Relativistic $1/N$ expansion for the Dirac equation

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A relativistic $1/N$ expansion method has been developed for the Dirac equation. This formalism is applied to the screened Coulomb potential proposed by Mehta and Patil [Phys. Rev. A **17**, 34 (1978)]. The $1/N$ expansion result is compared with numerical results and the envelope-method approximation.

I. INTRODUCTION

The shifted $1/N$ expansion method has been used extensively to determine the energy eigenvalues of the Schrödinger equation for some important potentials.[1–4] A modified method which guarantees better convergence has been proposed by Maluendes *et al.*[5] Very recently, Atag[6] applied this method to the rotational-vibrational states of the H_2^+ molecules. The shifted $1/N$ expansion method is nonperturbative in nature and hence is useful in problems involving large coupling constants. But until very recently the use of this method has been restricted to nonrelativistic problems. Some time ago Nieto[7] extended $1/N$ expansion formalism to relativistic potentials but he discussed it in the framework of the Klein-Gordon equation only and it was not the shifted $1/N$ but the ordinary $1/N$ expansion. Miramontes and Pajares[8] studied the large-N limit of both the Klein-Gordon and Dirac equations. But their result is not of much practical use as it was applied to the pure Coulomb problem; they made use of the exact solution of the Dirac-Coulomb problem, and they did not develop any formalism to deal with nonsolvable cases. Very recently, the method has been used to obtain linear scalar potential in the Dirac equation.[9] Mathematically the scalar Dirac potential is comparatively easy to deal with. However, it will be interesting to see if the shifted $1/N$ method can be applied to Coulomb-like relativistic problems at least for the cases where the rest energy can be assumed to be large compared to the relativistic corrections. In this paper explicit analytical formulas for energy values for any radially symmetric Dirac potential $V(r)$ have been derived. For numerical comparison the screened Coulomb potential as proposed by Mehta and Patil[10] has been chosen as detailed numerical results are available[11] for this potential. The organization of the paper is as follows.

In Sec. II we develop the formalism for the shifted $1/N$ expansion procedure for the Dirac equation for a radially symmetric potential. In Sec. III we apply this method to the hydrogen atom problem. In Sec. IV the results for the screened Coulomb potential of Ref. 10 are presented together with the numerical results of Ref. 11. Section V is kept for discussions and conclusions.

II. $1/N$ EXPANSION FOR THE DIRAC EQUATION

The Dirac equation in N dimensions for radially symmetric potential $V(r)$ can be written as

$$\left[\frac{d^2}{dr^2}-\frac{(N_j-2)(N_j-2+2s)}{4r^2}+(W-V)^2-m^2\right]G(r) = -\frac{dV}{dr}F(r) \quad (1)$$

and

$$\left[\frac{d^2}{dr^2}-\frac{(N_j-2)(N_j-2-2s)}{4r^2}+(W-V)^2-m^2\right]F(r) = \frac{dV}{dr}G(r)\ , \quad (2)$$

where we have used the following factorization for Dirac spinors:

$$\psi_{js}^{M}=\frac{1}{r^{\frac{N-1}{2}}}\begin{cases}F(r)Y_{lj}^{M}, & l=j+\frac{s}{2}, s=\pm 1\\ G(r)Y_{l'j}^{M}, & l'=j-\frac{s}{2}\end{cases} \quad (3)$$

and

$$N_j=N+2j\ . \quad (4)$$

In deriving (1) and (2) the second-order radial form of the Dirac equation has been used and the Laplacian Δ has been written (in N dimensions) as

$$\Delta=\frac{1}{r^2}\Delta_B+\frac{\partial^2}{\partial r^2}+\frac{N-1}{r}\frac{\partial}{\partial r}\ , \quad (5)$$

where Δ_B is the Beltrami operator[12] with eigenvalue $l(l+N-2)$ where l can assume the value $j\pm(s/2)$ ($s=+1$). Equations (1) and (2) can be recast in the form

$$\frac{dF}{dr}-\frac{\chi}{r}F=(V-W-m)G\ , \quad (6)$$

$$\frac{dG}{dr}+\frac{\chi}{r}G=(W-V-m)F\ , \quad (7)$$

where

$$\chi=-\frac{(N_j-2)s}{2}, \quad N_j=N+2j \ . \tag{8}$$

When $s=+1$ and $N=3$, $\chi=1$, and when $s=-1$ and $N=3$, $\chi=-(l+1)$, and then (6) and (7) reduce to the usual set of Dirac equations for a radially symmetric potential. Eliminating G from (6) and (7) and writing

$$W=E+m \ , \tag{9}$$

we have

$$\frac{d^2F}{dr^2}-\frac{\chi(\chi-1)}{r^2}F(r)+2m(E-V)F$$
$$=-\frac{1}{2m+E-V}\frac{dV}{dr}\left[\frac{dF}{dr}-\frac{\chi}{r}F\right]+(E-V)^2F \ . \tag{10}$$

The first derivative dF/dr of the right-hand side (rhs) of (10) can be removed by the substitution

$$F(r)=\left[1+\frac{E-V(r)}{2m}\right]^{1/2}\varphi(r) \ , \tag{11}$$

where $\varphi(r)$ satisfies the following equation:

$$\frac{d^2\varphi}{dr^2}-\frac{\chi(\chi-1)}{r^2}\varphi+2m(E-V)\varphi$$
$$=\frac{1}{2m+E-V}\left[\frac{1}{2}\frac{d^2V}{dr^2}+\frac{\chi}{r}\frac{dV}{dr}\right]\varphi(r)-(E-V)^2\varphi$$
$$+\frac{3}{4(2m-E-V)^2}\left[\frac{dV}{dr}\right]^2\varphi \ . \tag{12}$$

In principle, the $1/N$ expansion can be applied now by expanding each term in (12) in powers of $1/N$. But if we are interested in problems where the rest energy is large, we can expand terms like $1/(2m+E-V)$ as

$$(1/2m)[1-(E-V)/2m+\cdots] \ ,$$

and since the contributions of $(E-V)/4m^2$ terms are small we can treat them as perturbations and calculate them after the leading $1/mc^2$ order calculations have been done. Thus neglecting terms of the order of $(E-V)/4m^2$ we get from (12)

$$-\frac{1}{2m}\frac{d^2\varphi}{dr^2}+\frac{(k-1)(k-3)}{8mr^2}\varphi-(E-V)\varphi$$
$$=-u(r)\varphi+\frac{(E-V)^2}{2m}\varphi \ , \tag{13}$$

where

$$u(r)=\frac{1}{4m^2}\left[\frac{1}{2}\frac{d^2V}{dr^2}+\frac{\chi}{r}\frac{dV}{dr}\right] \ ,$$

where

$$k=N+2j+1 \quad \text{when } j=l-\tfrac{1}{2}$$
$$\text{and} \tag{14}$$
$$k=N+2j-1 \quad \text{when } j=l+\tfrac{1}{2} \ .$$

Also, $\chi=(k-1)/2$ or $-(k-3)/2$ according as $j=l-\frac{1}{2}$ or $l+\frac{1}{2}$. Hence we can always write $k=N+2l$ in conformity with the nonrelativistic result. If we further neglect the $(E-V)^2/2m$ term then (13) reduces to a Schrödinger equation with the effective potential

$$\bar{V}(r)=V(r)+\frac{1}{4m^2}\left[\frac{1}{2}\frac{d^2V}{dr^2}+\frac{\chi}{r}\frac{dV}{dr}\right] \ , \tag{15}$$

and one can apply the standard $1/N$ shifted expansion method for the Schrödinger equation. In fact, that is how we obtain the $1S$ result for Mehta-Patil potentials. In fact, all the relativistic eigenvalues of the potential of Ref. 10 could be obtained in this way and they give very good approximations, through the fine-structure splitting would not be very accurate. In any case, since we propose to develop the formalism for general screened Coulomb potentials of which the potential of Ref. 10 is just one example, we proceed further to derive the formulas for relativistic eigenvalues up to about second order.

First we give a shift to the quantity k, i.e., we write

$$k=\bar{k}+a \ . \tag{16}$$

Then (13) can be written as

$$-\frac{1}{2m}\frac{d^2\varphi}{dr^2}+\frac{\bar{k}^2}{8mr^2}\left[1+\frac{a-1}{\bar{k}}\right]\left[1+\frac{a-3}{\bar{k}}\right]+\left[V-\frac{V^2}{2m}+\frac{EV}{m}\right]+u(r)\varphi(r)=\left[E+\frac{E^2}{2m}\right]\varphi \ , \tag{17}$$

where χ in $u(r)$ is given by

$$\chi=\frac{\bar{k}+a-1}{2} \quad \text{when } j=l-\tfrac{1}{2} \ ,$$
$$\chi=-\left[\frac{\bar{k}+a-3}{2}\right] \quad \text{when } j=l+\tfrac{1}{2} \ . \tag{18}$$

Now we expand E and $V(r)$ in powers of $1/N$. We write

$$E=\bar{k}^2E_0+\bar{k}E_1+E_2+\frac{E_3}{\bar{k}}+\cdots \tag{19}$$

and

$$V(r)=\frac{\bar{k}^2}{Q}\left[V(r_0)+gV'(r_0)xr_0+\frac{g^2}{2}V''(r_0)x^2r_0^2+\cdots\right] \ , \tag{20}$$

$$u(r)=\frac{\bar{k}^2}{Q}[u(r_0)+gu'(r_0)xr_0+\cdots] \ , \tag{21}$$

where Q is a scale introduced whose magnitude is to be determined later on and x,g are defined through

$$\frac{(r-r_0)}{r_0}\bar{k}^{1/2}=x, \quad g=\frac{1}{\bar{k}^{1/2}} \ . \tag{22}$$

The leading $1/N$ order energy term is obtained from solving the equation

$$\frac{\bar{k}^2}{8mr_0^2}+V(r_0)-\frac{V(r_0)^2}{2m}+\frac{2\bar{k}^2E_0V(r_0)}{2m}+u(r_0)=\bar{k}^2\left[E_0+\frac{\bar{k}^2E_0^2}{2m}\right], \quad (23)$$

which gives

$$\bar{k}^2E_0=V(r_0)-m+m\left\{1+\frac{\bar{k}^2}{4m^2r_0^2}+\frac{\bar{U}(r_0)}{2m^3}\right\}^{1/2}, \quad (24)$$

where

$$\bar{U}(r_0)=\frac{1}{2}\frac{d^2V}{dr^2}+\frac{\chi}{r}\frac{dV}{dr}. \quad (25)$$

r_0 is chosen as to make $\bar{k}^2E_0$ a minimum. This gives

$$\left[r^3\frac{dV}{dr}\left\{1+\frac{\bar{k}^2}{4m^2r^2}+\frac{\bar{U}(r)}{2m^3}\right\}^{1/2}\right]\Bigg|_{r=r_0}=\frac{\bar{k}^2}{4m}-\frac{r_0^3\bar{U}'(r_0)}{4m^2}. \quad (26)$$

In the above derivations Q is chosen to be $\bar{k}^2$, which gives back the correct Dirac equation for any N. Neglecting terms of the order of $\bar{U}'(r_0)^2/m^6$, $\bar{k}^2$ is given by

$$\bar{k}^2=mr_0^3\left\{\frac{\bar{U}'(r_0)}{m^2}+\frac{2r_0}{m}\left|\frac{dV}{dr_0}\right|^2+\left[16\left|\frac{dV}{dr_0}\right|^2+\frac{4r_0^2}{m^2}\left|\frac{dV}{dr_0}\right|^4+\frac{4r_0}{m^3}\bar{U}'(r_0)\left|\frac{dV}{dr_0}\right|^2+\frac{8}{m^3}\bar{U}(r_0)\left|\frac{dV}{dr_0}\right|^2\right]^{1/2}\right\}. \quad (27)$$

The terms of order $\bar{k}$, $1/k$, etc. can be obtained in exactly the same manner as was done in the case of the Schrödinger equation in Ref. 2. We here quote the results and explain the appropriate modification whenever applicable. The next order contribution to E is given by

$$\frac{\bar{k}}{r^2}\left[(n_r+\tfrac{1}{2})w-\frac{(2-a)}{4m}\right], \quad (28)$$

where

$$w=\frac{1}{2m}\left\{3+4mr_0^4\frac{Y''(r_0)}{Q}\right\}^{1/2} \quad (29)$$

and $Y''(r_0)$ is given by

$$Y''(r_0)=V''(r_0)+\frac{\bar{U}''(r_0)}{4m^2}-\frac{V'(r_0)^2}{m}+\frac{V''(r_0)}{8m^2r_0^2}\bar{k}^2. \quad (30)$$

In analogy with the nonrelativistic case we choose a such that the contribution (28) vanishes. It will be shown in Sec. III that this choice gives the correct result for the hydrogen atom up to the appropriate order in $1/m$. Apart from the analytical demonstration we have checked exhaustively the fact that for the hydrogen atom case the procedure mentioned here reproduces the exact numerical values for the relativistic energy. Now the vanishing of expression (28) gives the required equation for r_0 given below,

$$N+2l-2+(2n_r+1)2mW=\bar{k}. \quad (31)$$

The energy up to second order is given by

$$E=\bar{E}_0+\bar{E}_2, \quad (32)$$

where

$$\bar{E}_0=k^2E_0 \quad (33)$$

and

$$\bar{E}_2=\frac{e_2}{1-\dfrac{\bar{E}_0-V(r_0)}{m}}, \quad (34)$$

where

$$e_2=\frac{\beta'}{r_0^2}, \quad (35)$$

$$a=2-(2n_r+1)\left\{3+4mr_0^4\frac{Y''}{\bar{k}^2}\right\}^{1/2}, \quad (36)$$

and

$$\beta'=\frac{1}{8m}(1-a)(3-a)+(1+2n_r)\bar{\epsilon}_2+3(1+2n_r+2n_r^2)\bar{\epsilon}_4-\frac{1}{w}[\bar{\epsilon}^2+6(1+2n_r)\bar{\epsilon}_1\bar{\epsilon}_3+(11+30n_r+30n_r^2)], \quad (37a)$$

where

$$\bar{\epsilon}_j=\frac{\epsilon_j}{(2mw)^{1/2}}, \quad j=0,1,2,\ldots \quad (37b)$$

and

$$\epsilon_1=\frac{(2-a)}{2m}, \quad \epsilon_2=-\frac{3(2-a)}{4m}, \quad (37c)$$

$$\epsilon_3=-\frac{1}{2m}+\frac{r_0^5}{6Q}Y'''(r_0), \quad (38)$$

$$\epsilon_4=\frac{5}{8m}+\frac{r_0^6}{24Q}Y^{\mathrm{IV}}(r_0). \quad (39)$$

Y''' and Y^{IV} are given by

$$Y'''=V'''(r_0)+\frac{\bar{U}'''(r_0)}{4m^2}-\frac{3V'(r_0)V''(r_0)}{m}+\frac{V'''(r_0)\bar{k}^2}{8m^2r_0^2}, \quad (40)$$

$$Y^{\mathrm{IV}}(r_0)=V^{\mathrm{IV}}(r_0)+\frac{\bar{U}^{\mathrm{IV}}(r_0)}{4m^2}+\frac{V^{\mathrm{IV}}(r_0)\bar{k}^2}{8m^2r_0^2}-\frac{3V''(r_0)^2}{m}-\frac{4V'(r_0)V'''(r_0)}{m}. \quad (41)$$

III. HYDROGEN ATOM PROBLEM

Here $V(r)=-v/r$ where $v=Z\alpha$ where α is the fine-structure constant and Z is the atomic number. We have from (24)

$$\bar{E}_0 \simeq V(r_0)+\frac{\bar{k}^2}{8mr_0^2}-\frac{m}{8}\left(\frac{\bar{k}^2}{8m^2r_0^2}\right)^2 . \tag{42}$$

$\bar{k}$ is given by $\partial\bar{E}_0/\partial r_0=0$ which gives [neglecting terms of order $(1/m^2)$]

$$\frac{\bar{k}^2}{4mr_0}=v+\frac{v^2}{2mr_0} . \tag{43}$$

Hence from (42)

$$\bar{E}_0 \simeq -\frac{v}{2r_0}+\frac{v^2}{8mr_0^2} . \tag{44}$$

Taking $N=3$ and $n_r=l+1=n$, r_0 can be obtained from (43), (29) and (31). After some manipulations and keeping only terms of the order up to v^3/n^4, we get

$$\frac{1}{r_0} \simeq \frac{mv}{n^2}+\frac{mv^3}{2n^4}+\frac{mv^3}{n^5}n_r . \tag{45}$$

Hence from (44) we get

$$\bar{E}_0=-\frac{mv^2}{2n^2}-\frac{mv^4}{8n^4}-\frac{mv^4}{2n^5}n_r . \tag{46}$$

Let us compare the result with the exact solution of the Dirac equation for the pure Coulomb potential:[13]

$$V(r)=-\frac{v}{r} , \tag{47}$$

$$E=-\frac{mv^2}{2n^2}-\frac{mv^4}{8n^3}\left\{\frac{4}{|k_1|}-\frac{3}{n}\right\} , \tag{48}$$

where we have considered only first-order relativistic correction. k_1 is defined as follows. When $k_1>0$, $k_1=n-n_r$ and when $k_1<0$, $k_1=n-n_r-1$. Taking $k_1>0$ and expanding $1/(n-n_r)$ assuming n to be large compared with n_r (this is equivalent to $1/N$ expansion), we have from (48)

$$E=-\frac{mv^2}{2n^2}-\frac{mv^4}{8n^4}-\frac{mv^4}{2n^5}n_r , \tag{49}$$

which is identical with (46). Hence the choice of the shift a is consistent with the Dirac Coulomb result. As mentioned before, apart from the above simplistic calculation exhaustive checks were made to ensure that this choice gives the exact numerical result for the relativistic hydrogen problem.

IV. RESULTS FOR THE SCREENED COULOMB POTENTIAL

The screened Coulomb potential is of great importance because of its application in atomic phenomena involving transitions and they are known to adequately describe the effective interaction in many-body atomic phenomena. There are a few popular three-dimensional models of the

TABLE I. Eigenvalues $E_{n_r}^P$ where P denotes parity for the screened Coulomb potential given by (50) obtained from the $1/N$ expansion. The figures in the parentheses and square brackets are the exact numerical values and envelope-approximation results, respectively, taken from Ref. 11.

Z	$E_{1,0}$	$E_{2,1}$	$E_{1,0}$	$E_{3,0}$
14	−2.0003	−0.2752	−0.2182	−0.2172
	(−1.9998)	(−0.2493)	(−0.2157)	(−0.2147)
	[−1.9591]	[−0.1877]	[−0.1877]	[−0.1870]
19	−3.8656	−0.5667	−0.4770	−0.4729
	(−3.8646)	(−0.5249)	(−0.4724)	(−0.4685)
	[−3.8090]	[−0.4269]	[−0.4269]	[−0.4237]
24	6.3843	0.9847	−0.8624	−0.8511
	(6.3829)	(−0.9268)	(−0.8543)	(−0.8438)
	[−6.3130]	[−0.7904]	[−0.7904]	[−0.7810]
29	−9.5754	−1.5388	1.3867	−1.3606
	(9.5740)	(1.466)	(1.373)	(−1.349)
	[9.491]	[1.290]	[−1.290]	[−1.268]
34	−13.4585	−2.2374	−2.0610	−2.0085
	(−13.460)	(−2.151)	(−2.039)	(−1.989)
	[−13.363]	[−1.935]	[−1.935]	[1.890]
39	−3.0889	−3.0889	−2.8967	−2.8010
	(−18.063)	(−2.993)	(−2.860)	(−2.771)
	[−17.954]	[−2.736]	[−2.736]	[−2.653]
44	23.3858	−4.1018	−3.9066	−3.7436
	(23.410)	(−4.001)	(−3.849)	(−3.698)
	[23.288]	[−3.703]	[−3.703]	[3.561]
49	−29.4776	−5.2852	−5.1049	−4.8419
	(−29.532)	(−5.188)	(−5.015)	(4.773)
	[−29.398]	[−4.847]	[4.847]	[4.619]
54	−36.3569	−6.6493	−6.5084	6.1014
	(−36.465)	(−6.564)	(6.371)	(−6.002)
	[36.320]	[6.181]	[−6.181]	[−5.829]
59	−44.0532	8.2055	−8.1373	−7.5278
	(44.251)	(−8.145)	(−7.931)	(−7.386)
	[44.095]	[−7.718]	[−7.718]	[−7.195]
64	−52.5988	−9.9669	−10.0166	−9.1273
	(−52.942)	(−9.947)	(−9.713)	(−8.930)
	[−52.774]	[−9.476]	[−9.476]	[−8.721]
69	−62.0281	11.948	12.178	10.906
	(62.597)	(11.991)	(11.736)	(10.638)
	[−62.418]	[−11.473]	[−11.473]	[−10.411]
74	−72.3784	−14.168	−14.661	−12.872
	(−73.287)	(−14.298)	(−14.023)	(−12.512)
	[−73.098]	[−13.734]	[−13.734]	[−12.267]
79	−83.6895	−16.647	−17.521	−15.032
	(85.101)	(−16.898)	(−16.603)	(−14.557)
	[84.901]	[−16.287]	[−16.287]	[−14.294]
84	−96.0038	−19.410	−20.835	−17.395
	(−98.145)	(−19.826)	(19.510)	(16.776)
	[−97.934]	[−19.165]	[−19.165]	[−16.496]

screened Coulomb potential. Among such quantum-mechanical models the screened Coulomb potential of the form

$$V(r)=-\frac{v}{r}\left|1-r\lambda\left|1-\frac{1}{Z}\right|\right/(1+r\lambda)\left|\right. \tag{50}$$

has been studied by some authors.[10,11] In the above formula for $V(r)$, $v=\alpha Z$, λ is the screening parameter, α is the fine-structure constant, and Z is the nuclear charge. This potential is the representative of the more general potential of the form

$$V(r)=-\frac{Z}{r}+\sum_{i=0}^{\infty}a_i(\lambda r)^i$$

studied by Pratt and Tseng[14] for analyzing the screening effect. Since relativistic numerical eigenvalues for the potential discussed by Mehta and Patil exist[11] we have used our $1/N$ expansion technique to calculate the eigenvalues for this potential. For comparison with the published numerical result λ is taken as the following:

$$\lambda=0.98\alpha Z^{1/3}\ . \tag{51}$$

In Table I our $1/N$ results have been compared with the numerical and envelope results.[11] It is to be noted that for $Z>74$ in Eqs. (43), (29), and (31) a real value of r_0 for the $1S$ case could not be determined. This is not very surprising as the shifted $1/N$ expansion (in the modified version) gives good results except for the ground state where N is not large. However, for the $1S$ state, as mentioned earlier, we have solved a Schrödinger equation with a modified potential

$$V(r)+\frac{1}{4m^2}\left[\frac{1}{2}\frac{d^2V}{dr^2}+\frac{\chi}{r}\frac{dV}{dr}\right],$$

which takes account of the relativistic correction, and we found that the agreement with the numerical result is fairly good though the $1/N$ expansion is not expected to give very accurate results for the lowest-lying state. Other states have been calculated using the formulas (24)–(31), i.e., $\bar{E}_0$ was calculated. It is clear that even our lowest-order calculation gives a better approximation to the exact value than the result obtained by the envelope method. Also the envelope approximation gives $E_{2\,1/2}^{-}=E_{1\,1/2}$ which is not true in our case. For $Z\geq 79$ the agreement is not as good as it is for $Z<79$.

V. DISCUSSION

To summarize, we have developed a formalism of the relativistic $1/N$ expansion method for the Dirac equation with radially symmetric potentials. For simplicity we have considered the case where the rest energy can be assumed to be large compared to the binding energy and we have restricted ourselves to first-order corrections in $1/N$. It has been shown that the shift chosen by us leads to the correct result for hydrogen atom. Our result can be generalized to the modified $1/N$ expansion method to yield very accurate results. It can be applied to the relativistic potentials in quantum mechanics and particle physics. Work is in progress along these lines.

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