

Large- N expansion method for a spin- $\frac{1}{2}$ particle in the presence of vector and scalar potentials

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The shifted large- N technique (SLNT) has been applied to study the relativistic motion of a particle in the presence of vector and scalar interactions with special emphasis on the construction of both large- and small-component Dirac radial wave functions. Numerical results for the binding energy for a particle in the presence of the Coulomb plus linear confining potential compare very well with those obtained by the elaborate analytic approximation method using the Padé-approximation technique. We illustrate that one recovers not only the exact analytic results for binding energies for vector and scalar Coulomb potentials, but also exact wave functions from the leading-order SLNT calculation. This motivates future applications of the same method to more realistic atomic systems governed by screened Coulomb potentials where the knowledge of the large and small components of the radial wave function is essential.

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I. INTRODUCTION

The shifted large- N expansion technique [1–4] has been widely applied to the calculation of nonrelativistic bound-state energies and wave functions for a variety of potential problems. In a recent review article, Chatterjee [5] has elucidated in great detail the perspective of this method which has already received interest in view of its analytic simplicity and numerical accuracy. However, it seems that the scope of its applicability to relativistic problems, in particular, to atomic and molecular physics, has not been adequately explored. Perhaps this is due to the fact that the coupled nature of the radial Dirac equation causes difficulties in applying the large-dimension expansion to it as compared to the nonrelativistic Schrödinger equation.

In spite of this intrinsic difficulty in handling the Dirac equation, attempts have been made to develop $1/N$ expansions for the eigenenergy and eigenfunctions for a relativistic particle. Some time ago, Nieto [6] developed a $1/N$ formalism to the relativistic potential only in the context of the Klein-Gordon (KG) equation. Subsequently, Miramontes and Pajares [7] and Chatterjee [8] studied the large- N limit of the Dirac equation using the unshifted $1/N$ method. Obviously, these attempts were plagued with a slow convergence problem in comparison to the shifted large- N technique (SLNT) developed by Sukhatme and co-workers [1,2]. In this modified approach a new degree of freedom, the so-called shift parameter a , was introduced with a view to improving the convergence leading to higher accuracy of the numerical results. The first successful application of the SLNT to the Dirac equation with a linear scalar potential was made by Roychoudhury and Varshni [9]. Mathematically the scalar Dirac potential is comparatively easier to deal with. Application of the same to vector and/or scalar Dirac potentials was

carried out by several workers [10–16]. It was demonstrated that the SLNT is capable of predicting accurate eigenvalues in a simpler way in contrast to analytic perturbation and other approximation methods [17–20] which involve lengthy analytic expressions and more computational time.

In the context of screened atomic problems, Panja, Dutt, and Varshni [13] have shown that results for both binding energies and eigenfunctions can be obtained with reasonable accuracy by making an optimum choice for the shift parameter. However, it was mentioned clearly that the SLNT wave function is equivalent to the large-component Dirac radial wave function only. It is then quite logical to examine whether the small-component radial wave function can be constructed within this framework at all. Encouraged by our earlier work, we feel tempted to extend the SLNT to the combination of both vector and scalar potentials [16,21–28] which have been used recently in the study of quark-antiquark bound-state problems. The purpose of this paper is to illustrate how SLNT formulas can be worked out (up to the first few leading orders) for a relativistic Dirac particle moving in the presence of vector and scalar potentials. For numerical illustration of the accuracy of our analytic formulas, we discuss the results for the vector Coulomb plus scalar and/or vector linear potential. Such combinations have been studied in the context of quarkonium physics. These models have been investigated recently by Vrscaj and Hamidian [29] using relativistic hypervirial and Hellmann-Feynman theorems for constructing the Rayleigh-Schrödinger (RS) expansion for eigenvalues of the perturbed radial Dirac equation to arbitrary order. However, this work involves large-order Padé approximants and the solution of multiple recursive formulas consuming large computational time. Furthermore, no information regarding the wave function can be obtained

due to the use of the Hellmann-Feynman and virial theorems. From this point of view, our SLNT calculation seems to be much more straightforward and algebraically tractable even with a simple computational device. The present scheme also works well for screened potentials with large screening parameters.

The plan of this paper is as follows. In Sec. II, we develop the formalism of the SLNT for obtaining the binding energy of a spin- $\frac{1}{2}$ particle moving in the presence of vector and scalar potentials. This part of calculation proceeds in a similar manner as discussed in our earlier paper [13], with the exception that the additional contributions due to the scalar potential to the appropriate expression are explicitly evaluated. It is interesting to note that one obtains exact analytic expressions for the relativistic binding energy and wave function for a spin- $\frac{1}{2}$ particle in the presence of vector and scalar Coulomb potentials. This part of the calculation is presented in Sec. III. In this section, we have explained how the small-component Dirac radial wave function can be obtained from the large component, which in our case is the leading-order SLNT wave function. Results and discus-

sion for a few interesting combinations of vector and scalar potentials are presented in Sec. IV. Our numerical results are found to be quite accurate and comparable to other analytic results obtained through many elaborate and time-consuming analytic procedures. Possible extensions of the present approach to the computation of bound-bound and bound-free atomic transitions for neutral atoms are discussed.

II. SHIFTED $1/N$ FORMULAS FOR VECTOR AND SCALAR POTENTIALS

We present here the relevant formulas obtained in the SLNT framework for relativistic motion of a spin- $\frac{1}{2}$ particle bound in radially symmetric vector and scalar potentials $V(r)$ and $S(r)$, respectively. In Ref. [13], we already mentioned that the shifted $1/N$ expansion can be applied to the Dirac equation by considering the KG equation, including the spin-dependent term, in a manner similar to the way Pauli considered the spin in the Schrödinger equation. Following our earlier work, we begin with the N -dimensional radial KG equation (in atomic units $\hbar = m = e^2 = 1$)

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

where $K = N + 2l$.

To get the correct threshold behavior of the wave function, one is required to extract the $1/r^2$ piece (if it exists at all) from $[V(r)]^2$ and $[S(r)]^2$. We thus define

$$u(r) = [V(r)]^2 - \frac{\Lambda_1^2}{r^2}, \quad (2a)$$

$$v(r) = [S(r)]^2 - \frac{\Lambda_2^2}{r^2},$$

where Λ_1, Λ_2 are the coupling constants for the Coulomb

potentials

$$V_c(r) = -\frac{\Lambda_1}{r}, \quad S_c(r) = -\frac{\Lambda_2}{r}. \quad (2b)$$

These constants are taken to be zero for non-Coulombic potentials. Collecting terms containing $1/r^2$ and replacing K by K' related through the relation

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

with $\Lambda^2 = (\Lambda_1^2 - \Lambda_2^2)$, one obtains

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

It is important to mention that the effect of spin was incorporated [15] in the KG-like equation, such as Eq. (4), by redefining the quantum numbers in a suitable fashion. Although the exact Coulomb eigenvalues were restored, the method fails to generate spin-orbit splitting of energy levels for potentials other than the Coulomb potential as is evident from Eq. (29) of Ref. [15]. Hence a spin-dependent term has to be included in such a manner that one should not get a term of the form $1/r^3$ for the Coulomb problem. This is dictated by the exact calculation of Su [30], in which the radial equation for the Dirac-Coulomb problem has been converted to a KG-like equation [Eq. (2.13) of Ref. [30]] without the appearance of such a singular term. We thus include at this stage a

spin-dependent term [13]

$$V_{\text{spin}}(r) = -(\kappa/4c^2)H(r) \quad (5)$$

with

$$H(r) = \frac{1}{r} \frac{d}{dr} \left[\left[V(r) + \frac{\Lambda_1}{r} \right] - \left[S(r) + \frac{\Lambda_2}{r} \right] \right]. \quad (6)$$

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

$$\kappa = -2(j-l)(j + \frac{1}{2}). \quad (7)$$

The terms in the square brackets of Eq. (6) imply a vanishing spin-orbit interaction term for equally mixed four-vector and scalar interactions [31]. Furthermore, for harmonic potentials, Eq. (6) produces a constant energy shift

which is consistent with the result obtained from Pauli's spin-orbit interaction term [32]. Introducing the shift parameter through the relation $\bar{k} = K' - a$, Eq. (4) thus becomes

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

In order to obtain the leading-order as well as higher-order corrections to the energy and the SLNT parameters such as r_0, \bar{K}, w , etc., we now proceed along in the manner described in Ref. [13]. The leading-order binding energy is given by

$$\bar{K}^2 E_0 = -c^2 + V(r_0) + c^2 \left[1 + \frac{Q}{4c^2 r_0^2} + \frac{\Lambda_1^2}{c^4 r_0^2} + \frac{2S(r_0)}{c^2} + \frac{v(r_0)}{c^4} - \frac{\kappa H(r_0)}{2c^4} \right]^{1/2}, \quad (9)$$

where r_0 satisfies the equation

$$\frac{r_0^3 V'(r_0)}{Q} \left[1 + \frac{Q}{4c^2 r_0^2} + \frac{\Lambda_1^2}{r_0^2 c^4} + \frac{2S(r_0)}{c^2} + \frac{v(r_0)}{c^4} - \frac{\kappa H(r_0)}{2c^4} \right]^{1/2} = \frac{1}{4} + \frac{\Lambda_1}{c^2 Q} - \frac{r_0^3 S'(r_0)}{Q} - \frac{r_0^3 V'(r_0)}{2c^2 Q} + \frac{\kappa r_0^3 H'(r_0)}{4c^2 Q}. \quad (10)$$

Expanding all the quantities in powers of $1/\bar{K}$ as described in Eqs. (10) and (11) of Ref. [13], one finally gets the second- and third-order corrections E_2 and E_3 of the energy E as

$$E_2 = \frac{[(1-a)(3-a)]/8 + \Sigma_{n_r}^{(1)}}{r_0^2 \{ [\bar{K}^2 E_0 + c^2 - V(r_0)] / c^2 \}}, \quad (11)$$

$$E_3 = \frac{\Sigma_{n_r}^{(2)}}{r_0^2 \{ [\bar{K}^2 E_0 + c^2 - V(r_0)] / c^2 \}}, \quad (12)$$

in which

$$\bar{K} = 2 + \{ [N + 2(l + s/2) - 2]^2 - 4\Lambda^2/c^2 \}^{1/2} - a, \quad (13)$$

$$a = 2 - [1 + 2(n_r - s/2)]2w, \quad (14)$$

$$w = \left[\frac{3}{4} + \frac{r_0^4 V''(r_0)}{Q} \left[\frac{\bar{K}^2 E_0 + c^2}{c^2} \right] + \frac{r_0^4 S''(r_0)}{Q} - \frac{r_0^4}{2c^2 Q} [u''(r_0) - v''(r_0)] - \frac{\kappa r_0^4 H''(r_0)}{4c^2 Q} \right]^{1/2}. \quad (15)$$

The expressions for $\Sigma_{n_r}^{(1)}$ and $\Sigma_{n_r}^{(2)}$ and other parameters are given in the Appendix.

The leading-order SLNT wave function is given by [13]

$$\phi^{(0)}(r) = -sN' r^{(K'-1+s)/2} \exp \left[-\frac{\bar{K}}{2\bar{w}} \left(\frac{r}{r_0} \right)^{\bar{w}} \right] \times {}_1F_1 \left[-n_r, \frac{K'-2}{\bar{w}} + 1; \frac{\bar{K}}{\bar{w}} \left(\frac{r}{r_0} \right)^{\bar{w}} \right], \quad (16)$$

where $s = \pm 1$ denotes the sign of κ . It is crucial to note that one of the limitations of the SLNT approach is that one gets only one component radial wave function instead of two (large and small) for a true Dirac particle. However, it has been shown in Ref. [13] that the SLNT wave function in (16) is equivalent to the large component for almost the entire range of r . In Sec. III we

shall illustrate that starting from this wave function, one may obtain an exact analytic expression for the large-component radial wave function for both vector and scalar Coulomb potentials. In addition to that, one may proceed to obtain the corresponding small-component wave functions.

III. EXACT RESULTS FOR VECTOR AND SCALAR COULOMB POTENTIALS

Before making numerical applications of our SLNT formulas given in Sec. II, we demonstrate the elegance of this expansion scheme by recovering exact analytic results both for binding energies and wave functions for vector and scalar Coulomb potentials in (2b). The expressions (10), (13)–(15) give

$$r_0 = \frac{\bar{K}^2}{4(\Lambda_2^2 - \Lambda_1^2)} \left[\Lambda_2 - \Lambda_1 \left[1 + \frac{4\Lambda^2}{\bar{K}^2} \right]^{1/2} \right],$$

$$\bar{K} = 2(p + \gamma), \quad (17)$$

$$w = \frac{1}{2}$$

with

$$\gamma = \left[\left(j + \frac{1}{2} \right)^2 - \frac{\Lambda^2}{c^2} \right]^{1/2}.$$

Using (17) in (9) and (16) we get the total energy $W = E + mc^2$,

$$W = c^2 \left[\frac{-\frac{\Lambda_1 \Lambda_2}{c^2} + (p + \gamma) \left[(p + \gamma)^2 + \frac{\Lambda^2}{c^2} \right]^{1/2}}{(p + \gamma)^2 + \frac{\Lambda_1^2}{c^2}} \right], \quad (18)$$

and the wave function

$$\phi^{(0)}(r) = -sN'r^\gamma e^{-(\bar{K}/2r_0)r} \times {}_1F_1 \left[-n_r, 2\gamma + 1 + s; \left[\frac{\bar{K}}{r_0} \right] r \right]. \quad (19)$$

The correction terms in Eqs. (11) and (12) vanish identically. Expression (18) is the exact energy expression [Eq. (A.1) of Ref. [29]]. Our wave function (19) for the point Coulomb potential has the following shortcomings. First, it contains only one confluent hypergeometric function (CHF) instead of two CHF's (see Ref. [32]) in the exact expression for the Coulomb problem. Second, it fails to give the correct threshold behavior for $s = +1$ cases. To recast (19) in the standard form and for restoring the correct threshold behavior, one proceeds as follows. Us-

ing the recurrence relation [33]

$$b {}_1F_1(a, b; z) = a {}_1F_1(a + 1, b + 1; z) - (a - b) {}_1F_1(a, b + 1; z) \quad \text{for } s = -1 \quad (20a)$$

and

$$z {}_1F_1(a, b + 1; z) = b [{}_1F_1(a, b; z) - {}_1F_1(a - 1, b; z)] \quad \text{for } s = 1. \quad (20b)$$

Equation (19) may be written as

$$\phi_{s=-1}^{(0)}(r) = N'_{-} r^\gamma e^{-(\bar{K}/2r_0)r} [-n_r {}_1F_1(-n_r + 1, 2\gamma + 1, (\bar{K}/r_0)r) + (n_r + 2\gamma) {}_1F_1(-n_r, 2\gamma + 1, (\bar{K}/r_0)r)], \quad (21a)$$

$$\phi_{s=+1}^{(0)}(r) = N'_{+} r^\gamma e^{-(\bar{K}/2r_0)r} [-(n_r + 1) {}_1F_1(-n_r, 2\gamma + 1, (\bar{K}/r_0)r) + (n_r + 1) {}_1F_1(-n_r - 1, 2\gamma + 1, (\bar{K}/r_0)r)]. \quad (21b)$$

Expressions (21a) and (21b) can be expressed in a single compact form if one replaces the nonrelativistic quantum number n_r by the relativistic Dirac quantum number p given by

$$p = \begin{cases} n_r & \text{for } s = -1 \\ n_r + 1 & \text{for } s = +1. \end{cases}$$

We thus write (21a) and (21b) as (with $c = 1$ units)

$$\phi^{(0)}(r) = \bar{N} \left[\frac{1 + E_c}{2} \right]^{1/2} r^\gamma e^{-(\bar{K}/2r_0)r} [-p {}_1F_1(-p + 1, 2\gamma + 1; (\bar{K}/r_0)r) + [p + \gamma(1 - s)] {}_1F_1(-p, 2\gamma + 1; (\bar{K}/r_0)r)], \quad (22)$$

in which the factor $[(1 + E_c)/2]^{1/2}$ has been extracted out from the normalization factor for convenience. It is easy to check that our expression is identical to that of the large component except for the coefficients of the CHF's. The reason is quite obvious. What we have obtained is basically the Schrödinger-like wave function and in order to recast it in the form of the relativistic wave function one essentially must follow the procedure given by Flügge [34] in a backward manner. We thus replace the coefficient $[p + \gamma(1 - s)]$ of the second CHF by $(\Gamma - \kappa)$ in which

$$\Gamma = \frac{\frac{\bar{K}}{2r_0}(r_0 - \Delta)}{[1 - (\bar{K}^2/4r_0^2)]^{1/2}} \quad (23)$$

with

$$\Delta = \frac{\frac{\bar{K}^2}{2r_0} \left[\{1 + [(\kappa^2 - \gamma^2)/\bar{K}^2]\}^{1/2} - \frac{16r_0^2}{\bar{K}^4} (\kappa^2 - \gamma^2) [1 - (\bar{K}^2/4r_0^2)]^{1/2} \right]}{[1 - (\bar{K}^2/4r_0^2)]^{1/2} + \{1 + [(\kappa^2 - \gamma^2)/\bar{K}^2]\}^{1/2}}.$$

Using the expressions for r_0, \bar{K} as given by (17) in (23), one obtains from (22)

$$g_{\text{SLNT}}^{(0)}(r) = -N \left[\frac{1 + E_c}{2} \right]^{1/2} r^\gamma e^{-(\bar{K}/2r_0)r} [p {}_1F_1(-p + 1, 2\gamma + 1; (\bar{K}/r_0)r) - (\Gamma - \kappa) {}_1F_1(-p, 2\gamma + 1; (\bar{K}/r_0)r)]. \quad (24)$$

This is the exact large component of the reduced radial wave function.

For the construction of the small-component reduced radial wave function from the knowledge of the large component, we follow the artifice mentioned in Ref. [32]. The large- and small-component wave functions are connected through the differential operator given by

$$f(r) = \frac{c}{[E + c^2 + V(r)]} \left[\frac{d}{dr} + \frac{\kappa}{r} \right] g(r). \quad (25)$$

Using (24) and the recurrence relations [33]

$$z {}_1F_1'(a, b; z) = (z - b - a) {}_1F_1(a, b; z) - (a - b) {}_1F_1(a - 1, b; z) \quad \text{for } a = -p + 1,$$

$$z {}_1F_1'(a, b; z) = a [{}_1F_1(a + 1, b; z) - {}_1F_1(a, b; z)] \quad \text{for } a = -p$$

in (25), one obtains after some algebraic rearrangements

$$f_{\text{SLNT}}^{(0)}(r) = -N \left[\frac{1 - E_c}{2} \right]^{1/2} r^\gamma e^{-(\bar{K}/2r_0)r} \left[p {}_1F_1 \left[-p + 1, 2\gamma + 1; \left[\frac{\bar{K}}{r_0} \right] r \right] + (\Gamma - \kappa) {}_1F_1 \left[-p, 2\gamma + 1; \left[\frac{\bar{K}}{r_0} \right] r \right] \right]. \quad (26)$$

Expression (26) is the exact small-component reduced radial Dirac wave function for the point Coulomb potential.

IV. RESULTS AND DISCUSSION

For numerical application of our method, we consider the addition of vector or scalar linear potentials to the vector Coulomb potential. Such combinations are known to support bound states and have been considered as a model for quark confinement. In Tables I and II we present the binding energies obtained from our SLNT formula (9), (11), and (12). For the sake of comparison, we also cite the average values of the Padé-approximant results obtained by Vrscay and Hamidian who used [24,24] and [24,25] Padé approximants to the RS perturbation series. Excellent agreement is observed in general for various values of the coupling of Coulomb and linear terms. Departure is only appreciable when the strength of the linear potential is as large as that of the Coulomb term. It is remarkable that our algebraic expression is capable of giving results within the same order of accuracy consuming about one-tenth of the computation time needed by the authors of Ref. [29]. For interested readers, we would like to mention that our method works quite well for the screened Coulomb potential without extracting the Coulomb term explicitly. For illustration, we work with the potential

$$V(r) = -\frac{2Z}{r} \left[1 - \frac{(Z-1)}{Z} (1 - 1/[1 + H(e^{r/d} - 1)]) \right] \quad (27)$$

TABLE I. Estimates of ground-state energies for the combination of vector Coulomb potential $V(r) = -\Lambda_1/r$ plus scalar linear potential $S(r) = \lambda_s r$ in units of $\hbar = c = m = 1$. The first row of entries corresponds to our SLNT results and the second in italics corresponds to the average of the upper and lower bounds of the Padé-approximant results of Ref. [28].

$\lambda_s \backslash \Lambda_1$	0.9	0.7	0.5
0.0	0.436	0.714	0.866
	<i>0.436</i>	<i>0.714</i>	<i>0.866</i>
0.1	0.489	0.804	1.000
	<i>0.475</i>	<i>0.810</i>	<i>1.024</i>
0.2	0.536	0.877	1.101
	<i>0.506</i>	<i>0.882</i>	<i>1.131</i>
0.3	0.579	0.943	1.189
	<i>0.534</i>	<i>0.942</i>	<i>1.219</i>
0.4	0.621	1.004	1.269
	<i>0.558</i>	<i>0.995</i>	<i>1.296</i>
0.5	0.660	1.061	1.343
	<i>0.580</i>	<i>1.043</i>	<i>1.366</i>

suggested by Darewych, Green, and Sellin [35]. In Table III we cite the electronic energies for a wide range of neutral atoms corresponding to small as well as large screening parameters. The agreement of our results with the numerical values of Ref. [35] are in general excellent.

As far as the achievement for the computation of the relativistic wave function is concerned, we would like to make the following comments. Although it was shown [13] that the SLNT wave function resembles the large component of the reduced radial Dirac wave function over a wide range of radial variables, knowledge of the small component was obscure in this framework. We have shown here that the SLNT is at least an exact formalism for the relativistic point Coulomb problem of both vector and scalar nature. Furthermore, the small component of the Coulomb wave function can be systematically obtained starting from the SLNT leading-order wave function. This certainly highlights the possibility of constructing both large- and small-component Dirac radial wave functions for a potential which is not exactly solvable but may be solved approximately by the present method.

As a concluding remark, we would like to mention that the spirit of our work is quite similar to that of Su [30] who used a similarity transformation on the Dirac equation and obtained KG-like equations for two functions. Su suggested that these equations can be approximately solved by using the WKB method for non-exactly-

TABLE II. Estimates of first excited-state energies for the combination of vector Coulomb plus vector linear potential $V(r) = -\Lambda_1/r + \lambda_v r$ in units of $\hbar = c = m = 1$. The first row of entries corresponds to our SLNT results and the second in italics corresponds to the average of the upper and lower bounds of the Padé-approximant results of Ref. [28].

$\lambda_v \backslash \Lambda_1$	0.9	0.7	0.5
0.0	0.847	0.925	0.965
	<i>0.847</i>	<i>0.925</i>	<i>0.965</i>
0.1	1.091	1.268	1.378
	<i>1.095</i>	<i>1.272</i>	<i>1.394</i>
0.2	1.257	1.485	1.639
	<i>1.260</i>	<i>1.485</i>	<i>1.640</i>
0.3	1.391	1.659	1.843
	<i>1.395</i>	<i>1.656</i>	<i>1.85</i>
0.4	1.506	1.809	2.017
	<i>1.512</i>	<i>1.805</i>	<i>2.05</i>
0.5	1.609	1.943	2.172
	<i>1.617</i>	<i>1.935</i>	<i>2.2</i>

TABLE III. Electronic energies for several neutral atoms in Rydberg units ($\hbar=2m_e=e^2/2=1$) for the potential (27) with the parameters taken from Table II of Ref. [35]. The first row of entries corresponds to our SLNT results and the second in italics corresponds to the numerical values of Darewych *et al.*

Z	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
30	7.119(+2) <i>7.129</i>	8.608(+1) <i>8.622</i>	7.596(+1) <i>7.713</i>	7.725(+1) <i>7.524</i>
40	1.322(+3) <i>1.324</i>	1.864(+2) <i>1.843</i>	1.712(+2) <i>1.701</i>	1.664(+2) <i>1.635</i>
50	2.170(+3) <i>2.172</i>	3.334(+2) <i>3.318</i>	3.172(+2) <i>3.142</i>	2.973(+2) <i>2.961</i>
60	3.227(+3) <i>3.231</i>	5.271(+2) <i>5.250</i>	5.055(+2) <i>5.011</i>	4.624(+2) <i>4.610</i>
70	4.557(+3) <i>4.563</i>	7.768(+2) <i>7.754</i>	7.532(+2) <i>7.467</i>	6.654(+2) <i>6.657</i>
80	6.188(+3) <i>6.196</i>	1.101(+3) <i>1.101</i>	1.075(+3) <i>1.066</i>	9.140(+2) <i>9.157</i>
90	8.159(+3) <i>8.170</i>	1.513(+3) <i>1.512</i>	1.480(+3) <i>1.468</i>	1.202(+3) <i>1.204</i>

solvable potentials and one may retrieve the Dirac radial wave function in the Sommerfeld form by invoking back the similarity transformation. It is well known that the higher-order WKB calculation is quite complicated and in that respect our algebraic procedure based on the SLNT will have an advantage over it.

An N -dimensional generalization of the work of Su [30] has been done recently by Wong [36] for only the Coulomb problem. A further extension of this work based on the similarity transformation for an arbitrary radially symmetric potential may be a good starting point for carrying out relativistic $1/N$ calculations. This aspect is currently under investigation.

The present work hints at the possibility of applying the SLNT to more complicated relativistic problems. In particular, computations of hyperfine splitting, bound-

bound transition rates, etc. in atomic systems governed by screened Coulomb potentials require both large- and small-component radial wave functions. Computation of the continuum-state wave function from the knowledge of the bound-state wave function through the analytic continuation procedure is also worthwhile.

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APPENDIX

We cite here the explicit expressions for $\Sigma_{n_r}^{(1)}$ and $\Sigma_{n_r}^{(2)}$ and the parameters ϵ'_i, δ'_j s in order to calculate the second- and third-order corrections E_2 and E_3 to the energy:

$$\Sigma_{n_r}^{(1)} = (1 + 2n'_r)\bar{\epsilon}_2 + 3(1 + 2n'_r + 2n_r'^2)\bar{\epsilon}_4 - [\bar{\epsilon}_1^2 + 6(1 + 2n'_r)\bar{\epsilon}_1\bar{\epsilon}_3 + (11 + 30n'_r + 30n_r'^2)\bar{\epsilon}_3^2],$$

$$\Sigma_{n_r}^{(2)} = (1 + 2n'_r)\bar{\delta}_2 + 3(1 + 2n'_r + 2n_r'^2)\bar{\delta}_4 + 5(3 + 8n'_r + 6n_r'^2 + 4n_r'^3)\bar{\delta}_6$$

$$- \frac{1}{w} [(1 + 2n'_r)\bar{\epsilon}_2^2 + 12(1 + 2n'_r + 2n_r'^2)\bar{\epsilon}_2\bar{\epsilon}_4 + 2(21 + 59n'_r + 51n_r'^2 + 34n_r'^3)\bar{\epsilon}_4^2 \\ + 2\bar{\epsilon}_1\bar{\delta}_1 + 6(1 + 2n'_r)\bar{\epsilon}_1\bar{\delta}_3 + 30(1 + 2n'_r + 2n_r'^2)\bar{\epsilon}_1\bar{\delta}_5 + 6(1 + 2n'_r)\bar{\epsilon}_3\bar{\delta}_1 \\ + 2(11 + 30n'_r + 30n_r'^2)\bar{\epsilon}_3\bar{\delta}_3 + 10(13 + 30n'_r + 42n_r'^2 + 28n_r'^3)\bar{\epsilon}_3\bar{\delta}_5]$$

$$+ \frac{1}{w^2} [4\bar{\epsilon}_1^2\bar{\epsilon}_2 + 36(1 + 2n'_r)\bar{\epsilon}_1\bar{\epsilon}_2\bar{\epsilon}_3 + 8(11 + 30n'_r + 30n_r'^2)\bar{\epsilon}_2\bar{\epsilon}_3^2$$

$$+ 8(31 + 78n'_r + 78n_r'^2)\bar{\epsilon}_1\bar{\epsilon}_3\bar{\epsilon}_4 + 12(57 + 189n'_r + 225n_r'^2 + 150n_r'^3)\bar{\epsilon}_3^2\bar{\epsilon}_4 + 24(1 + 2n'_r)\bar{\epsilon}_1^2\bar{\epsilon}_4]$$

$$- \frac{1}{w^3} [8\bar{\epsilon}_1^3\bar{\epsilon}_3 + 108(1 + 2n'_r)\bar{\epsilon}_1^2\bar{\epsilon}_3^2 + 48(11 + 30n'_r + 30n_r'^2)\bar{\epsilon}_1\bar{\epsilon}_3^3 + 30(31 + 109n'_r + 141n_r'^2 + 94n_r'^3)\bar{\epsilon}_3^3]$$

with

$$n'_r = n_r - s/2, \quad \tilde{\epsilon}_i = \frac{\epsilon_i}{(2w)^{i/2}}, \quad \tilde{\delta}_j = \frac{\delta_j}{(2w)^{j/2}}, \quad i = 1, 2, \dots, 4; \quad j = 1, \dots, 6,$$

where

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

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

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

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

$$\delta_1 = -\frac{1}{4}(1-a)(3-a) + \frac{E_2 r_0^3 V''(r_0)}{c^2},$$

$$\delta_2 = \frac{3}{8}(1-a)(3-a) + \frac{E_2 r_0^2 V''(r_0)}{2c^2},$$

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

$$\delta_4 = -\frac{5}{8}(2-a),$$

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

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

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