Coulomb energy of a proton in the relativistic nuclear shell model

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We examine the Dirac equation for a proton in a nucleus, with a shell-model potential consisting of nuclear and Coulomb parts. When the Dirac equation is reduced to a Schrödinger-like equation, the effective potential W in it exhibits two Coulomb-related effects that are absent in the usual nonrelativistic treatment: (I) W contains a Coulomb-nuclear interference term; (II) W depends strongly on the proton energy, which in turn depends on the Coulomb energy. If the shell-model potential consists of a strongly attractive Lorentz scalar and a strongly repulsive Lorentz vector, effect I by itself is very large. However, effect II counteracts effect I, leaving a small yet significant decrease in the Coulomb energy as compared with its nonrelativistic counterpart.

I. INTRODUCTION

Consider the relativistic nuclear shell model. The potential for a proton consists of nuclear and Coulomb parts. Let us assume that the potential is a sum of an attractive Lorentz scalar S and a repulsive (zeroth component of) Lorentz vector V, and that S and V are both large in magnitude. Such a combination of S and V is strongly hinted at by the successful Dirac phenomenology.[1-3] We write V for proton as $V=V_N+V_C$, where V_N is the nuclear part and V_C is the Coulomb potential. We also consider a fictitious "neutral proton" for which $V=V_N$. We refer to it as neutral proton rather than neutron because in a realistic shell model V_N should differ between proton and neutron. For light to medium nuclei, however, the difference between the neutral proton and neutron would not be very significant.

If we reduce the Dirac equation to the nonrelativistic Schrödinger equation by means of the Foldy-Wouthuysen transformation, the nonrelativistic potential that emerges is $S+V$ plus corrections of higher order with respect to $1/m$. However, S and V_N within the nucleus are believed to be 300–400 MeV in magnitude and, although $S+V_N$ is much smaller than the nucleon rest mass m, S and V_N are individually not.[4] Hence, the nonrelativistic reduction of the Dirac equation by means of the Foldy-Wouthuysen transformation is misleading in this case and one must solve the Dirac equation as such. Even then, the Dirac equation can be reduced to a Schrödinger-like equation with an effective potential W. As it turns out the W for proton contains a term $-V_N V_C/m$. For $V_N \simeq 400$ MeV, we find $-V_N V_C/m \simeq -0.4V_C$; hence, this interference term reduces the Coulomb potential within the nucleus by about 40%. This would result in an enormous reduction of the Coulomb energy. Would this be true? This is the riddle that motivated us to scrutinize relativistic effects on the Coulomb energy.[5]

W has another aspect that is of crucial importance regarding the Coulomb energy: W is strongly energy dependent. W becomes less attractive as the binding energy decreases. The Coulomb energy decreases the binding energy, making W less attractive. We refer to the effect due to the Coulomb-nuclear interference as effect I, and that due to the energy dependence of W as effect II. Although effects I and II are individually very large, they counteract each other leaving a small yet significant reduction of the Coulomb energy of a bound proton as compared with its nonrelativistic counterpart.

In order to avoid possible confusion, let us emphasize the "novelty" of the two effects. Suppose one takes the usual nonrelativistic approach with the shell-model potential for the proton, $V_{N,\mathrm{NR}}+V_C$, where $V_{N,\mathrm{NR}}$ is the nuclear part of the potential. If one solves the Schrödinger equation with this potential, the solution, of course, contains Coulomb-nuclear interference effects. This should not be confused with effect I in which the Coulomb-nuclear interference shows up in the potential W for the Schrödinger-like equation; it is there before the equation is solved. One may say that $V_{N,\mathrm{NR}}$ contains Coulomb-nuclear interference effects if $V_{N,\mathrm{NR}}$ is, say, a Hartree-Fock potential. This is correct, but this is not of relativistic origin. We are ignoring this aspect of the nuclear shell-model potential. A similar point may be raised regarding effect II. The Hartree-Fock potential is nonlocal and energy dependent. This is due to many-body effects, and should be distinguished from our effect II, which is of a relativistic origin. In a more realistic calculation, these many-body effect must be incorporated.

In Sec. II, we illustrate how effects I and II are individually large and how they tend to cancel. We discuss implications of the results in Sec. III.

II. MODEL

We start with the Dirac equation

$$[\boldsymbol{\alpha}\cdot\mathbf{p}+\beta(m+S)+V]\psi=E\psi\ . \tag{2.1}$$

We use units such that $c=\hbar=1$ and the standard notation.[6] The Dirac wave function ψ can be written in the form of a two-component function, the upper and lower components being G and F, respectively. Then Eq. (2.1) becomes

$$F'-\kappa F/r=-(E-V-m-S)G\ , \tag{2.2}$$

$$G'+\kappa G/r=(E-V+m+S)F\ , \tag{2.3}$$

where $F'=dF/dr$, and κ is related to the angular momentum j by $\kappa=\pm(j+\frac{1}{2})=\pm1, \pm2, \ldots$. If we eliminate F in favor of G, and define χ by

$$\chi=(E-V+m+S)^{-1/2}G\ , \tag{2.4}$$

Eqs. (2.2) and (2.3) can be reduced to

$$-\chi''/(2m)+W\chi=[(E^2-m^2)/(2m)]\chi\ , \tag{2.5}$$

which is of the form of the Schrödinger equation except that E is the relativistic energy including the rest mass m. The effective potential W is given by

$$W=S+\frac{2EV+S^2-V^2}{2m}+\frac{\kappa(1+\kappa)}{2mr^2} -\frac{1}{8mD}\left[2D''-\frac{4\kappa D'}{r}-\frac{3D'^2}{D}\right], \tag{2.6}$$

where

$$D=E-V+m+S\ . \tag{2.7}$$

The reduction of the Dirac equation to the Schrödinger-like equation given above is exact. If S and V are both much smaller than m, the leading term in the $1/m$ expansion of W is $S+V$, as expected. In comparing the W's for proton and neutral proton, we denote them by W_p and W_n, respectively: W_p (W_n) is given by Eq. (2.6) with $V=V_N+V_C$ ($V=V_N$).

There are two crucial features to be observed. If one works entirely in nonrelativistic quantum mechanics, one would think that W_p and W_n are simply related by $W_p=W_n+V_C$. This is not the case for W_p and W_n. Secondly, unlike the potentials usually used in nonrelativistic calculations, W is energy dependent. In fact, for the combination of strong S and V, W depends on energy strongly. Effects I and II mentioned in Sec. I are due to these two features, respectively.

For the model interaction, we assume the following: S and V_N are of the form

$$S(r)=-g_S f(r),\quad V(r)=g_V f(r)\ , \tag{2.8}$$

where $f(r)$ is the Woods-Saxon function for the nuclear density,

$$f(r)=\frac{1+e^{-R/a}}{1+e^{(r-R)/a}}\ . \tag{2.9}$$

Parameter a is related to the surface thickness s by[7]

$$s=4a\ \ln 3\simeq 4.40a\ . \tag{2.10}$$

For the strength parameters g_S and g_V, for example, Noble took $g_S=420$ MeV and $g_V=328$ MeV.[8] He chose these values such that W conforms to the standard empirical low-energy ($E\simeq m$) shell-model parameters. With his parameters, however, we found that the single-particle binding energy tends to be somewhat too large. This is because Noble used W for $E=m$ (instead of the W for the average value of E of bound nucleons) in determining the strength parameters. Instead, we take

$$g_S=420\text{ MeV},\quad g_V=340\text{ MeV}\ . \tag{2.11}$$

Then the ground-state energy comes out about right. For the Coulomb potential we use the one for a sphere of radius R with uniform charge $(Z-1)e$, i.e., $V_C(r)=(Z-1)e^2/r$ for $r>R$, and

$$V_C(r)=\frac{(Z-1)e^2}{2R}\left[3-\frac{r^2}{R^2}\right]\quad\text{for } r<R\ . \tag{2.12}$$

We consider the following two sets of parameters,[2] one corresponding to ^{208}Pb,

$$Z=82,\quad R=6.5\text{ fm},\quad s=2.3\text{ fm}\ , \tag{2.13}$$

and the other to ^{40}Ca,

$$Z=20,\quad R=3.64\text{ fm},\quad s=2.5\text{ fm}\ . \tag{2.14}$$

We refer to the above two sets of the parameters as models Pb and Ca, respectively. We use the nucleon mass $m=939$ MeV.

We have solved Eq. (2.5) with W_p and with W_n for the ground ($\kappa=-1$) and the first excited ($\kappa=1$) states; we require the consistency with respect to energy E such that the E in W of Eq. (2.6) is the eigenvalue E determined by Eq. (2.5). Unless otherwise specified, by W_p we mean $W_p(E_p)$, where E_p is the energy determined as we have just stated.

We compare the results for W_p with its nonrelativistic counterpart. The latter is obtained by using

$$W_{p,\mathrm{NR}}=W_n+V_C \tag{2.15}$$

in Eq. (2.5). Here it is important to specify the W_n in $W_{p,\mathrm{NR}}$ clearly. This W_n is for $E=E_n$, where E_n is the energy determined earlier using W_n alone; the energy that enters in this W_n is fixed once and for all. Unlike the relativistic version W_p, $W_{p,\mathrm{NR}}$ is hence *energy independent*.

Table I lists the binding energies calculated in three ways, i.e., using W_p, W_n, and $W_{p,\mathrm{NR}}$, for the two models.

TABLE I. The binding energies in MeV determined by the potentials W_p, $W_{p,\mathrm{NR}}$, and W_n.

State	Potential	Pb	Ca
$\kappa=-1$	W_p	47.67	46.93
	$W_{p,\mathrm{NR}}$	46.10	46.27
	W_n	71.64	56.70
$\kappa=1$	W_p	39.84	25.77
	$W_{p,\mathrm{NR}}$	38.53	25.37
	W_n	62.91	34.82

The energies determined by W_p and W_n are what we have been calling E_p and E_n, respectively. Let $E_{p,\mathrm{NR}}$ denote the energy determined by $W_{p,\mathrm{NR}}$.[9] The empirical binding energy of the proton in the ${}^1S_{1/2}$ state of Ca is 55 ± 9 MeV,[10] which can be compared with $E_p=46.93$ MeV of Ca of Table I. The Coulomb energy of the proton is given by[11]

$$E_C=E_p-E_n \; , \tag{2.16}$$

and its nonrelativistic counterpart by

$$E_{C,\mathrm{NR}}=E_{p,\mathrm{NR}}-E_n \; . \tag{2.17}$$

Table II lists E_C, $E_{C,\mathrm{NR}}$, and the relativistic correction $E_C-E_{C,\mathrm{NR}}$. This correction is as important as various other corrections to the Coulomb energy. Consider, for example, the ground state of Pb. The relativistic correction is -1.57 MeV, which is 6.6% of $E_C=23.96$ MeV. This can be compared with the proton-neutron atomic mass difference of 0.78 MeV, and the exchange correction, which is of the order of 4% of the Coulomb energy for ^{208}Pb.[11,12] For the ground state of Ca, the relativistic correction is -0.66 MeV, which is 6.8% of $E_C=9.76$ MeV. The exchange correction to the Coulomb energy is about 10%.[12,13]

Figure 1 shows the potentials (for the ground state with $\kappa=-1$) for model Pb, and Fig. 2 those for model Ca. The small dip in the potential near the origin is due to the term proportional to D'/r in W of Eq. (2.6); it is noticeable only for model Ca of Fig. 2. Figures 3–5 are all for model Pb. Figure 3 compares V_C and $W_p(E_p)-W_n(E_p)$; here, note that $W_n(E_p)$ is for the same energy as for W_p. The difference between the two curves shows the reduction of the Coulomb potential within the nucleus due to the Coulomb-nuclear interference; this is a relativistic effect. Figure 4 exhibits the energy dependence of W_n. In a consistent calculation, the potential that binds the neutral proton is $W_n(E=E_n)$, but if we artificially substitute energy $E=E_p$ of $E=m$, $W_n(E)$ changes as shown. Crudely speaking, the reduction of the Coulomb repulsion from V_C to $W_p(W_p)-W_n(E_p)$, shown in Fig. 3, is almost compensated by the reduction of attraction from $W_n(E_n)$ to $W_n(E_p)$ of Fig. 4. Finally, Fig. 5 compares $W_p(E=m)$ and $W_n(E=m)+V_C$. We will discuss Fig. 5 in the next section.

TABLE II. The Coulomb energies E_C and $E_{C,\mathrm{NR}}$, and the relativistic correction $E_C-E_{C,\mathrm{NR}}$, in units of MeV.

State		Pb	Ca
$\kappa=-1$	E_C	23.96	9.76
	$E_{C,\mathrm{NR}}$	25.54	10.43
	$E_C-E_{C,\mathrm{NR}}$	-1.57	-0.66
$\kappa=1$	E_C	23.07	9.05
	$E_{C,\mathrm{NR}}$	24.39	9.46
	$E_C-E_{C,\mathrm{NR}}$	-1.32	-0.40

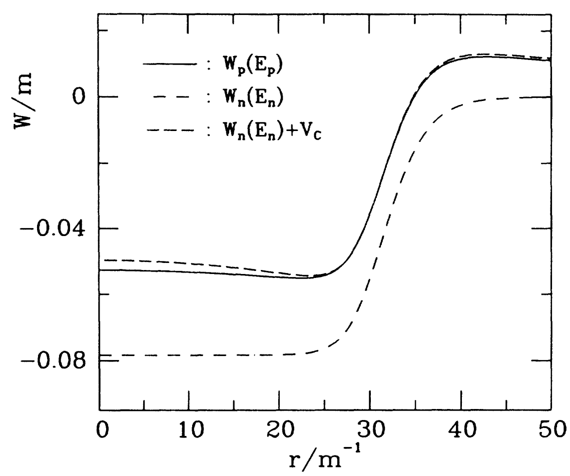

FIG. 1. The effective potentials W_p and W_n in the Schrödinger-like equation for model Pb, compared with the nonrelativistic version $W_{p,\mathrm{NR}}$.

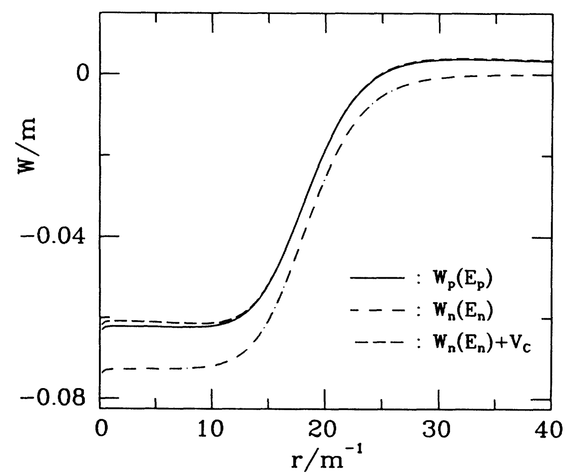

FIG. 2. The same as for Fig. 1, but for model Ca.

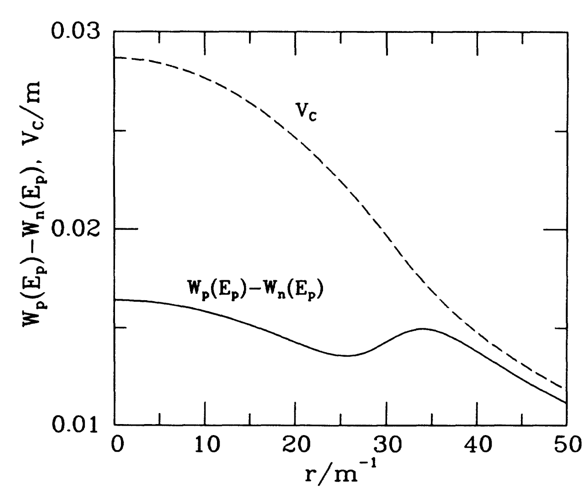

FIG. 3. Comparison between the Coulomb potential V_C and the (Coulomb plus Coulomb-nuclear interference term) of the relativistic model Pb.

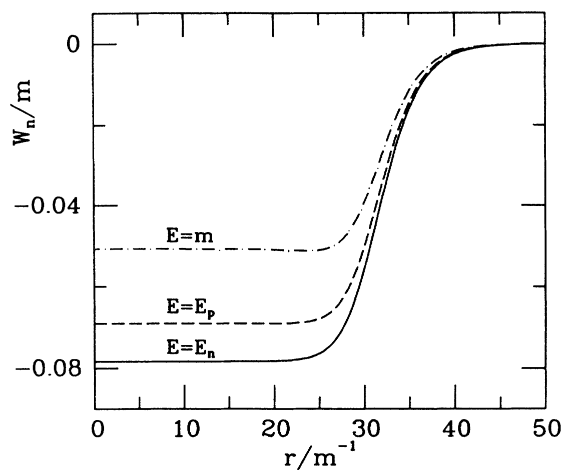

FIG. 4. The energy dependence of W_n for model Pb; E_n is the energy of the "neutral proton" determined by $W_n(E_n)$, while E_p is the energy of the proton determined by $W_p(E_p)$.

III. DISCUSSIONS

We examined the Coulomb energy of a proton in a relativistic shell model and found that there are two effects, I and II, which are both absent in the usual nonrelativistic treatment. For the relativistic shell-model potential consisting of strong S and V, the two effects are individually very large but they counteract each other resulting in a small yet significant departure from the nonrelativistic treatment. The net effect on the Coulomb energy is comparable with and of the same sign as the exchange effect. Since there are two large effects involved, the variation of the Coulomb energy from one nucleus to another may be more appreciable in a relativistic model than in its nonrelativistic counterpart. This should be remembered in examining the Coulomb energies of very heavy nuclei.

The Coulomb energies of nuclei have been a subject of considerable interest for many years, in particular since

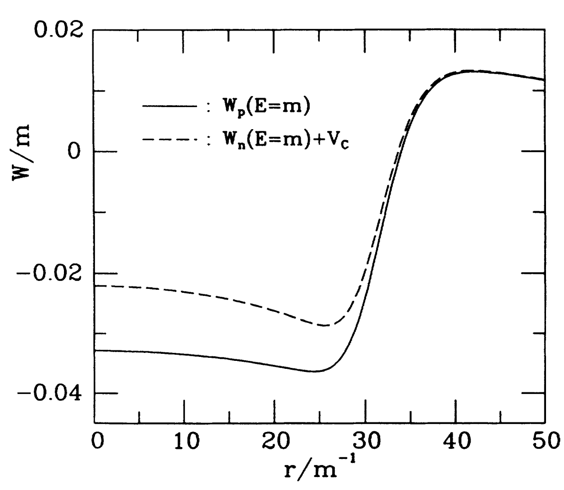

FIG. 5. The proton-nucleus potential $W_p(E=m)$ for model Pb compared with its nonrelativistic analog $W_n(E=m)+V_C$.

Nolen and Schiffer pointed out a systematic discrepancy regarding the Coulomb energies of a large number of nuclei.[12] Also, there is a well-known discrepancy regarding the difference between the binding energies of ^{3}H and ^{3}He. Theoretical estimates based on charge symmetric nucleon-nucleon interactions account for about 90% of the empirical value of the binding-energy difference of this pair of mirror nuclei.[14] The relativistic effect will probably reduce the Coulomb energy of ^{3}He, resulting in an enhancement of the discrepancy. This discrepancy calls for charge-symmetry-breaking (CSB) nuclear interactions of some other origins, somewhat stronger than those considered so far.

In order to avoid possible confusion regarding the usage of the term CSB, let us make the following point clear. In this paper, we assumed that the relativistic nuclear interaction $(S+V_N)$ is charge symmetric. However, when the relativistic model is transcribed into the form of an effective nonrelativistic model as we have done, the effective nonrelativistic interaction that emerges obtains a CSB term like $-V_N V_C/m$ of effect I. This illustrates the point that what one means by CSB depends on the framework in which one chooses to work. This kind of symmetry breaking occurs whenever some degrees of freedom are eliminated in a theory with a higher symmetry. The CSB effect that we mentioned towards the end of the preceding paragraph is the one which exists even in the relativistic interaction; for example, the nuclear interaction mediated by the ρ-ω mixing or by the γ-π exchange.[15]

We have seen that effects I and II on the Coulomb energy are individually large but they almost cancel. This prevents the Coulomb energy of the relativistic model from being drastically reduced than its nonrelativistic counterpart. This is an answer to the riddle that motivated us to examine the Coulomb energy in the relativistic Hartree-Fock calculations including the Coulomb interaction, and the features that we have discussed must be there implicitly in these calculations.[2,3]

In scattering problems, however, effect II is absent in the sense that the energy is externally fixed rather than determined by the interaction. In principle, therefore, one would be able to see effect I in its unsuppressed form. We can think of two model potentials for proton-nucleus scattering. One is derived from a relativistic interaction as we did, say, for $E=m$; this is the $W_p(E=m)$ shown in Fig. 5. The other is its nonrelativistic analog defined by $W_n(E=m)+V_C$, also shown in Fig. 5. The difference between these two potentials is a manifestation of effect I; the difference amounts to about 40% of V_C within the nucleus. To detect consequences of this difference may be rather impractical for nucleon-nucleus scattering. However, one can imagine a similar situation for nucleon-nucleon scattering. For the nucleon-nucleon system, the singlet scattering lengths for pp and nn are both known; the uncertainty is still rather large for nn though. For these quantities, there will be a CSB effect of type I (but not II) that arises in nonrelativistic reduction of a relativistic equation. Recall that all analyses of CSB effects with respect to low-energy nucleon-nucleon scattering have been done within the nonrelativistic framework using the Schrödinger equation. We will discuss this problem in a separate paper.[16]

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[9]Let us reiterate that the energy that is substituted into the W_n of $W_{p,\mathrm{NR}}$ of Eq. (2.14) is the energy determined by using W_n alone.

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