

**Approximate treatment of the Dirac equation with scalar and vector potentials of rectangular shapes**

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The Dirac equation with a scalar potential  $U_S(r)$  and the fourth component of a vector potential  $U_V(r)$  is considered in the case of rectangular shapes of these potentials with the same radius  $R$ ; approximate analytic expressions are derived for the single-particle energy of bound states in certain cases. The results obtained with these expressions are compared with the corresponding "exact" results obtained by solving the eigenvalue equation numerically. It is found that very good results are obtained for the ground state and for quite a wide range of values of  $R$  with one of the proposed expressions. Even the corresponding nonrelativistic version of this expression has not been derived before, to our knowledge.

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The Dirac equation with a scalar potential  $U_S(r)$  and the fourth component of a vector potential  $U_V(r)$  [1,2],

$$[c\alpha \cdot \mathbf{p} + \beta\mu c^2 + \beta U_S(r) + U_V(r)]\Psi = E\Psi, \quad (1)$$

has attracted much interest in the past (see Refs. [2,3], and references therein). In this equation  $\alpha$  and  $\beta$  are the usual Dirac matrices,  $\Psi$  the Dirac spinor, and  $E$  the total energy  $E = \epsilon + \mu c^2$ .

By expressing the Dirac spinors in terms of large ( $G$ ) and small ( $F$ ) component:

$$\Psi = \Psi_{Nljm} = \begin{pmatrix} \frac{iG_{Nlj}(r)}{r} \\ F_{Nlj}(r)\sigma \cdot \mathbf{r} \\ r \end{pmatrix} \varphi_{ljm}, \quad (2)$$

where

$$\varphi_{ljm} = (Y_l^{m_l} \otimes \chi_{1/2}^{m_s})_{jm} \quad (3)$$

and  $\chi_{1/2}^{m_s}$  are the Pauli spinors, one may derive from (1) the following Schrödinger-type equation (for central potentials) [4]:

$$g''(r) - \left[ \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} (V_{\text{central}} + V_{\text{SO}} - \epsilon) \right] g(r) = 0, \quad (4)$$

where

$$g(r) = D^{-1/2}(r)G(r), \quad (5)$$

$$D(r) = \frac{1}{\hbar c} [2\mu c^2 + \epsilon + U_-(r)].$$

$G$  is the large component of the Dirac wave function and

$$G(r) = \tilde{N}nr \left[ [1 - \Theta(r - R)]j_l(nr) + \Theta(r - R)\frac{j_l(nR)}{h_l^{(1)}(in_0R)}h_l^{(1)}(in_0r) \right], \quad (10)$$

$$V_{\text{central}} = U_+(r) + \frac{\hbar^2}{2\mu} \left[ \frac{1}{\hbar^2 c^2} [U_+(r) - \epsilon][U_-(r) + \epsilon] - D^{-1}(r)D'(r)r^{-1} - [2D(r)]^{-1}D''(r) + \frac{3}{4}D^{-2}(r)[D'(r)]^2 \right], \quad (6)$$

$$V_{\text{SO}}(r, \epsilon) = -\frac{\hbar}{2\mu} \frac{1}{[2\mu c^2 + \epsilon + U_-(r)]} \frac{1}{r} \frac{dU_-(r)}{dr} \mathbf{l} \cdot \boldsymbol{\sigma}. \quad (7)$$

The potentials  $U_{\pm}(r)$  are defined as

$$U_{\pm}(r) = U_S(r) \pm U_V(r). \quad (8)$$

We consider the case in which  $U_+(r)$  and  $U_-(r)$  are square wells with the same radius  $R$  [5] and depths  $D_+$  and  $D_-$ , respectively, i.e.,

$$U_{\pm}(r) = -D_{\pm}[1 - \Theta(r - R)], \quad (9)$$

where  $\Theta$  is the unit step function.

Square-well potentials, in particular of infinite depth, have been used in applications of nonrelativistic quantum mechanics in spite of their crudeness because of the analytic expressions to which they lead. As it was also pointed out recently [6], the eigenvalues of the one-dimensional Schrödinger equation with a potential which is a sum of even powers of  $x$  may be calculated, by using the eigenfunctions and eigenvalues of the infinite square well.

The generalized Dirac equation with the square-well potentials we are discussing may be solved (semi)analytically, for every bound state [7]. The expressions for  $G$  and  $F$  are given in terms of spherical Bessel functions  $j_l$  and spherical Hankel functions of the first kind  $h_l^{(1)}$  and are

$$F(r) = \tilde{N} nc\hbar \left[ [1 - \Theta(r - R)] \frac{1}{\varepsilon + 2\mu c^2 - D_-} [nrj_{l-1}(nr) + (k-l)j_l(nr)] \right. \\ \left. + \Theta(r - R) \frac{1}{\varepsilon + 2\mu c^2} \frac{j_l(nR)}{h_l^{(1)}(in_0R)} [in_0rh_{l-1}^{(1)}(in_0r) + (k-l)h_l^{(1)}(in_0r)] \right] \quad (11)$$

while the energy eigenvalue equation is [7]

$$\left[ 1 - \frac{D_-}{2\mu c^2 + \varepsilon} \right] \frac{in_0R h_{l-1}^{(1)}(in_0R)}{h_l^{(1)}(in_0R)} \\ = \frac{(k-l)D_-}{2\mu c^2 + \varepsilon} + \frac{nR j_{l-1}(nR)}{j_l(nR)}. \quad (12)$$

In these expressions the quantities  $n$  and  $n_0$  are defined as follows:

$$n = \left[ \frac{2\mu}{\hbar^2} (D_+ + \varepsilon) [1 - (D_- - \varepsilon)(2\mu c^2)^{-1}] \right]^{1/2}, \quad (13)$$

$$n_0 = \left[ \frac{2\mu}{\hbar^2} \{-\varepsilon[1 + \varepsilon(2\mu c^2)^{-1}]\} \right]^{1/2}, \quad (14)$$

and  $k = \pm(j + \frac{1}{2})$  for  $j = (l \mp \frac{1}{2})$ . The quantum numbers in  $G, F, \varepsilon$ , and  $\tilde{N}$  have been suppressed.

The disadvantage with eigenvalue equation (12) is that, in general, it cannot be solved for  $\varepsilon$  and thus it is not possible to have an explicit expression for the energy in terms of the potential parameters. We show in this paper, however, that in certain cases this can be achieved approximately in a rather satisfactory way. Thus one is led to fairly simple approximate analytic expressions for  $\varepsilon$ . Before proceeding we recall that usually in practice  $D_-$  is adequately smaller than  $2\mu c^2$  and  $D_+$  much smaller than  $D_-$ .

Let us consider the case in which  $nR$  and  $n_0R$  are sufficiently larger than  $(l/2)(l+1)$  (see also Refs. [8,9]) so that we may use the following asymptotic form for  $j_l(nR)$  and  $h_l^{(1)}(in_0R)$ :

$$j_l(nR) \simeq \frac{1}{nR} \sin \left[ nR - \frac{l\pi}{2} \right], \\ h_l^{(1)}(in_0R) \simeq \frac{-1}{n_0R} e^{-n_0R - il\pi/2}. \quad (15)$$

Thus Eq. (12) may be written in the form

$$n_0R + nR \cot \left[ nR - \frac{l\pi}{2} \right] = \frac{D_-}{2\mu c^2 + \varepsilon} [n_0R - (k-l)]. \quad (16)$$

It is seen immediately that for the ground state  $1s_{1/2}$  ( $l=0, k=-1$ ) this equation coincides with the exact eigenvalue equation for this state (see Appendix of Ref. [5]). For the excited states, however, it is approximate.

Equation (16) may be written in the following form, which is suitable for our treatment:

$$n^2 R^2 = \frac{2\mu}{\hbar^2} D_+ R^2 (1 + C_R) \sin^2 \left[ (2N + l) \frac{\pi}{2} - nR \right], \quad (17)$$

where  $N = 1, 2, 3, \dots, l = 0, 1, 2, \dots$ , and

$$C_R = \left[ \frac{\varepsilon}{D_-} - \frac{\varepsilon}{D_+} - 1 \right] D_- (2\mu c^2)^{-1} \\ + \frac{1}{(2\mu/\hbar^2) D_+ R^2} \left\{ -(n_0R)^2 \right. \\ \left. + \left[ n_0R \left[ 1 - \frac{D_-}{2\mu c^2 + \varepsilon} \right] \right. \right. \\ \left. \left. + \frac{(k-l)D_-}{2\mu c^2 + \varepsilon} \right]^2 \right\}. \quad (18)$$

We are interested in the case of a well of sufficiently large depth  $D_+$  and radius  $R$ . Thus if we write Eq. (17) in terms of the arcsin of the small quantity

$$x = nR [(2\mu/\hbar^2) D_+ R^2 (1 + C_R)]^{-1/2}$$

we may keep only the leading term in the expansion of arcsin  $x$  and obtain the eigenvalue equation in the approximate form

$$(nR)^2 = \frac{(2N + l)^2 \pi^2}{4(1 + \lambda_R)^2}, \quad (19)$$

where

$$\lambda_R = \lambda_0 [1 + C_R]^{-1/2}, \quad (20a)$$

$$\lambda_0 = \left[ \frac{2\mu}{\hbar^2} D_+ R^2 \right]^{-1/2}. \quad (20b)$$

It is interesting to note that if we neglect completely the terms of order  $(2\mu c^2)^{-1}$  the eigenvalue equation (12) goes over to the corresponding nonrelativistic one. In this case Eq. (19) may be written in the form

$$\varepsilon_{NR1} = -D_+ + \frac{\hbar^2}{8\mu} \frac{(2N + l)^2 \pi^2}{(1 + \lambda_0)^2 R^2}. \quad (21)$$

This is an approximate expression of the nonrelativistic energy for a particle of mass  $\mu$  in a square-well potential of depth  $D_+$  and radius  $R$ . In the case of the  $s$  states the above expression is reduced to a known approximate expression [10] derived from the corresponding Schrödinger eigenvalue equation.

An approximate relativistic expression for the energy may be derived from expression (19) if the unknown energy which appears in terms which are expected to be small is estimated by means of (21). In this way we obtain the following approximate expression for the relativistic energy which we shall denote by  $\varepsilon_{R1}$ :

$$\varepsilon_{R1} = -D_+ + \frac{\hbar^2}{8\mu_{g1}^*} \frac{(2N+l)^2\pi^2}{(1+\lambda_{R1})^2 R^2}, \quad (22)$$

where  $\mu_{g1}^*$  is a type of "effective mass" given by

$$\mu_{g1}^* = \mu[1 + (\varepsilon_{NR1} - D_-)(2\mu c^2)^{-1}] \quad (23)$$

and  $\lambda_{R1}$  is given by (20a) in which the energy in the expression of  $C_R$  has been substituted by  $\varepsilon_{NR1}$  [expression (21)]. The above procedure may be iterated. Thus we may use as expressions for the energy in  $\mu_{g1}^*$  and  $\lambda_{R1}$  which appear in (22) the ones obtained in the previously described way and so on.

An improved expression for  $\varepsilon$  may be obtained if instead of retaining only the leading term  $x$  in the expansion of  $\arcsin x$ :

$$\begin{aligned} \arcsin x &= x + \frac{x^3}{2(3)} + \frac{1(3)}{2(4)5}x^5 + \dots \\ &= x[1 + F(x)], \end{aligned} \quad (24)$$

that is, instead of setting  $F(x)=0$  we write, as in a similar expansion [11],  $F(x) \approx F(x^{ap})$  where  $x^{ap}$  is the expression resulting from the eigenvalue equation solved approximately with  $\arcsin x \approx x$ . This procedure leads in the nonrelativistic case to the following expression for the energy which we shall denote by  $\varepsilon_{NR2}$ , i.e.,

$$\varepsilon_{NR2} = -D_+ + \frac{\hbar^2}{8\mu} \frac{(2N+l)^2\pi^2}{(1+F_0)^2 R^2}, \quad (25)$$

where

$$F_0 = \frac{\arcsin\{\lambda_0(2N+l)\pi/[2(1+\lambda_0)]\}}{(2N+l)\pi/[2(1+\lambda_0)]}. \quad (26)$$

In the relativistic case the corresponding expression is

$$\varepsilon_{R2} = -D_+ + \frac{\hbar^2}{8\mu_{g2}^*} \frac{(2N+l)^2\pi^2}{(1+F_{R2})^2 R^2}, \quad (27)$$

where

$$F_{R2} = \frac{\arcsin\{\lambda_{R2}(2N+l)\pi/[2(1+\lambda_{R2})]\}}{(2N+l)\pi/[2(1+\lambda_{R2})]}, \quad (28)$$

$$\mu_{g2}^* = \mu[1 + (\varepsilon_{NR2} - D_-)(2\mu c^2)^{-1}], \quad (29)$$

and  $\lambda_{R2}$  is given by (20a) in which the energy in the ex-

pression of  $C_R$  has now been estimated with  $\varepsilon_{NR2}$  [expression (25)].

We discuss also the case of states for which in addition  $|\varepsilon| \ll D_+$ . This condition is satisfied for loosely bound states in a sufficiently deep well. In this case it may be seen from Eq. (16), in analogy with the corresponding nonrelativistic treatment [9], that the cotangent should be close to zero. Thus we arrive at the following approximate expression:

$$\varepsilon_{R3} = 2D_+ \left[ -1 + \tilde{\lambda}_0(2N+l-1)\frac{\pi}{2} \right], \quad (30)$$

where

$$\tilde{\lambda}_0 = \lambda_0 \left[ \frac{\mu}{\mu_{g3}^*} \right]^{1/2} \quad (31)$$

and  $\mu_{g3}^*$  is calculated from the expression of

$$\mu_{g3}^* = \mu[1 + (\varepsilon - D_-)(2\mu c^2)^{-1}] \quad (32)$$

by using for the energy the corresponding nonrelativistic expression [9]

$$\varepsilon_{NR3} = 2D_+ \left[ -1 + \lambda_0(2N+l-1)\frac{\pi}{2} \right]. \quad (33)$$

Expressions (30) and (33) gave usually poor results in the cases we studied. However, an alternative expression which gives considerably improved results in a variety of cases (see below) may be derived by using expression (17) and the following expansion for the  $\arcsin(1-z)$  (see expression 4.4.42 of Ref. [12]):

$$\begin{aligned} \arcsin(1-z) &= \frac{\pi}{2} \\ &- (2z)^{1/2} \\ &\times \left[ 1 + \sum_{k=1}^{\infty} \frac{1(3)5 \cdots (2k-1)}{2^{2k}(2k+1)k!} z^k \right], \end{aligned} \quad (34)$$

$|z| < 2$ .

We write, on the basis of Eqs. (17) and (34),

TABLE I. Energy eigenvalues of various states obtained with  $D_+ = 30, 55$  MeV,  $D_- = 300$  MeV and various values of  $R$  ( $R = 1.01 A_{\text{core}}^{1/3}$  fm). The values (in MeV) obtained with the numerical solution of the eigenvalue equation (12) are denoted by  $\varepsilon_{ex}$  while those obtained with the approximate expressions by  $\varepsilon_{R1}$  and  $\varepsilon_{R2}$  (see text for these expressions and also for the expressions of  $\lambda_0$ ,  $nR$ , and  $n_0R$ ).

$A_{\text{core}}$	$1s_{1/2}$							$1p_{3/2}$					$1d_{5/2}$					
	$R$	$\lambda_0$	$nR$	$n_0R$	$-\varepsilon_{ex}$	$-\varepsilon_{R1}$	$-\varepsilon_{R2}$	$nR$	$n_0R$	$-\varepsilon_{ex}$	$-\varepsilon_{R1}$	$-\varepsilon_{R2}$	$nR$	$n_0R$	$-\varepsilon_{ex}$	$-\varepsilon_{R1}$	$-\varepsilon_{R2}$	
12	2.31	0.35	2.14	1.76	11.2	9.2	11.8											
15	2.49	0.31	2.21	2.07	13.1	11.6	13.4											
39	3.45	0.22	2.47	3.61	19.8	19.4	19.8	3.4	2.5	9.5	5.5	9.0						
50	3.72	0.21	2.50	4.03	21.1	20.8	21.1	3.5	3.0	11.9	8.8	10.9	4.1	1.1	1.6			
88	4.49	0.17	2.60	5.16	23.6	23.5	23.6	3.7	4.3	16.7	14.8	15.6	4.7	3.1	8.4			
137	5.21	0.15	2.68	6.18	25.1	25.1	25.1	3.8	5.5	19.7	18.3	18.7	4.8	4.5	13.0	8.8	10.5	
207	5.98	0.13	2.72	7.27	26.3	26.2	26.3	3.9	6.6	21.9	21.0	21.1	4.9	5.8	16.5	13.5	14.3	

TABLE II. Energy eigenvalues of various states obtained with  $D_+ = 30.55$  MeV,  $D_- = 300$  MeV, and various values of  $R$  ( $R = 1.01 A_{\text{core}}^{1/3}$  fm). The values (in MeV) obtained with the numerical solution of the eigenvalue equation (12) are denoted by  $\epsilon_{\text{ex}}$  while those obtained with the approximate expression by  $\epsilon_{R4}$  (see text).

$A_{\text{core}}$	$s_{1/2}$		$p_{3/2}$		$p_{1/2}$		$d_{5/2}$		$d_{3/2}$	
	$-\epsilon_{R4}$	$-\epsilon_{\text{ex}}$	$-\epsilon_{R4}$	$-\epsilon_{\text{ex}}$	$-\epsilon_{R4}$	$-\epsilon_{\text{ex}}$	$-\epsilon_{R4}$	$-\epsilon_{\text{ex}}$	$-\epsilon_{R4}$	$-\epsilon_{\text{ex}}$
12	11.3	11.2								
15	13.2	13.1								
19	15.1	15.0	1.4	1.8	0.3	0.5				
27	17.6	17.5	4.4	5.6	3.2	4.5				
31	18.5	18.4	5.8	7.12	4.7	6.1				
39	19.8	19.8	8.1	9.5	7.3	8.7				
50	21.1	21.1	10.6	11.9	9.9	11.3				
88	23.6	23.6	15.5	16.7	15.2	16.3	5.5	8.4	4.5	7.5
137	25.2	25.1	18.7	19.7	18.5	19.4	10.3	13.0	9.6	12.4
207	26.3	26.3	21.1	21.9	21.0	21.8	14.2	16.5	13.8	16.2

$$(2N + l) \frac{\pi}{2} - nR = \arcsin(\lambda_R nR)$$

$$\simeq \frac{\pi}{2} - (2z)^{1/2} \left[ 1 + \frac{z}{12} \right], \quad (35)$$

where  $\lambda_R nR = 1 - z$ . This equation may be easily solved to a good approximation with respect to  $1 - z$  for  $z$  sufficiently small. Such a procedure has not been followed, to our knowledge, even in the nonrelativistic case. The final result for the energy eigenvalue is

$$\epsilon_{R4} = -D_+ + \frac{\hbar^2}{2\mu_g^*} \frac{\theta_{NI}^2}{R^2}, \quad (36)$$

where

$$\theta_{NI} = \left\{ \frac{(4\lambda_R - 3\alpha_{NI})}{(\lambda_R^2 - 3)} \right. \\ \left. \times \left[ 1 + \left[ 1 - \frac{(\lambda_R^2 - 3)(7 - 3\alpha_{NI}^2)}{(4\lambda_R - 3\alpha_{NI})^2} \right]^{1/2} \right] \right\}, \quad (37)$$

with  $\alpha_{NI} = (2N + l - 1)(\pi/2)$ .

The energies entering  $\mu_g^*$  and  $\lambda_R$  may be evaluated by using for  $\epsilon$  the  $\epsilon_{NR4}$  which is of the same structure as (36) but with  $\mu$  instead of  $\mu_g^*$  and with  $\lambda_0$  instead of  $\lambda_R$  in the expression of  $\theta_{NI}$ .

In order to test the accuracy of the approximate expressions  $\epsilon_{R1}$  and  $\epsilon_{R2}$ , numerical calculations have been performed and the results were compared with those obtained by solving numerically the eigenvalue equation (12). The following values of the parameters were used (see Ref. [5]):  $D_+ = 30.55$  MeV,  $D_- = 300$  MeV, and  $R = r_0 A_{\text{core}}^{1/3}$  ( $r_0 = 1.01$  fm),  $A_{\text{core}}$  being the mass number of the core nucleus. These are rather reasonable values for the potential parameters of a  $\Lambda$  particle in its ground state in hypernuclei. It should be noted that there is not much difference if the values  $D_+ = 30.77$  MeV,  $D_- = 443$  MeV, and  $r_0 = 1.022$  fm are used instead.

The results obtained for the  $1s_{1/2}$ ,  $1p_{3/2}$ , and  $1d_{5/2}$  states and for various values of  $R$  (and therefore of  $\lambda_0$ ) are displayed in Table I. The results for the states  $1p_{1/2}$  and  $1d_{3/2}$  are usually rather similar. The smallest value of  $A_{\text{core}}$  used corresponds to  $^{13}_{\Lambda}\text{C}$  while the largest to  $^{208}_{\Lambda}\text{Pb}$ . In each case the values of the "exact" relativistic energy  $\epsilon_{\text{ex}}$  for the rectangular potentials that is the one obtained by solving numerically the eigenvalue equation (12) and the approximate ones  $\epsilon_{R1}$  and  $\epsilon_{R2}$  are shown. In addition the quantities  $nR$  and  $n_0R$  calculated with  $\epsilon_{\text{ex}}$  are also displayed. It is seen from the results of this table that for the  $1s$  and  $1p$  states and mainly for the larger values of  $R$  which correspond also to larger values of  $nR$  and  $n_0R$  the approximate expressions  $\epsilon_{R1}$  and  $\epsilon_{R2}$  are good approximations to  $\epsilon_{\text{ex}}$ . From the same table it is also seen that the results with  $\epsilon_{R2}$  are better compared to those obtained with  $\epsilon_{R1}$ . In some cases the improvement is considerable.

In Table II the results obtained with  $\epsilon_{R4}$  are displayed for various states and values of  $R$  and are compared with those obtained with the numerical solution of the eigenvalue equation. It is seen that for the ground state the accuracy of  $\epsilon_{R4}$  is very good both for the smaller and for the larger values of  $R$ . We further observe from both tables that for the higher states the accuracy of the various approximate expressions is deteriorating quite rapidly. It should be noted, however, that the accuracy depends on the values of  $D_+$  and  $R$ . If in a physical problem the values of these quantities were larger, the accuracy for each state should have been improved.

We may conclude that the analytic expressions  $\epsilon_{R1}$  and  $\epsilon_{R2}$  give, in a number of cases, single-particle energy values which are fairly close to those obtained from the numerical solution of the eigenvalue equation, derived by means of the Dirac equation with potentials  $U_S$  and  $U_V$  of rectangular shape and of the same radius. Expression  $\epsilon_{R4}$  gives in general better results than  $\epsilon_{R1}$  (or than  $\epsilon_{R2}$ , for the ground state).

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