(r_0)}{2c^4}\right]^{1/2}=\frac{1}{4}+\frac{\Lambda^2}{c^2Q}+\frac{\kappa H'(r_0)r_0^3}{4c^2Q} . \tag{13}$$

Since this expression involves $\bar{K}$ (through the rescaled parameter Q) containing the unknown shift parameter a, r_0 can be determined only after we give the prescription for fixing a.

Using (10)–(13), Eq. (9) can be recast into the form

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}+\epsilon_0+\tfrac{1}{2}\omega^2x^2+\frac{1}{\bar{K}^{1/2}}(\epsilon_1x+\epsilon_3x^3)+\frac{1}{\bar{K}}(\epsilon_2x^2+\epsilon_4x^4)+\frac{1}{\bar{K}^{3/2}}(\delta_1x+\delta_3x^3+\delta_5x^5)+\frac{1}{\bar{K}^2}(\delta_2x^2+\delta_4x^4+\delta_6x^6)+\cdots\right]\tilde{\phi}(x)=r_0^2\left[\mathcal{E}_{(1)}+\frac{1}{\bar{K}}\mathcal{E}_{(2)}+\frac{1}{\bar{K}^2}\mathcal{E}_{(3)}+\cdots\right]\tilde{\phi}(x) , \tag{14}$$

where

$$\epsilon_0=\left[-\frac{1}{4}(2-a)+\frac{E_1r_0^2V(r_0)}{c^2}\right]+\frac{1}{\bar{K}}\left[\frac{1}{8}(1-a)(3-a)+\frac{E_2r_0^2V(r_0)}{c^2}\right]+\frac{1}{\bar{K}^2}\left[\frac{E_3r_0^2V(r_0)}{c^2}\right] , \tag{15}$$

$$\omega=\left\{\tfrac{3}{4}+\frac{r_0V''(r_0)}{4V'(r_0)}\left[1+\frac{4}{c^2Q}\left[\Lambda^2+\frac{\kappa r_0^3H'(r_0)}{4}\right]\right]+\frac{r_0^4}{2c^2Q}(2VV''-u''-\tfrac{1}{2}\kappa H'')\right\}^{1/2}, \tag{16}$$

$$\epsilon_1=\tfrac{1}{2}(2-a),$$

$$\epsilon_2=-\tfrac{3}{4}(2-a),$$

$$\epsilon_3=-\frac{1}{2}+\frac{r_0^5V'''(r_0)}{6Q}\left[\frac{\bar{K}^2E_0+c^2}{c^2}\right]-\frac{r_0^5}{12Qc^2}[u'''(r_0)+\tfrac{1}{2}\kappa H'''(r_0)], \tag{17}$$

$$\epsilon_4=\frac{5}{8}+\frac{r_0^6V''''(r_0)}{24Q}\left[\frac{\bar{K}^2E_0+c^2}{c^2}\right]-\frac{r_0^6}{48Qc^2}[u''''(r_0)+\tfrac{1}{2}\kappa H''''(r_0)],$$

$$\delta_1=-\tfrac{1}{4}(1-a)(3-a)+\frac{E_2r_0^3V'(r_0)}{c^2},$$

$$\delta_2=\tfrac{3}{8}(1-a)(3-a)+\frac{E_2r_0^4V''(r_0)}{2c^2},$$

$$\delta_3=(2-a),$$

$$\delta_4=-\tfrac{5}{4}(2-a), \tag{18}$$

$$\delta_5=-\tfrac{3}{4}+\frac{r_0^7V'''''(r_0)}{120Q}\left[\frac{\bar{K}^2E_0+c^2}{c^2}\right]-\frac{r_0^7}{240Qc^2}[u'''''(r_0)+\tfrac{1}{2}\kappa H'''''(r_0)],$$

$$\delta_6=\tfrac{7}{8}+\frac{r_0^8V''''''(r_0)}{720Q}\left[\frac{\bar{K}^2E_0+c^2}{c^2}\right]-\frac{r_0^8}{1440Qc^2}[u''''''(r_0)+\tfrac{1}{2}\kappa H''''''(r_0)],$$

$$\mathcal{E}_{(1)}=E_1\left[\frac{\bar{K}^2E_0+c^2}{c^2}\right],$$

$$\mathcal{E}_{(2)}=E_2\left[\frac{\bar{K}^2E_0+c^2}{c^2}\right]+\frac{QE_1^2}{2c^2}, \tag{19}$$

$$\mathcal{E}_{(3)}=E_3\left[\frac{\bar{K}^2E_0+c^2}{c^2}\right]+\frac{QE_1E_2}{c^2}.$$

Equation (14) is the same as Eq. (A1) of Ref. 11. Hence following the steps of Ref. 11, one may easily fix the shift parameter by setting the first nonleading correction term E_1 to zero. Furthermore, as we are dealing with a spin-$\frac{1}{2}$ particle, we follow Ref. 20 and replace the nonrelativistic radial and orbital angular momentum quantum numbers n_r and l by $(n_r-s/2)$ and $(l+s/2)$, respectively, where $s=\pm1$ denotes the sign of κ given in (7). We thus get

$$a=2-[1+2(n_r-s/2)]2w, \tag{20}$$

$$\bar{K}=\left[[N+2(l+s/2)-2]^2-\frac{4\Lambda^2}{c^2}\right]^{1/2}+2w[1+2(n_r-s/2)]. \tag{21}$$

Setting $Q=\bar{K}^2$ and using (21) in (13), r_0 can be determined. Once r_0 is evaluated, computations of binding energies and leading-order wave functions are fairly straightforward. Omitting the algebraic complexities, we just present the final expressions:

$$E_2=\frac{\left[\frac{(1-a)(3-a)}{8}+\sum_{n_r}^{(1)}\right]}{r_0^2\left[\frac{\bar{K}^2E_0+c^2-V(r_0)}{c^2}\right]}, \tag{22}$$

$$E_3=\frac{\sum_{n_r}^{(2)}}{r_0^2\left[\frac{\bar{K}^2E_0+c^2-V(r_0)}{c^2}\right]}, \tag{23}$$

where $\sum_{n_r}^{(1)}$ and $\sum_{n_r}^{(2)}$ are given in the Appendix. The

leading-order wave function $\phi^{(0)}(r)$ is given by[12]

$$\phi^{(0)}(r)=Nr^{(K'-1-s)/2}\exp\left[-\frac{\bar{K}}{2\tilde{\omega}}\left[\frac{r}{r_0}\right]^{\tilde{\omega}}\right]\times L_{n_r}^{(K'-2-s)/\tilde{\omega}}\left[\frac{\bar{K}}{\tilde{\omega}}\left[\frac{r}{r_0}\right]^{\tilde{\omega}}\right], \tag{24}$$

in which $\tilde{w}=2w$ and $L_\alpha^\beta(x)$ is the associated Laguerre polynomial. It may be pointed out that the term s has been included in (24) with a view to obtaining the correct nonrelativistic expression for the wave function in the appropriate limit. The wave function in (24) is equivalent to the large component of the Dirac wave function. The normalization factor is obtained to be

$$N=\tilde{\omega}^{1/2}\left[\frac{\bar{K}}{\tilde{\omega}r_0^{\tilde{\omega}}}\right]^{(K'-s)/2\tilde{\omega}}\left[\sum_{m=0}^{n_r}(-1)^m\frac{\left[n_r+\frac{K'-2-s}{\tilde{\omega}}\right]!\Gamma\left[\frac{K'-s}{\tilde{\omega}}+m\right]\Gamma\left[n_r+1-m-\frac{2}{\tilde{\omega}}\right]}{(n_r-m)!m!n_r!\left[\frac{K'-2-s}{\tilde{\omega}}+m\right]!\Gamma\left[1-m-\frac{2}{\tilde{\omega}}\right]}\right]^{-1/2}. \tag{25}$$

The expressions (24) and (25) are new and to the best of our knowledge, were not obtained in SLNT previously.

III. POINT-COULOMB PROBLEM

Before discussing realistic screened Coulomb potential problems it is worthwhile to illustrate that our formulas (12), (22), (23), and (24) reproduce correct results for the binding energies as well as eigenfunctions for point-Coulomb potential $V(r)=-Z/r$. For this case one obtains from Eqs. (13), (16), and (21)

$$w=\tfrac{1}{2},\quad \bar{K}=2\{p+[(j+1/2)^2-(Z\alpha)^2]^{1/2}\},\quad r_0=\frac{\bar{K}^2}{4Z}\left[1+\frac{4Z^2}{c^2\bar{K}^2}\right]^{1/2}, \tag{26}$$

where $p=(n_r+1/2-s/2)$ is the Dirac radial quantum number[23] and $j=l+s/2$. Using (26) in (12), (23) and (24) one obtains

$$E_c=c^2\left[\left[1+\frac{(Z\alpha)^2}{\{p+[(j+\frac{1}{2})^2-(Z\alpha)^2]^{1/2}\}^2}\right]^{-1/2}-1\right], \tag{27}$$

which is the exact Coulomb binding energy that one obtains from the solution of the Dirac equation.

From (24) and (25), the leading-order Coulomb wave function and the normalization factor become

$$\phi_c^{(0)}=N_c r^{(2\nu+1-s)/2}\exp\left[-\left[\frac{c^4-E^2}{c^2}\right]^{1/2}r\right]L_{n_r}^{2\nu-s}\left[2\left[\frac{c^4-E^2}{c^2}\right]^{1/2}r\right], \tag{28}$$

$$N_c=\left[2\left[\frac{c^4-E^2}{c^2}\right]^{1/2}\right]^{(2\nu+2-s)/2}\left[\sum_{m=0}^{n_r}(-1)^m\frac{(n_r+2\nu-s)!\Gamma(2\nu+2-s+m)\Gamma(n_r-m-1)}{(n_r-m)!m!n_r!(m+2\nu-s)!\Gamma(-1-m)}\right]^{-1/2}. \tag{29}$$

Regarding these results, we make the following observation: For states with $p=0$ ($n_r=0, s=+1$), Eqs. (28) and (29) lead to

$$\phi_c^{(0)}=\left[2\left[\frac{c^4-E^2}{c^2}\right]^{1/2}\right]^{\nu+(1/2)}\frac{1}{\sqrt{\Gamma(2\nu+1)}}r^\nu\exp\left[-\left[\frac{c^4-E^2}{c^2}\right]^{1/2}r\right], \tag{30}$$

which is the exact large component of the Dirac-Coulomb wave function.[24,25] For $p\neq 0$ states, although our leading-order wave function (28) does not retrieve the exact analytic expressions,[25] the numerical agreement between our approximate functions and the exact ones is remarkable. This may be visualized from Figs. 1(a) and 1(b), which display excellent agreement between our approximate wave functions and the exact ones for $2s_{1/2}$

and $2p_{1/2}$ states for $Z=30$. This indicates the correctness of our leading-order calculation for the wave function.

IV. APPLICATIONS TO SCREENED COULOMB POTENTIALS

The method of Sec. II has been applied to the first four bound states of screened Coulomb potentials, which may be expanded in the form[2,8]

$$V(r)=-\frac{Z}{r}+\sum_{i=1}^{\infty}V_i(\lambda r)^i\ , \tag{31}$$

in which λ is the screening parameter. Screened Coulomb potentials which have great utility in a variety of fields such as atomic, nuclear, and plasma physics, were studied extensively by various authors.[2,3,5,8] Using our formulas (12), (22), and (23), we compute energy eigenvalues for the Yukawa potential [$V(r)=-(Z/r)e^{-\lambda r}$; $\lambda=1.13\alpha Z^{1/3}$], self-consistent Kohn-Sham (KS) potential,[2] and Mehta-Patil (MP) potential[26]

$$V(r)=-\frac{Z}{r}\left[1-\frac{\lambda r\left[1-\frac{1}{Z}\right]}{1+\lambda r}\right],\quad \lambda=0.98\alpha Z^{1/3}\ ,$$

and compare the results with the predictions of other analytic methods as well as with the values obtained numerically. For the KS potential, we take the form (31) with only three coefficients V_1, V_2, and V_3 for which the values are taken from Ref. 2. In Tables I and II, we present the results for low-, intermediate-, and high-Z atoms. For an assessment of the level of accuracy of each theoretical prediction, the percentage of error is also shown in the tables. In comparison to other analytic results, the agreement of our predicted results, particularly for the Yukawa and MP potentials, with the exact ones is better in general and improves significantly for large-Z cases. For these potentials, the order of accuracy is within 3% for the entire range of Z except for $n=2$ and $Z=14$. As indicated in Table II, results for such states are not even calculable within the framework of analytic perturbation theory[2] (APT).

For the KS potential, however, the percentage of error becomes relatively large and shoots up to about 13% for intermediate Z. The reason for this may be attributed to the fact that the potential coefficients V_i's given in Ref. 2 are obtained from numerical fit in a small region of r which is essential for the validity of this method. But SLNT is not restricted in any manner by a particular domain of the variable and it works well only when the behavior of the potential is correctly known for the entire range of r. This is evident from our results for the Yukawa and the MP potentials, where we have taken the full form of the potentials and not the first four terms of their expansions. We have verified that, if we expand these two analytic potentials in the form of (31) and compute with only the first four terms, the percentage of error for each state becomes as large as that for the KS potential given in Table I.

As mentioned clearly in the preceding section, we have given analytic expressions for the relativistic wave function (large component) and normalization for a spin-$\frac{1}{2}$ particle only up to the leading-order term. We demon-

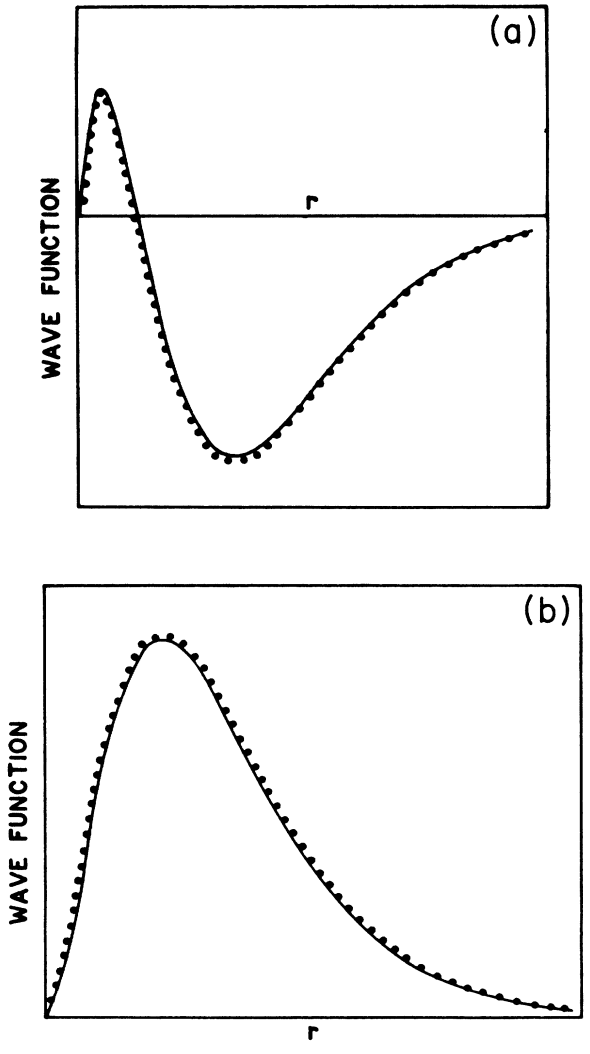

FIG. 1. (a) Radial part of the large-component (unnormalized) Dirac relativistic $2s_{1/2}$-state wave function vs radial distance for $Z=30$. The solid line represents our analytic expression [Eq. (28)] obtained in SLNT. The dotted line corresponds to the point-Coulomb shape for the same. (b) Radial part of the large-component (unnormalized) Dirac relativistic $2p_{1/2}$-state wave function vs radial distance for $Z=30$. The solid line represents our analytic expression [Eq. (28)] obtained in SLNT. The dotted line corresponds to the point-Coulomb shape for the same.

TABLE I. Relativistic binding energies (in keV) for the Yukawa and KS potentials as a function of N, κ, and Z. For comparison we also give the results of APT and numerical calculation taken from Ref. 2.

				Binding energies in keV				
							% of errors	
Potential	Z	n	κ	Present work [Eq. (11)]	APT (Ref. 2)	Numerical calculation (Ref. 2)	Present work	APT
Yukawa	13	1	+1	0.1487(+1)	0.1489	0.1493	0.4	0.3
	30	1	+1	0.9744(+1)	0.9758	0.9758	0.1	0.0
		2	+1	0.1050(+1)	0.9647(0)	0.1045(+1)	0.5	8.0
			−1	0.9635(+0)	0.8740	0.9377	3.0	7.0
			+2	0.9000(+0)	0.8442	0.9096	1.0	7.0
	74	1	+1	0.7170(+2)	0.7175	0.7175	0.1	0.0
		2	+1	0.1252(+2)	0.1250	0.1254	0.2	0.3
			−1	0.1238(+2)	0.1226	0.1230	0.7	0.3
			+2	0.1070(+2)	0.1073	0.1077	0.7	0.4
KS	13	1	+1	0.1471(+1)	0.1503	0.1505	2.0	0.1
	30	1	+1	0.9469(+1)	0.9552	0.9506	0.4	0.5
		2	+1	0.1094(+1)	0.1099	0.1157	5.0	5.0
			−1	0.1095(+1)	0.9547(+1)	0.1021(+1)	7.0	7.0
			+2	0.8619(+0)	0.9299	0.9969	14.0	7.0
	74	1	+1	0.6990(+2)	0.7014	0.6934	0.8	1.0
		2	+1	0.1186(+2)	0.1194	0.1196	0.8	0.2
			−1	0.1187(+2)	0.1146	0.1144	4.0	0.2
			+2	0.9747(+1)	0.1005(+2)	0.1009(+2)	3.0	0.4

TABLE II. Relativistic binding energies (in keV) for the MP potential as a function of n, κ, and Z. For comparison we give the results of APT (calculated from Ref. 2) and Roychoudhury and Varshni (Ref. 19). Numerical results are taken from Ref. 27. The occurrence of the opposite signature of the binding energy is referred to here as "Unphy."

			Binding energies in keV						
							% of errors		
Z	n	κ	Present work (Eq. 11)	RV (Ref. 19)	APT (Ref. 2)	Numerical calculation (Ref. 27)	Present work	RV	APT
14	1	+1	0.1999(+1)	0.2000	0.1979	0.2000	0.0	0.0	1.0
	2	+1	0.2630(+0)	0.2752	Unphy.	0.2493	5.0	10.0	
		−1	0.2105(+0)	0.2182	Unphy.	0.2157	2.0	1.0	
		+2	0.2364(+0)	0.2172	Unphy.	0.2147	10.0	1.0	
29	1	+1	0.9564(+1)	0.9575	0.9561	0.9574	0.1	0.0	0.1
	2	+1	0.1483(+1)	0.1539	0.1006	0.1466	1.0	5.0	31.0
		−1	0.1380(+1)	0.1387	0.1059	0.1373	0.5	1.0	23.0
		+2	0.1370(+1)	0.1361	0.1024	0.1349	2.0	1.0	23.0
44	1	+1	0.2339(+2)	0.2338	0.2340	0.2341	0.1	0.1	0.0
	2	+1	0.4016(+1)	0.4102	0.3621	0.4001	0.4	3.0	10.0
		−1	0.3874(+1)	0.3907	0.3590	0.3849	0.6	2.0	7.0
		+2	0.3708(+1)	0.3744	0.3419	0.3698	0.3	1.0	8.0
59	1	+1	0.4421(+2)	0.4405	0.4425	0.4425	0.1	0.4	0.0
	2	+1	0.8155(+1)	0.8206	0.7830	0.8145	0.1	0.7	4.0
		−1	0.7979(+1)	0.8137	0.7721	0.7931	0.6	2.0	2.0
		+2	0.7381(+1)	0.7528	0.7142	0.7386	0.1	2.0	3.0
74	1	+1	0.7322(+2)	0.7238	0.7330	0.7329	0.1	1.0	0.0
	2	+1	0.1430(+2)	0.1417	0.1404	0.1430	0.0	0.9	1.8
		−1	0.1410(+2)	0.1466	0.1385	0.1402	0.6	4.6	1.1
		+2	0.1249(+2)	0.1287	0.1230	0.1251	0.2	2.9	1.7
84	1	+1	0.9806(+2)	0.9600	0.9818	0.9814	0.1	2.2	0.0
	2	+1	0.1982(+2)	0.1941	0.1961	0.1983	0.1	2.1	1.1
		−1	0.1960(+2)	0.2084	0.1937	0.1951	0.5	6.8	0.7
		+2	0.1674(+2)	0.1740	0.1658	0.1678	0.2	3.7	1.7

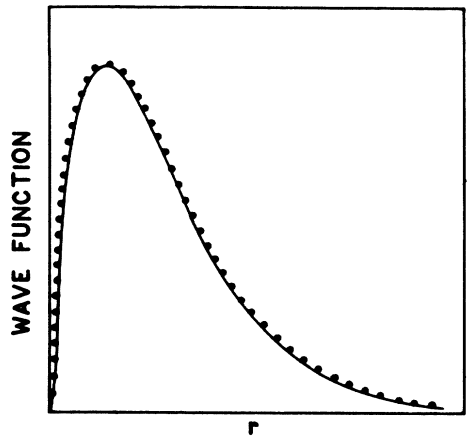

FIG. 2. Relativistic large-component (unnormalized) wave function for the $1s_{1/2}$-state of aluminum ($Z=13$) for the KS potential. The solid line represents the shape obtained from SLNT [Eq. (24)], while the dotted line represents the results as obtained from APT [Ref. 2].

strate here that even the leading-order wave function, which is analytically much simpler than the complicated expression obtained in APT, is capable of reproducing results with high accuracy. In Fig. 2 we have shown the comparison between the results obtained in SLNT and APT for the shape of the wave function of the $1s_{1/2}$ state for $Z=13$. Both methods give almost identical results for the entire range of r. The same feature is found to be true for other states as well. The departure seems to be gradually prominent as Z increases. For better agreement, one may in principle calculate nonleading corrections to the wave function for which calculation becomes as complicated as one encounters in APT. We avoid it purposely as it is contrary to our motivation.

A comparison of our expression for the relativistic bound-state normalizations with those obtained in APT and exact numerical results is given in Table III. In general, we see that the behavior of the normalizations as a function of Z and quantum numbers is comparatively worse for the $2s_{1/2}$ and $2p_{1/2}$ states. The reason may be due to the fact that in the Coulomb limit, one does not restore exact analytic expressions for the Coulomb wave functions for these states. It is clear that higher-order corrections to the leading-order wave function are essential in SLNT in order to reproduce more accurate results for $2s_{1/2}$ and $2p_{1/2}$ states.

V. CONCLUDING REMARKS

In this paper we have succeeded in extending SLNT in obtaining compact analytic expressions as well as accurate numerical results for the relativistic bound-state energies, wave functions, and normalizations for a spin-$\frac{1}{2}$ particle in a spherically symmetric potential. This has been achieved by a new prescription in which a spin-dependent term has been included in the KG equation to

TABLE III. Bound-state normalizations for the Yukawa and KS potentials as a function of n, κ, and Z. For comparison we also give the results of APT and numerical calculation taken from Ref. 2.

				Bound-state normalization				
							% of errors	
Potential	Z	n	κ	Present work (Eq. 25)	APT (Ref. 2)	Numerical calculation (Ref. 2)	Present work	APT
Yukawa	13	1	+1	0.2910(−1)	0.2893	0.2885	0.9	0.3
	30	1	+1	0.1072(+0)	0.1072	0.1071	0.1	0.1
		2	+1	0.3831(−1)	0.3590	0.3435	12.0	5.0
			−1	0.3301(−1)	0.3428	0.3282	0.6	4.0
			+2	0.1097(−2)	0.1047	0.1074	2.0	3.0
	74	1	+1	0.4831(+0)	0.4881	0.4840	0.2	0.8
		2	+1	0.1764(+0)	0.1852	0.1842	4.0	0.6
			−1	0.1873(+0)	0.1833	0.1822	3.0	0.6
			+2	0.1254(−1)	0.1240	0.1212	3.5	2.3
KS	13	1	+1	0.2890(−1)	0.2861	0.2854	1.0	0.2
	30	1	+1	0.1067(+0)	0.1065	0.1062	0.5	0.3
		2	+1	0.3750(−1)	0.3431	0.3312	13.0	4.0
			−1	0.2972(−1)	0.3113	0.3003	1.0	4.0
			+2	0.9810(−2)	0.9555	0.9163	7.0	4.0
	74	1	+1	0.4812(+0)	0.4866	0.4848	0.7	0.4
		2	+1	0.1674(+0)	0.1795	0.1770	5.0	1.0
			−1	0.1897(+0)	0.1754	0.1703	11.0	3.0
			+2	0.1213(+1)	0.1177	0.1143	6.0	3.0

simulate the results of the Dirac equation as far as practicable. In this respect, the present approach indicates substantial modifications of the earlier work of Papp and Roychoudhury and Varshni. Needless to mention, our work is, we believe, the first attempt to obtain relativistic wave functions in SLNT. From the comprehensive analysis of a variety of screened Coulomb potentials in the light of SLNT presented in this paper, it is made evident that in spite of the simplicity of the analytic forms of the energy levels and wave functions, the numerical accuracy of the predicted results is quite satisfactory. Nevertheless, we would like to point out that the contribution from the spin-orbit interaction term considered in Eq. (5) is only 2% and is less than what is required to explain the actual splitting. For example, the binding energy for $Z=14$ is -1.999 keV (column 4, Table II), whereas it is -1.965 keV if the spin-orbit term is ignored. Similar results also occur for higher-Z atoms. We suspect that this shortcoming is due to use of the KG framework rather than Dirac.

The present method is quite flexible in the sense that it is applicable to any radially symmetric potential in contrast to other perturbative methods for which the applications are restricted not only to the Coulomb-like potentials, but also to a limited region of the motion of the electron in an atom. Encouraged by our results, we are motivated to examine thoroughly the relativistic corrections to the dipole transitions and radiative rates, quantum defects, etc.[3] for the inner shell electrons in a complex atomic system. Also it is within the scope of our method to consider a mixture of scalar and vector potentials[20] which may be useful to study the bound-state properties of the quarkonia.[7,28] This work is now in progress and will be reported later.

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APPENDIX

To calculate second- and third-order terms in the $1/\bar{K}$ expansion of the energy eigenvalues, we give here the expressions for $\sum_{n_r}^{(1)}$ and $\sum_{n_r}^{(2)}$ explicitly:

$$\sum_{n_r}^{(1)} = (1+2n_r')\tilde{\epsilon}_2 + 3(1+2n_r'+2n_r'^2)\tilde{\epsilon}_4 - \frac{1}{\tilde{\omega}}[\tilde{\epsilon}_1^2 + 6(1+2n_r')\tilde{\epsilon}_1\tilde{\epsilon}_3 + (11+30n_r'+30n_r'^2)\tilde{\epsilon}_3^2] ,$$

$$\begin{aligned}\sum_{n_r}^{(2)} &= (1+2n_r')\tilde{\delta}_2 + 3(1+2n_r'+2n_r'^2)\tilde{\delta}_4 + 5(3+8n_r'+6n_r'^2+4n_r'^3)\tilde{\delta}_6 \\ &\quad - \frac{1}{\omega}[(1+2n_r')\tilde{\epsilon}_2^2 + 12(1+2n_r'+2n_r'^2)\tilde{\epsilon}_2\tilde{\epsilon}_4 + 2(21+59n_r'+51n_r'^2+34n_r'^3)\tilde{\epsilon}_4^2 + 2\tilde{\epsilon}_1\tilde{\delta}_1 \\ &\qquad + 6(1+2n_r')\tilde{\epsilon}_1\tilde{\delta}_3 + 30(1+2n_r'+2n_r'^2)\tilde{\epsilon}_1\tilde{\delta}_5 + 6(1+2n_r')\tilde{\epsilon}_3\tilde{\delta}_1 + 2(11+30n_r'+30n_r'^2)\tilde{\epsilon}_3\tilde{\delta}_3 \\ &\qquad + 10(13+30n_r'+42n_r'^2+28n_r'^3)\tilde{\epsilon}_3\tilde{\delta}_5] \\ &\quad + \frac{1}{\omega^2}[4\tilde{\epsilon}_1^2\tilde{\epsilon}_2 + 36(1+2n_r')\tilde{\epsilon}_1\tilde{\epsilon}_2\tilde{\epsilon}_3 + 8(11+30n_r'+30n_r'^2)\tilde{\epsilon}_2\tilde{\epsilon}_3^2 + 24(1+2n_r')\tilde{\epsilon}_1^2\tilde{\epsilon}_4 \\ &\qquad + 8(31+78n_r'+78n_r'^2)\tilde{\epsilon}_1\tilde{\epsilon}_3\tilde{\epsilon}_4 + 12(57+189n_r'+225n_r'^2+150n_r'^3)\tilde{\epsilon}_3^2\tilde{\epsilon}_4] \\ &\quad - \frac{1}{\omega^3}[8\tilde{\epsilon}_1^3\tilde{\epsilon}_3 + 108(1+2n_r')\tilde{\epsilon}_1^2\tilde{\epsilon}_3^2 + 48(11+30n_r'+30n_r'^2)\tilde{\epsilon}_1\tilde{\epsilon}_3^3 + 30(31+109n_r'+141n_r'^2+94n_r'^3)\tilde{\epsilon}_3^4] ,\end{aligned}$$

where

$$n_r' = n_r - s/2, \quad \tilde{\epsilon}_j = \frac{\epsilon_j}{(2\omega)^{j/2}}, \quad \tilde{\delta}_j = \frac{\delta_j}{(2\omega)^{j/2}} \quad (j=1,2,\ldots) .$$

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