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Improved Coulomb Potential*

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Abstract

An improved Coulomb potential is presented for use in the relativistic Schrödinger equation. This potential takes into account contributions of all two-photon exchange diagrams and gives the lowest-order relativistic corrections to the static Coulomb potential for arbitrary masses of the two particles. The cases spin 0-spin 0, spin 0-spin $\frac{1}{2}$, and spin $\frac{1}{2}$-spin $\frac{1}{2}$ are considered. When the mass of one of the particles goes to infinity, then the well-known corrections to the binding energy and to the phase shifts as obtained with either the Klein-Gordon or the Dirac equation are reproduced.

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The electromagnetic interaction between two charged point particles is for many purposes not accurately enough describd by the $1/r$ Coulomb potential inserted in the nonrelativistic Schrödinger equation. Often one needs relativistic corrections. Some of such corrections can be obtained when one uses the Klein-Gordon (KG) or the Dirac equation. These equations suffer from the disadvantage that they are essentially one-particle equations and not very well suited for a two-body problem. For example, recoil corrections are not easily obtained. Another way to improve the nonrelativistic descirption is to go to the Breit equation. [1] When used in coordinate representationthis equation suffers from the difficulty that it is really a fourth-order differential equation because of the correction term $-p^4/8m^3$ to the kinetic energy.

In this Letter we present an improved Coulomb potential which gives correctly the lowest-order relativistic and recoil corrections to the scattering amplitude, phase shifts, and bound-state energies, when this potential is inserted in the "relativistic" Schrödinger equation. We do this for the following cases: spin 0-spin 0, spin $\frac{1}{2}$-spin 0, and spin $\frac{1}{2}$-spin $\frac{1}{2}$. This improved potential takes into account contributions of the planar- and crossed-box two-photon-exchange diagrams, and in the case of spin 0 also of the seagull graphs. This relativistic Schrödinger equation is the coordinate-space version of the Blankenbecler-Sugar-Logunov-Tavkhelidze (BSLT) equation. [2–5] The (nonrelativistic as well as relativistic) Schrödinger equation in the coordinate representation is

$$(\Delta + p^2)\psi(\vec{r}) = 2mV\psi(\vec{r})$$

where $m = m_1 m_2/(m_1 + m_2)$ for a two-body system with masses m_1 and m_2. The difference between the nonrelativistic and relativistic Schrödinger equation is the relation between the center of mass (c.m.) relative momentum p and the c.m. energy E. In the nonrelativistic case $E = p^2/2m$ and relativistically $E = (p^2 + {m_1}^2)^{1/2} + (p + {m_2}^2)^{1/2} - m_1 - m_2$. This improved Coulomb potential has been constructed [6,7] in order to give an accurate description of the low-energy proton-proton scattering experiments. In that case the vacuum polarization potential [8] has to be added and one must also include form factors to describe the extended electric and magnetic charge distributions of the protons. [9] However, we can think of several other cases where this potential could be very useful.

The derivation [7] of this improves Coulomb potential will be published elsewhere, but let us indicate how it was obtained. We follow the well-known road [4,5] from the Bethe-Salpeter equation [10] for the relativistic scattering amplitude via the BSLT equation to a potential V for the relativistic Schrödinger equation. This potential is constructed in a way that it reproduces the relativistic scattering amplitude (its pole positions are the bound-state energies) as well as possible. When one wants to obtain in a consistent way relativistic corrections to the Coulomb potential one must calculate in addition to the one-photon-exchange diagrams also the two-photon-exchange diagrams. The pseudopotential W for the BSLT equation is to order e^4 given by [11]

$$W = M_1 + M_{\rm V} + (M_{\rm X} + M_{\rm V} + M_{\rm II} - M_1 g M_1). \tag{1}$$

The contributions to this potential W come from one-photon exchange M_1 (where we can include the vacuum polarization $M_{\rm VP}$) and from two-photon exchange like planar-box $M_{\rm II}$, crossed-box $M_{\rm X}$, and in the case of spin 0 also the seagull graphs $M_{\rm V}$. When one computes these different contributions then one notices first of all a large cancellation between $M_{\rm II}$ and the twice-iterated one-photon exchange $M_1 g M_1$, and also a sizable cancellation [12] between $M_{\rm X}$ and the rest of $M_{\rm II}$. Next we use the freedom [13] still existing in the choice of the off-shell behavior of the BSLT propagator g. We choose this propagator in such a way that we obtain in the low-energy region *another* cancellation between the sums of all two-photon-exchange contributions $M_{\rm II} + M_{\rm X} + M_{\rm V}$ and the twice-iterated one-photon-exchange contribution to W [the term in parentheses in Eq. 1] vanishes in the order of accuracy of our calculation. Then our pseudopotential $W \approx M_1 + M_{\rm VP}$ does not contain two-photon-exchange contributions anymore. However, this statement is not true for our improved Coulomb potential V for the relativistic Schrödinger equation. The off-shell behavior of this potential [the term proportional to b in Eq. 3] is such that by iteration it will give the main contribution of the two-photon-exchange diagrams.

The off-shell matrix elements of the improved Coulomb potential (neglecting the vacuum polarization) for two spin-0 particles with point charges $Z_1 e$ and $Z_2 e$ are

$$(\vec{\rm p}_f|V|\vec{\rm p}_i) = (Z_1 Z_2 e^2/k^2)(a + X_0/4m^2), \tag{2}$$

with

$$X_0 = b(q^2 + \tfrac{1}{4}k^2 - p^2) + c_0 k^2 + 4d(\vec{\rm q}\cdot\vec{\rm k}/k)^2. \tag{3}$$

We have introduced the vectors

$$\vec{\rm q} = (\vec{\rm p}_f + \vec{\rm p}_i)/2, \quad \vec{\rm k} = \vec{\rm p}_f + \vec{\rm p}_i, \quad \vec{\rm n} = \vec{\rm p}_i \times \vec{\rm p}_f = \vec{\rm q}\times\vec{\rm k}.$$

The coefficients a to d are

$$\begin{aligned} a &= (E_1E_2 + p^2)/m(E_1+E_2) \approx 1 + p^2(1 - m/M)/2m^2, \\ b &= 1 - \lambda, \\ c_0 &= -m/M, \\ d &= \lambda, \end{aligned} \tag{4}$$

where $M = m_1 + m_2$ and $E_1 = ({m_1}^2 + p^2)^{1/2}$. Equations 2 and 3 indicate the approximations made. We include in V all corrections to the static Coulomb potential $V_{\rm C}$ which are of order $[(\text{momentum})^2/m^2]V_{\rm C}$. The improved Coulomb potential depends on the gauge in which we perform the calculations and on the definition of the relative four-momentum. [5] This can be expressed by only one arbitrary parameter λ in the potential. Our lowest-order corrections to measurable quantities (like binding energies and cross sections) are *independent* of λ.

When particle 1 has spin $\frac{1}{2}$ instead of spin 0 and a magnetic moment $\vec{\mu}_1 = (1 + \kappa_1)(Z_1 e/m_1)\vec{\rm s}_1$, with $\vec{\rm s}_1 = \frac{1}{2}\vec{\sigma}_1$ the spin, then we must add to X_0 of Eq. 3 the term

$$X_1 = c_1 k^2 + e_1 i\vec{\rm s}_1\cdot\vec{\rm n}, \tag{5}$$

where

$$c_1 = -\tfrac{1}{2}(1 + 2\kappa_1)(m/m_1)^2, \tag{6a}$$

$$e_1 = -2(1 + 2\kappa_1)(m/m_1)^2 - 4(1+\kappa_1)m/M. \tag{6b}$$

Here e_1 gives the spin-orbit interaction and c_1 the corresponding Darwin term of particle 1.

When also particle 2 has spin $\frac{1}{2}$ instead of spin 0, then we must add to X moreover the terms

$$\begin{aligned}X_2 &= c_2 k^2 + e_2 i \vec{\mathrm{s}}_2 \cdot \vec{\mathrm{n}},\\ X_{12} &= f[(\vec{\sigma}_1 \cdot \vec{\mathrm{k}})(\vec{\sigma}_2 \cdot \vec{\mathrm{k}}) - k^2 \vec{\sigma}_1 \cdot \vec{\sigma}_2],\end{aligned}$$

with $f = (1+\kappa_1)(1+\kappa_2)m/M$ and c_2 and e_2 given by Eq. 6. Here X_2 gives the spin-orbit interaction and the Darwin term of particle 2 and X_{12} the tensor and spin-spin interaction between the two spin-$\frac{1}{2}$ particles.

The improved Coulomb potential in the coordinate representation is

$$V = V_1 + V_2 = Z_1 Z_2 \alpha'/r + (Z_1 Z_2 \alpha/4m^2)\phi, \tag{7}$$

with

$$\begin{aligned}\phi = &-bp^2/r - \tfrac{1}{2}b[\Delta(1/r) + (1/r)\Delta]\\ &+(c + d - \tfrac{2}{3} f \vec{\sigma}_1 \cdot \vec{\sigma}_2)4\pi\delta^3(\vec{\mathrm{r}})\\ &+(2dL^2 + e_1 \vec{\mathrm{L}} \cdot \vec{\mathrm{s}}_1 + e_2 \vec{\mathrm{L}} \cdot \vec{\mathrm{s}}_2 - fS_{12})/r^3.\end{aligned} \tag{8}$$

Here $\alpha = e^2/(4\pi)$, $\alpha' = \alpha a$, $c = c_0 + c_1 + c_2$, Δ is the Laplacian, $\vec{\mathrm{L}}$ the orbital angular momentum, and $S_{12} = (\vec{\sigma}_1 \cdot \vec{\mathrm{r}})(\vec{\sigma}_2 \cdot \vec{\mathrm{r}})/r^2 - \vec{\sigma}_1 \cdot \vec{\sigma}_2/3$.

The bound-state energies $E(n,l,j)$ for a hydrogenlike atom ($Z_1 Z_2 = -Z$) can easily be calculated by use of the potential ad given in Eqs. 7 and 8. In order to demonstrate the accuracy of this improved potential we will give these bound-state energies in an expansion in α. When particle 1 has either spin 0 or spin $\frac{1}{2}$ and particle 2 has spin 0, then up to α^4 we get

$$E(n,l,j) = -(m/2)(Z\alpha/n)^2[1 + (Z\alpha/n)^2 A], \tag{9}$$

with

$$A = -\frac{3}{4} + \frac{m}{4M} + \frac{2n}{2l+1}(b + d + \frac{1}{2}e_1) - \frac{n}{2j+1}e_1 + (c_0 + c_1 - \frac{1}{4}e_1)2n\delta(l,0). \tag{10}$$

We observe using Eqs. 4 and 6 that A is independent of λ, i.e., "gauge" inependent. For teo spin-0 particles Eq. 10 becomes

$$A = \frac{2n}{2l+1} - \frac{3}{4} + \frac{m}{4M} - \delta(l,0)2n\frac{m}{M}.$$

The first two terms represent the standard KG result [15] and the last two terms are corrections to this. For a system with spin $\frac{1}{2}$ and spin 0 we get

$$A = \frac{2n}{2j+1} - \frac{3}{4} + \frac{m}{4M} + \frac{4n(l-j)}{(2j+1)(2l+1)}\left[2\kappa_1\left(1 - \frac{m_1}{M}\right) - \left(\frac{m_1}{M}\right)^2\right] + 2\kappa_1 n\frac{m}{M}\delta(l,0).$$

This expression is valid for all values of m_1 and m_2. However, we have grouped the terms such that for the case $m_1 \ll m_2$ (like the H atom) the result can be compared with well-known results. The first two terms give the standard result as obtained with the Dirac equation. The third term is a well-known recoil correction. [16] The last two terms represent another recoil correction and the contribution to the Lamb shift due to the anomalous magnetic moment.

Not included in the binding energy is the contribution due to the vacuum polarization potential which is of order $\alpha(Z\alpha)^4 m^3/[m_e(Z\alpha M + m_e)^3]^{1/2}$, where m_e is the electron mass. However, this potential can easily be included. In that case the most important term not obtained with this potential is due to the mass renormalization. Its contribution to the binding energy is of the order $\alpha(Z\alpha)^4 \ln(Z\alpha)$.

The phase shifts due to this improved Coulomb potential can easily be calculated. To illustrate once more the accuracy of this improved potential we calculate in distorted-wave Born approximation explicitly the lowest order corrections to the nonrelativistic Coulomb phase shift $\sigma l^{(0)}(\eta) = \arg\Gamma(l+1+i\eta)$. Here $\eta = Z_1 Z_2 \alpha m/p = Z_1 Z_2 \alpha/v$ with v the nonrelativistic velocity in the c.m. system. The Schrödinger equation with the potential $v_1 = Z_1 Z_2 \alpha'/r$ can easily be solved. It leads to a phase shift $\sigma_l^{(0)}(\eta')$, where we have defined the modified Coulomb parameter [17]

$$\eta' = Z_1 Z_2 \alpha' m/p = Z_1 Z_2 \alpha/v_{\text{lab}}. \tag{11}$$

The total phase shift due to our improved Coulomb potential V we write as $\sigma_l = \sigma_l^{(0)}(\eta') + \rho_l$. The correction ρ_l can easily be calculated in distorted-wave Born approximation from the potential $V_2 = V - V_1$. Then

$$\tan\rho_1 = -\frac{2m}{p}\int_0^\infty dr F_l(\eta', pr) V_2 F_l(\eta', pr),$$

where $F_l(\eta', pr)$ is the regular Coulomb wave function.

In the case of scattering two spin-0 particles we find

$$\rho_l = -\frac{Z\alpha p}{2m}\lambda + \frac{Z\alpha Z\alpha'}{2l+1}\left(\frac{\pi}{2} - \frac{\partial\sigma_l^{(0)}(\eta')}{\partial l}\right) + \frac{Z\alpha p}{2M} C_0^2(\eta')\delta(l,0). \tag{12}$$

The first term in Eq. 12 is due to the $(\vec{\mathrm{q}}\cdot\vec{\mathrm{k}}/k)^2$ part of the potential. This gauge-dependent part of the phase shift is independent of l and is thus unobservable. The second term in Eq. 12 is in the limit $m_2 \to \infty$ exactly equal to the term that would be obtained when one solves the KG equation to the same order of accuracy. [15] The last term is an extra correction for s waves only.

It is also easy to calculate ρ_l in the case of spin $\frac{1}{2}$-spin 0 scattering. In order to compare with the exact solution of the Dirac equation we take $\kappa_1 = 0$ and in the limit $m_2 \to \infty$; then we get

$$\rho(l,j) = -\frac{Z\alpha p}{2m}\lambda + \frac{(Z\alpha)^2}{2j+1}\left(\frac{\pi}{2} - \frac{\partial\sigma_l^{(0)}}{\partial l} + \frac{j-l}{\eta}\right). \tag{13}$$

We see here again a gauge-dependent but unobservable part and a second part that agrees with the exact solution [15] of the Dirac equation expanded to the same order of accuracy. When $\kappa_1 \neq 0$ and/or $m_2 \neq \infty$ we find some corrections to Eq. 13.

The difference between the nonrelativistic Coulomb phase shift $\sigma_l^{(0)}(\eta)$ and the modified Coulomb phase σ_l is twofold. Firstly we have the replacement of η by η' in $\sigma_l^{(0)}$ and secondly we have the extra phase ρ_l.

What are the advantages of our potential? (i) The potential is for use in the very familiar Schrödinger equation. (ii) Relativistic as well as recoil corrections are included. Because the potential has a clear field-theoretic derivation one knows explicitly the approximations made. (iii) Extensions to higher spin particles can easily be postulated: Add the Darwin terms, the electric and magnetic multipole interactions, and the terms due to the Thomas presession, as is done in Eqs. 5 and 6 for the magnetic dipole. (iv) When one or both of the particles have extended charge distributions then the form factors can be included exactly. [9] By exactly we mean that the same type of cancellations as discussed here for the two-photon-exchange contributions to the potential V will also happen in that case. (v) Strong-interaction potentials can be added easily. Corrections to additivity can be calculated in principle. (vi) An improved Coulomb and vacuum polarization modified effecttive range expansion has been derived. [7]

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