Abstract

For the S-states of muonium and positronium, the hyperfine shifts to the order $\alpha^6$ of a recently derived two-fermion equation with explicit $CPT$-invariance are checked against the results of a nonrelativistic reduction, and the leading $\alpha^8$ shifts are calculated. An additional hyperfine operator is discovered which can milder the singularity for $r \to 0$ of the Dirac hyperfine operator, such that the resulting extended operator can be used nonperturbatively. The binding correction to magnetic moments is mentioned.

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I. INTRODUCTION

The energy levels of one-electron atoms are well described by the Dirac equation, particularly when the nuclear hyperfine operators are included, and when radiative corrections are computed from the vector potential operator that is part of the electron momentum operator (Erickson 1977). But the Dirac equation applies also to muonium ($e^-\mu^+$), where the “nucleus” is a structureless muon. A simple recoil correction reduces the electron mass $m_1$ by a factor $m_2/m = m_2/(m_1 + m_2)$, where $m_2$ is the muon mass. The resulting reduced mass $\mu_{nr} = m_1 m_2/m$ is familiar from the two-body Schrödinger equation, but apart from the limit $m_2/m \approx 1 - m_1/m_2$ (Braun 1973), the correctness of this factor in the Dirac equation has not been proven.

For positronium ($e^-e^+$), $m_2/m = 1/2$ excludes a perturbative treatment of recoil. In the past, precise calculations of muonium and positronium have used the Bethe-Salpeter equation, which treats both particles relativistically (Sapirstein and Yennie 1990). However, the complicated higher-order radiative corrections contain only few relativistic effects. An alternative method has been elaborated in which all relativistic effects are treated perturbatively, by effective operators added to the nonrelativistic two-body Schrödinger Hamiltonian $p^2/2\mu_{nr} + V(r)$ (Caswell and Lepage 1986). By this “nonrelativistic quantum electrodynamics method” (NRQED), the energy levels of muonium and positronium have been calculated to the order $\alpha^6$ (Pachucki 1997). To that order at least, all results of the Dirac equation with the above reduction factor are confirmed at the lowest nonvanishing power of $\mu_{nr}/m$, not...
only in the coarse and fine structures, but also in the hyperfine structure. In the calculation of the muonium hyperfine splitting, the term $\alpha^8\mu_{nr}^2/m$ must also be included, but only in the approximation $\mu_{nr}^2/m \approx m_1^2/m_2$ (Kinoshita 1998). It is clearly more convenient to rely on the correctness of the Dirac expectation value of the relativistic hyperfine operator than to extract this term from four-photon exchange graphs in NRQED.

Recently, a relativistic two-body equation with only eight components and explicit $\mathcal{CPT}$-invariance has been constructed from the QED scattering matrix (Häckl et al. 1998) for two structureless fermions (a short rederivation is presented in appendix A). Although both particles are treated symmetrically, the equation looks like a one-body Dirac equation, in which the mass $m_1$ and energy $E_1$ of particle 1 are replaced by a relativistic reduced mass $\mu$ and reduced energy $\varepsilon$:

$$\mu = m_1m_2/E, \quad \varepsilon/\mu = (E^2 - m_1^2 - m_2^2)/2m_1m_2,$$

where $E$ is the total cms energy ($c = 1$). This equation has predictive power for all values of $\mu_{nr}/m$, including the positronium value $\mu_{nr}/m = 1/4$. For the nS-states, $E$ is $\mu_{nr}$ times a polynomial in $\mu_{nr}/m$, which has the order 2 to the order $\alpha^6$ and 3 to the order $\alpha^8$. In this paper, the second-order polynomial is checked against the NRQED results, and the third-order polynomial is constructed to an extent that may become relevant in the near future.

For a simple understanding of the origin of the polynomial, the hyperfine operator is neglected in section 2. The energy levels are then obtained from those of the static Dirac equation, $E_1/m_1 = f(n^*)$, by the replacement $E_1/m_1 \to \varepsilon/\mu$, and by the subsequent evaluation of $E - m$ as a power series in $f - 1$. The resulting terms of order $\mu_{nr}$ and $\mu_{nr}^2/m$ give directly the hyperfine-averaged energy levels, while the order $\mu_{nr}^3/m^2$ contains additional second-order hyperfine effects in the hyperfine-averaged levels, beginning at the order $\alpha^6$.

The argument $n^*$ in $f(n^*)$ denotes the effective principal quantum number, $n^* = n + \delta \ell$, where $\delta \ell$ is a (negative) quantum defect. With $\delta \ell$ unspecified, the results of section 2 are more general than their derivation. This is so because the function

$$f(n^*) = (1 + \alpha^2/n^*)^{-1/2} \approx 1 - \alpha^2/2n^*$$

solves not only the Dirac equation, but also the Klein-Gordon equation. The latter case has $\delta \ell_{KG} = [(\ell + 1/2)^2 - \alpha^2]^{1/2} - \ell - 1/2$, while the Dirac case has the orbital angular momentum $\ell$ replaced by $j = 1/2$ for $\ell = 0$ and by $j = \ell \pm 1/2$ for $\ell > 0$:

$$\delta \ell_D = \gamma - j - \frac{1}{2}, \quad \gamma = [(j + 1/2)^2 - \alpha^2]^{1/2}. \quad (3)$$

Thus expressions (1) and (2) occur also in the bound states of two spinless particles such as $\pi^-K^+$ and $\pi^-\pi^+$. On the other hand, bound states of one lepton and one spinless particle ($\mu^-\pi^+$ or $e^-^4\text{He}$) require a more complicated equation with an asymmetric dependence on $m_1$ and $m_2$, which produces the so-called Barker-Glover term at the order $\alpha^4$ (Atomic hydrogen requires also an asymmetric interaction, due to the proton’s large anomalous magnetic moment.) In section 3, the expectation values of the Dirac hyperfine operator of the two-fermion Dirac equation are expanded in powers of $f(n_D^*) - 1$ to order $\alpha^8\mu_{nr}^3/m^2$. The first-order expansion for Zeeman operators is mentioned, in which the $\mathcal{CPT}$ origin is particularly evident.
Radiative corrections are ignored so far, but for the more complicated graphs, they may again be evaluated nonrelativistically. The simpler graphs can be evaluated by Dirac methods also for the new equation. There are however other effective two-photon exchange operators that must be added in the two-fermion equation. For \( \ell > 0 \), they are
\[
\frac{7 \alpha^2}{6 \pi \mu_{nr} m r^3} \quad \text{and} \quad \frac{\alpha^2 L^2}{2 \mu_{nr}^2 m r^4}.
\]
The first of these contributes at the order \( \alpha^5 / \pi \), where it is part of the so-called Salpeter shift. Its precise form for S-states is
\[
\frac{7 \alpha^2}{6 \pi \mu_{nr} m r^3} \frac{p^2}{m} \frac{G}{r} = -\nabla^2 \left( \frac{\ln(\gamma \mu r)}{r} \right) - \frac{2}{r} \left[ \partial_r, \frac{\ln(\gamma \mu r)}{r} \right],
\]
with \( \gamma = e^C \) and \( C = \) Euler’s constant \( 0.577... \), with the prescription that expectation values of \( p^2 G \) are calculated by partial integration. This operator is mentioned here because its relativistic analogue occurs in the hyperfine interaction at the order \( \alpha^6 \mu_{nr}^3/m^2 \), to be discussed in section 4.

II. THE ENERGY LEVELS OF THE TWO-FERMION DIRAC-COULOMB EQUATION

When the hyperfine operators are neglected, the resulting Dirac-Coulomb equation has exact solutions. In units of the relativistic reduced mass \( \mu \), the equation reads (\( \hbar = c = 1 \))
\[
\left( \frac{\varepsilon}{\mu} - V(\rho) - \beta - \gamma_5 \sigma_1 p_\rho \right) \psi_{DC} = 0, \quad \rho = \mu r, \quad V = -\frac{\alpha}{\rho}
\]
with \( \beta = \gamma^0 \), \( \gamma_5 \sigma_1 = \alpha = \gamma^0 \gamma \) as usual, and \( p_\rho = p/\mu \).

The solutions are
\[
\frac{\varepsilon}{\mu} = f_D = \left( 1 + \frac{\alpha^2}{n_D^2} \right)^{-1/2}, \quad n_D^* = n + \gamma - j - \frac{1}{2}
\]
with \( \gamma \) defined in \( \text{(3)} \). With the definitions \( \text{(4)} \) of \( \mu \) and \( \varepsilon \), the binding energy \( E - m \) is expanded in powers of \( f_D - 1 \) as follows:
\[
E - m = \sqrt{m^2 + 2m_1 m_2 (f_D - 1)} - m = \mu_{nr} (f_D - 1) - \frac{1}{2} (f_D - 1)^2 \frac{\mu_{nr}^2}{m} + \frac{1}{2} (f_D - 1)^3 \frac{\mu_{nr}^3}{m^2} \ldots
\]
The precise expansion parameter is \( m_1 m_2 (\alpha/n_{D^*} m)^2 \), but as \( n_{D^*} \) is also expanded in terms of \( \alpha \) at a later stage, the mass dependence must be kept explicitly in \( \text{(4)} \). To the order \( \alpha^8 \), one needs
\[
f_D - 1 = -\frac{\alpha^2}{2n_D^2} \left[ 1 - \frac{3}{4} \frac{\alpha^2}{n_D^2} + 5 \frac{\alpha^4}{8 n_D^4} \left( 1 - \frac{7}{8} \frac{\alpha^2}{n_D^2} \right) \right]
\]
\[
(f_D - 1)^2 = \frac{\alpha^4}{4n_D^4} \left[ 1 - \frac{3}{2} \frac{\alpha^2}{n_D^2} + 29 \frac{\alpha^4}{16 n_D^4} \right]
\]
\[
(f_D - 1)^3 = -\frac{\alpha^6}{8n_D^6} \left[ 1 - \frac{9}{4} \frac{\alpha^2}{n_D^2} \right], \quad (f_D - 1)^4 = \frac{\alpha^8}{16n_D^8}
\]
It has been pointed out that the simple relation (1) between $\frac{\varepsilon}{\mu}$ and $E^2$ makes the expansion of $E^2 - m^2$ simpler than that of $E - m$, but for the check against present NRQED it is necessary to expand $E - m$. In particular, one sees that for $\alpha^6$ the mass dependence ends at $\frac{\mu_{nr}^3}{m^2}$. This order in $\mu_{nr}/m$ receives contributions also from second-order hyperfine effects, which are discussed in the next section.

In the frame of the two-fermion Dirac equation, all terms discussed so far originate from the one-photon exchange Born graph. Additional two-photon exchange graphs contribute already at the order $\alpha^5/\pi$. These have only been evaluated with nonrelativistic approximations, where most of them result in the operator $\delta(r)$, with matrix elements proportional to $\frac{\mu_{nr}}{m^3}$. The only two-photon exchange operator with a more complicated $n$-dependence is the “Gupta operator” (4), which has the following expectation value for $\ell = 0$

$$\langle \rho \rangle_{\ell=0} = 2\mu_{nr}^3 \frac{\alpha^3}{mn^3} \left[ \ln \frac{2\alpha}{n} + \sum_{i=1}^{n+1} \left( - \frac{1}{2n} + \frac{1}{2} \right) \right] = \frac{2}{m} \left( \frac{\mu_{nr}\alpha}{n} \right)^3 \left[ \ln \frac{2\alpha}{n} + \Psi + C + \frac{n+1}{2n} \right]$$ (11)

with $\Psi = \Psi(n) = d\Gamma(n)/dn$. At this order in $\alpha$, there is no finite-range two-photon exchange operator in the hyperfine structure. At the next order $\alpha^6$, there is no finite-range three-photon exchange operator for S-states in the Dirac-Coulomb equation, but there is one such operator to be added to the Dirac hyperfine operator, which is discussed in section 4.

All terms in (11) that require only the nonrelativistic values, $f_{D-1} = -\alpha^2/2n^2$, $(f_{D-1})^2 = \alpha^4/4n^4$ etc. are valid for all combinations of spins and magnetic moments. At the order $\alpha^4$, there is only one such term, originating from the second term in the expansion (11). It was originally discovered by Bechert and Meixner (1935). The complete series (11) was discovered for two spinless particles by Brezin et al (1970), with $n_{*D}^2$ replaced by the appropriate Klein-Gordon value $n_{*KG}^2$. It could not yet be confirmed experimentally. For positronium, on the other hand, the agreement between the NRQED calculation to the order $\alpha^6$ and experiment is not perfect, but it seems fair to say that all terms in the expansion (11) are now checked, for the extreme case $\mu_{nr}/m = 1/4$ (Pachucki and Karshenboim 1998, Czarnecki et al 1999).

### III. DIRAC HYPERFINE SPLITTING

Inclusion of the hyperfine operator in the dimensionless reduced Dirac equation (3) leads to (Häckl et al 1998)

$$\varepsilon - V(\rho) - \beta - \gamma_5(\sigma_1 + \sigma_{hf}^{(1)}p_\rho) \psi = 0, \quad \sigma_{hf}^{(1)} = -i\sigma_1 \times \sigma_2 V \frac{\mu}{E}$$ (12)

By standard perturbation theory, the first-order shift of $\varepsilon/\mu$ caused by the hyperfine operator is (Rose 1961)

$$\left( \frac{\varepsilon}{\mu} \right)_{hf}^{(1)} = \alpha^4 \frac{\mu}{E} f_{hf,D}^{(1)}, \quad f_{hf,D}^{(1)} = \frac{4(f - j)}{f + 1/2} \frac{\mu}{\gamma(2\gamma + 1)(2\gamma - 1)}$$ (13)

where $f = j \pm 1/2$ is the total angular momentum, and $\kappa_D = 2(\ell - j)(j + 1/2)$. Any small shift $\delta(\varepsilon/\mu) = \delta(E^{2}/2m_1m_2)$ corresponds to a small shift $\delta E$. 


\[ \delta(E^2) = 2E \delta E. \] (14)

Thus the first-order hyperfine shift is

\[ E_{hf}^{(1)} = \mu \left( \frac{\varepsilon}{\mu} \right)_{hf} f_{hf,D}^{(1)} \approx 2 \frac{\mu_{nr}^2}{m} \alpha^4 f_{hf,D}^{(1)} \left[ 1 + 3 \frac{\mu_{nr}}{m} (f_D - 1) + \frac{15}{2} \left( \frac{\mu_{nr}}{m} \right)^2 (f_D - 1)^2 \right]. \] (15)

In the hyperfine structure of muonium, \( \mu_{nr}/m < \alpha \) makes the last term in (13) negligible, while \( f_D - 1 \) is required at most to the order \( \alpha^4 \). Insertion of \( n_D^* \approx n^{-2} + \alpha^2/n^3(j + 1/2) \) gives

\[ E_{hf}^{(1)} = 2 \frac{\mu_{nr}^2}{m} \alpha^4 f_{hf,D}^{(1)} \left[ 1 + 3 \frac{\mu_{nr}}{m} \frac{\alpha^2}{2n^2} \left( 1 - \frac{3 \alpha^2}{4n^2} + \frac{\alpha^2}{n(j + 1/2)} \right) \right]. \] (16)

Turning now to \( f_{hf,D}^{(1)} \), we find to order \( \alpha^6 \) and for \( j = \ell + \frac{1}{2} \)

\[ f_{hf,D}^{(1)} = \frac{2(f - j)}{(2f + 1) n^3 j(j + 1/2)} (1 + \alpha^2 c_2 + \alpha^4 c_4), \] (17)

\[ c_2 = \frac{1}{j(j + 1)} + \frac{1}{2(j + 1/2)^2} + \frac{3}{2n(j + 1/2)} - \frac{3}{2n^2} - \frac{j + 1/2}{2n^2(j + 1)}. \] (18)

For \( j = \frac{1}{2} \) (nS-states), the \( \alpha^4 \) correction in (17) becomes

\[ c_4 = \frac{1}{4} \left( \frac{203}{18} + \frac{25}{2n} - \frac{67}{9n^2} - \frac{55}{3n^3} + \frac{21}{2n^4} \right). \] (19)

For the “circular” states with \( n = j + \frac{1}{2} \) (which include the ground state) (14) gives \( n_D^* = \gamma \), \( f_D = \gamma/n \), in which case \( f_{hf,D}^{(1)} \) is greatly simplified:

\[ f_{hf,D}^{(1)} \left( j = n - \frac{1}{2} \right) = 4 \frac{f - j}{f + 1/2} \frac{n \gamma + n/2}{n^3 \gamma (2 \gamma + 1) (2 \gamma - 1)} = 2 \left( \frac{f - j}{f + 1/2} \right) \frac{1}{n^2 (2 \gamma^2 - \gamma)}. \] (20)

This expression was used in the calculation of the muonium hyperfine splitting. For \( n = 1 \), the \( \alpha^4 \)-component of the last bracket is 17\( \alpha^4/4 \), in agreement with (19). It amounts to 12 ppb in the muonium hyperfine splitting, \( \Delta \nu = 4463 \, 302 \, 617(510) \) Hz (the error of 510 Hz arises from the uncertainty of \( m_n \)). As both \( c_2(j = 1/2) \) and its recoil correction (15) are positive, inclusion of the latter one gives an (insignificant) increase of \( \Delta \nu \). A recent experimental determination (Liu et al 1999) gives \( \Delta \nu = 4463 \, 302 \, 776(51) \) Hz.

The hyperfine splitting in P-states with total angular momentum \( f = 1 \) is complicated by the mixing of \( j = 1/2 \) and \( j = 3/2 \) states at the order \( \alpha^4 \); in this case the \( \mu_{nr}/m \)-expansion for a given power of \( \alpha \) does not terminate (Pilkuhn 1995). Fortunately, the S-states are simpler. At the order \( \alpha^6 \), the \( n^3 S_1 \) states have a mixing between \( j = 1/2 \) and \( j = 3/2 \) (the S-D-mixing), and all S-states have contributions from the squares of the diagonal hyperfine matrix elements. Both effects are of second order in the hyperfine operator; their energy shifts \( \langle \varepsilon/\mu \rangle_{hf}^{(2)} \) may be calculated with Schrödinger wave functions and then simply added to the higher-order relativistic terms of \( \langle \varepsilon/\mu \rangle_{hf}^{(1)} \). The S-D-mixing contributes \( -4\alpha^6 \mu_{nr}^3/9m^2n^5 \) to the hyperfine splitting, which combines with \( +4\alpha^6 \mu_{nr}^3/m^2n^5 \) from the second term of (16).
into a total of $32\alpha^6\mu_{nr}^3/9m^2n^5$, in agreement with the NRQED result (Pachucki 1997). This is presently the only confirmation of the expansion (I3). The squares of the diagonal matrix elements may be calculated from an effective Schrödinger equation, which in units of $\mu$ is

$$ (\tilde{p}_\rho^2/2 + V - \varepsilon/\mu + 1)\psi_{Sch} = 0 $$

(21)

where $\tilde{p}_\rho^2$ comprises $p_\rho^2$ and all other interaction that may be approximated by a $\rho^{-2}$-potential:

$$ \tilde{p}_\rho^2 = -(\partial_\rho + 1/\rho)^2 + \ell'(\ell' + 1)/\rho^2 $$

(22)

The case at hand has

$$ \ell' - \ell \equiv \delta \ell = \alpha^2 \left( -\frac{1}{2j+1} + \frac{2(f-j)}{f+1/2} \mu_{nr} \right) = \delta \ell_j + \delta \ell_{hf} $$

(23)

To order $\alpha^6$, one obtains

$$ E - m = -\alpha^2(1 - 2\delta \ell/n + 3\delta \ell^2/n^2)\mu_{nr}/2n^2 - \alpha^4\mu_{nr}^2(1 - 4\delta \ell/n)/8mn^4 - \alpha^6\mu_{nr}^3/16m^2n^6, $$

(24)

where the term $-3\alpha^2\delta \ell^2\mu_{nr}/2n^4$ contains the desired $\delta \ell_{hf}^2$. Its contribution to the hyperfine splitting is $-16\alpha^6\mu_{nr}^3/3m^2n^4$. Here, however, the NRQED results give only half that value, together with other terms, to be discussed in the next section.

Before leaving the subject, we wish to propose a minor modification of the binding correction to the leptonic $g$-factors that has been used in the measurement of the muon magnetic moment in muonium (Liu et al 1999). To order $\alpha^2$ and to second order in $m_1/m_2$, this correction has been calculated (Grotch and Hegstrom 1971, Faustov 1970) as

$$ g'_i \approx g_i \left[ 1 - \frac{\alpha^2}{3} + \alpha^2 \frac{m_1}{2m_2} \left( 1 - \frac{2m_1}{m_2} \right) \right], $$

(25)

where $g_i$ ($i=1,2$) are the $g$-factors of the two free leptons. The modification consists of replacing the mass factors by $\mu_{nr}/m$. More precisely, we propose

$$ g'_i = g_i \frac{2\gamma + 1}{3} \frac{m}{E}, \quad E \approx m - \frac{\mu_{nr}\alpha^2}{2n^2}. $$

(26)

The reason is that the Zeeman operator must be an odd function of $E$. In fact, any small change $\delta E$ caused by CPT-invariant perturbations must be odd in $E$. In the case at hand, CPT-invariance requires equal energy levels for muonium and antimuonium, even in the presence of a magnetic field. Both systems are described by a single eigenvalue equation, with $E^2$ as eigenvalue (Malvetti and Pilkuhn 1994). First-order perturbation theory produces a small shift $\delta(E^2)$, from which $\delta E$ follows as in eq. (14). For the hyperfine operator $\sigma_{hf}^{(1)}$ of equation (I2), $\delta(E^2)$ goes as $E^{-2}$, due to $\mu/E = m_1m_2/E^2$. For the Zeeman operators, $\delta(E^2)$ is obviously independent of $E$, to order $\alpha^2$. For positronium, (26) has been verified by a NRQED calculation (Grotch and Kashuba 1973).
IV. THE GUPTA HYPERFINE OPERATOR

According to the NRQED calculation to order $\alpha^6$, the total hyperfine splitting $\Delta E_{hf} = E(\text{triplet}) - E(\text{singlet})$ contains also the combination $-16\alpha^6\mu_n^3\ln(\alpha/n) + \Psi + C + 7/6 - 1/2n)/3n^3m^2$. The last term in the bracket may be decomposed into $-1/n + 1/2n$, where the $-1/n$ arises from the previously mentioned second-order hyperfine interaction. Comparison with (4) shows that the $n$-dependence of the remaining part is identical with that of the “Gupta operator”. The complete $\alpha^6$-result for S-states is

$$\Delta E_{hf,NRQED}^{(6)} = \Delta E_{hf,D}^{(6)} + \Delta E_{hf,G}^{(6)} + 8\alpha^6\mu_n^3 F'_{hf}/3n^3m^2,$$

where $\Delta E_{hf,D}^{(6)}$ contains all terms from the two-fermion Dirac equation, and

$$\Delta E_{hf,G}^{(6)} = \frac{16}{3} \alpha^3 \mu_n^3 \langle p^2 G/2 \mu \rangle,$$

$$F'_{hf} = \frac{91}{36} + \frac{13}{2} \ln \frac{3}{4} - 2 \ln 2 + f_{hf},$$

where $f_{hf}$ is a numerical function of $\mu_n/m$, which is presently known in analytic form only for $\mu_n/m = 0$ and 1/4. The “Gupta” part of (28) is the nonrelativistic expectation value of an operator that may be combined with the Dirac hyperfine operator in (12):

$$\sigma_{hf} = \sigma_{hf}^{(1)}[1 + 2(\mu/E)\alpha^2 \ln(\gamma \rho)].$$

With $\sigma_{hf}^{(1)} = -i \sigma_1 \times \sigma_2 \alpha \mu/E \rho$, the Gupta hyperfine operator goes as $\rho^{-1} \ln \rho$, which is even more singular than the $\rho^{-1}$ of the Dirac hyperfine operator. However, as it is only a first-order correction, it may be combined with the Dirac hyperfine operator into less singular forms, for example

$$\sigma_{hf} = -i \sigma_1 \times \sigma_2 V m_1 m_2 [E^2 - 2m_1 m_2 \alpha^2 \ln(\gamma \rho)]^{-1}.$$}

This combination goes as $(\rho \ln \rho)^{-1}$ for $\rho \to 0$, which appears to admit a nonperturbative use in the Dirac equation.

This extension is of little importance for QED bound states. But hyperfine operators appear also in quarkonium models, mainly in the form of Breit operators for heavy quarkonium. For the vector $(1^-)$ and pseudoscalar $(0^-)$ mesons, one expects a small and constant hyperfine splitting in $E^2$, $\Delta = E^2(1^-) - E^2(0^-)$ (Mannel 1998). However, a closer look reveals that $\Delta$ increases with decreasing meson masses, from 0.48 GeV$^2$ for the heavy b quarkonium (Review of Particle Physics 1998) up to 0.57 GeV$^2 \approx m_\rho^2$ for the $\rho - \pi$ system, where NRQED expansions would diverge. Moreover, $m_\rho^2/m_\pi^2 = 30$ excludes a perturbative treatment of the hyperfine operator. It is true that the quark model for pions must differ drastically from any QED analogue, for example in its dependence on $m_1$ and $m_2$. But the pion is only the lightest meson in a long list of light mesons whose quantum numbers all agree with the naive quark model. Until the masses of these mesons are calculated by fundamental methods such as lattice QCD, it may be allowed to replace the nonrelativistic QCD Breit operators by the relativistic QCD hyperfine operator. This operator has a similar structure as in QED. Even in the absence of a detailed quarkonium model, the experimental increase of $\Delta$ hints at an increase of the hyperfine operator for small $E^2$, in agreement with (30).
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APPENDIX A: REDERIVATION OF THE TWO-FERMION EQUATION

The standard 16-component formalism for two fermions contains two kinetic energy operators $\alpha_i p_i$ (i=1,2), with $\alpha_i = \gamma_i^5 \sigma_i$ and $\sigma_i$ = Pauli spin matrices. The essential point of the eight-component formalism in the cms ($p_1 = -p_2 = p$) is the absence of $\alpha_2 p_2 = -\gamma_2^5 \sigma_2 p$ in the free two-body equation, to which the interaction operator is added. The desired equation is easily constructed from the kinematical constraints: The direct product $\psi_0 = \psi_1 \otimes \psi_2$ of two free particle solutions $\psi_1$ and $\psi_2$ satisfies two Klein-Gordon equations, which are required in the cms, where one may use $p_1^2 = p_2^2 \equiv p^2$:

$$(p_1^{02} - m_1^2)\psi_0 = (p_2^{02} - m_2^2)\psi_0 = p^2 \psi_0.$$  

(A1)

After elimination of $p_1^0 - p_2^0 = i \partial_1 - i \partial_2$ using $(p_1^0 - p_2^0)\psi_0 = (m_1^2 - m_2^2)(p_1^0 + p_2^0)^{-1}\psi_0$, there remains a single equation containing $p_1^0 + p_2^0 \equiv E$:

$$(k^2 - p^2)\psi_0 = 0, \quad 4E^2k^2 = E^4 - 2E^2(m_1^2 + m_2^2) + (m_1^2 - m_2^2)^2.$$  

(A2)

The equation applies to particles of any spins. For fermions, it must be linearized in $p$. Here it suffices to write $p^2 = (\gamma_5 \sigma_1 p)^2$, with $\gamma_0^2 = 1$ and one set of Pauli matrices, $\sigma_1$. At the same time, $k^2$ must be factorized, writing

$$k^2 = (\varepsilon - \mu \beta)(\varepsilon + \mu \beta), \quad \beta^2 = 1.$$  

(A3)

For two structureless fermions, the symmetry of $k^2$ under the exchange $m_1^2 \leftrightarrow m_2^2$ must be preserved in the factorization, which leads to the expressions (11) for $\mu$ and $\varepsilon/\mu$. In the last step, the $E$ is removed from the denominators of $\mu$ and $\varepsilon$:

$$(E\varepsilon - E\mu \beta - \gamma_5 \sigma_1 E p)\psi_0 = 0, \quad E\varepsilon = \frac{1}{2}(E^2 - m_1^2 - m_2^2), \quad E\mu = m_1 m_2.$$  

(A4)

The factor $E$ in front of $p = -i \nabla$ is absorbed by a rescaling of the variable $r$, after which (A4) is an explicit eigenvalue equation for $E^2$. A slightly more convenient dimensionless form is obtained by dividing by $E\mu = m_1 m_2$ as in equation (5).

In the 16-component formalism, the direct product $\psi_0^{(16)} = \psi_{1D} \otimes \psi_{2D}$ of two free Dirac spinors satisfies two free Dirac equations,

$$(p_i^0 - \gamma_i^5 \sigma_i p_i - m_i \beta_i)\psi_0^{(16)} = 0, \quad \beta_i = \gamma_i^0, \quad p_i^0 = i \partial_i.$$  

(A5)

The sum of these equations in the cms gives, with $p_1 = -p_2 \equiv p$,

$$[E - (\gamma_1^5 \sigma_1 - \gamma_2^5 \sigma_2)p - m_1 \beta_1 - m_2 \beta_2]\psi_0^{(16)} = 0.$$  

(A6)

In the following, (A5) is transformed into (A4) before the corresponding interaction operator is added. The motivation for this step comes from the details of the interaction, but
the main point is easily stated: In a first approximation, the differential approach with interaction included replaces the $E$ in (A4) by $E - V^{(1)}$, where $V^{(1)} = -\alpha/r$ is the main part of the Fourier transform of the first Born approximation. When this form is reduced to (A4), then $E^2$ in $E\xi$ is replaced by $(E - V^{(1)})^2$. The second-order Born approximation provides several additional operators, which in leading order cancel the squares of the first-order operators, such as the $(V^{(1)})^2$ in $(E - V^{(1)})^2$. These cancellations occur not only in the differential equation sketched here, but also in the Bethe-Salpeter equation and in NRQED calculations. When the interaction is added in the eight-component form (A4), $E^2$ is automatically replaced by $E^2 - 2E V^{(1)}$; the operator $(V^{(1)})^2$ is absent. In this sense, the first Born approximation in the eight-component scattering includes the leading terms of the second Born approximation in the 16-component scattering.

To achieve the reduction from (A4) to (A4), $\psi_0^{(16)}$ is divided into two octets $\psi_{0P}$ and $\chi_{0P}$, which have $\gamma^5_1 = \gamma^5_2 \equiv \gamma_5$ and $\gamma^5_0 = -\gamma^5_2 = \gamma_5$, respectively. The round bracket is $\gamma_5(\sigma_1 - \sigma_2) \equiv \gamma_5 \Delta \sigma$ when acting on $\psi_{0P}$, and $\gamma_5(\sigma_1 + \sigma_2) \equiv \gamma_5 \sigma$ when acting on $\chi_{0P}$. In the chiral basis, $\gamma^5_1$ and $\gamma^5_2$ are diagonal:

$$
\gamma^5_i = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \beta_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \psi_i = \begin{pmatrix} \psi_{ir} \\ \psi_{\beta} \end{pmatrix}, \quad \psi_{0P} = \begin{pmatrix} \psi_{r} \\ \psi_{\beta} \end{pmatrix}, \quad \chi_{0P} = \begin{pmatrix} \psi_{r} \\ \psi_{\beta} \end{pmatrix},
$$

(A7)

where the indices $r$ and $l$ (= righthanded, lefthanded) refer to the eigenvalues $\pm 1$ of $\gamma^5_i$. Each $\beta_i$ exchanges $ir$ with $il$; $\beta_2$ exchanges $\psi_{0P}$ with $\chi_{0P}$, while $\beta \equiv \beta_1\beta_2$ exchanges each upper quartet with the lower one.

$$
\beta_2 \psi_{0P} = \chi_{0P}, \quad \beta_2 \chi_{0P} = \psi_{0P}, \quad \beta \gamma_5 + \gamma_5 \beta = 0.
$$

(A8)

Consequently, (A4) is decomposed as follows:

$$
(E - \gamma_5 p \Delta \sigma)\psi_{0P} = m_+ \chi_{0P}, \quad (E - \gamma_5 p \sigma)\chi_{0P} = m_+ \psi_{0P}, \quad m_+ = m_2 \pm \beta m_1.
$$

(A9)

Using the first equation for the elimination of $\chi_{0P}$, one obtains for the second one

$$
(E - \gamma_5 p \sigma)(m_+)^{-1}(E - \gamma_5 p \Delta \sigma)\psi_{0P} = m_+ \psi_{0P}.
$$

(A10)

Multiplying this equation by $m_+$ and using

$$
m_+ \gamma_5 = \gamma_5 m_-, \quad (p \sigma)(p \Delta \sigma) = 0,
$$

(A11)

one arrives at the following equation

$$
[E^2 - E \gamma_5(p \sigma m_-/m_+ + p \Delta \sigma) - m_+^2]\psi_{0P} = 0.
$$

(A12)

As a rule, an elimination of components produces operators of second order in $p$. This is prevented here by (A11). The factor $m_-/m_+$ is removed by the transformation

$$
\psi_{0P} = c \psi_0, \quad c^{-1} \gamma_5 = \gamma_5 c, \quad c \sigma c = \sigma m_+/m_- , \quad c \Delta \sigma c = \Delta \sigma.
$$

(A13)

$$
c = (m_+ m_-)^{-1/2}[m_2 + m_1 \beta(1 + \sigma_1 \sigma_2)/2] = (m_+ m_-)^{-1/2}(m_+ - 2m_1 \Lambda_s \beta),
$$

(A14)
where \( \Lambda_s = (1 - \sigma_1 \sigma_2)/4 \) is the projector on singlet spin states. The inner bracket in (A12) becomes \( 2p \sigma_1 \), and division by 2 produces (A13). As mentioned before, the result is trivial, but the \( c \)-transformation will be needed again for the \( S \)-matrix, \( S = 1 + iT \). The \( 16 \times 16 \) form of the fermion-fermion \( T \)-matrix in the cms is \( T_{if} = \pi_i \pi_f T_{uu12} \), where \( u_i \) and \( \pi_i \) are the free Dirac spinors for the in- and outgoing fermions, \( \psi_i = u_i e^{i \phi_i}, \phi_i = k_i r_i - E_i t \). In the \( (\psi, \chi) \) basis, analogous expressions are defined for the ingoing \( \psi_{0p} \) and \( \chi_{0p} \),

\[
\psi_{0p} = v e^{i \phi}, \quad \chi_{0p} = w e^{i \phi}, \quad \phi = \phi_1 + \phi_2,
\]

and for the outgoing \( \psi_{0i}^T, \chi_{0i}^T \). \( T_{if} \) is now expressed as \( v^T T_v v, \ v^T T_{vw} w, \ w^T T_{wu} v \) and \( w^T T_w w \). The first Born approximation \( T_{if}^{(1)} \) has \( T_{vw} = T_{wu} = 0 \). The product of Dirac matrices \( \gamma_i^\mu \gamma_2^\mu \) is \( \beta_1 \beta_2 (1 - \gamma_i^1 \sigma_1 \gamma_2^5 \sigma_2) \), with \( \gamma_5 \gamma_5 = +1 \) in the \( v \)-components and \( -1 \) in the \( w \)-components, respectively. Remembering \( \pi_i = u_i T \) and \( \beta_1^2 = 1 \), one finds

\[
T_{if}^{(1)} = -4 \pi \alpha q^{-2} [v^T (1 - \sigma_1 \sigma_2) v + w^T (1 + \sigma_1 \sigma_2) w],
\]

with \( q = k - k' \) (\( q^0 = 0 \)), where \( k \) and \( k' \) are the in- and outgoing momenta of particle 1. In general, \( T_{vw} \) and \( T_{wu} \) appear only for an odd number of matrices \( \beta_i \).

One-loop graphs contain two fermion propagators, the product of which may be written symbolically as

\[
P = (\not{p} - m)^{-1} X (\not{p}' - m')^{-1} = (\not{p} + m) X (\not{p}' + m')/(p^2 - m^2)(p'^2 - m'^2),
\]

where \( X \) may be any operator. When both propagators occur on one fermion line \( i \) as in radiative corrections, one has \( m = m' = m_i \), otherwise \( m = m_1, m' = m_2 \). The product (A17) may be decomposed as follows:

\[
\begin{align*}
P &= P_{++} - P_{--}, & P_{++} &= 2(\not{p} X \not{p}' + mm' X)/(p^2 - m^2)(p'^2 - m'^2), \\
P_{--} &= (\not{p} - m) X (\not{p}' - m')/(p^2 - m^2)(p'^2 - m'^2) = (\not{p} + m)^{-1} X (\not{p}' + m')^{-1}
\end{align*}
\]

For bound states, \( P_{--} \) is of higher order in \( \alpha \) because it contains a product of two antifermion poles. The leading radiative corrections contain no \( \beta \), just as (A16). Two-photon exchange is linear in \( \beta \), because \( \not{p} X \not{p}' \) contains \( \beta_1 \beta_2 = \beta \) in this case. \( T_{if} \) can always be put into the form \( w^T M v \) by means of (A9). For \( P_{--} \approx 0 \), one finds

\[
M = T_w m_+^{-1} (E - \gamma_5 k \Delta \sigma) + (E - \gamma_5 k' \sigma) m_+^{-1} T_v.
\]

Before insertion into (A4), \( M \) must also be \( c \)-transformed.

The form \( w^T M v \) is no longer hermitian. It may be compared with the \( 2 \times 2 \) single-fermion scattering matrix \( T_{if} = u_i^T M_u r \), which is also complete and nonhermitian.

The first Born approximation (A16) gives

\[
m_+ M^{(1)} = -4 \pi \alpha q^{-2} (E - i \gamma_5 k \sigma_1 \times \sigma_2).
\]

Notice the absence of \( k' \). Its Fourier transform produces the interaction operators, which in the dimensionless variable \( \rho = \mu r \) lead to equation (12). Thus the only addition to the almost trivial Dirac-Coulomb operator (3) is a hyperfine operator, which is not totally unexpected either. Apart from the replacement \( m_2^{-1} \rightarrow m^{-1} \), which was already found by Breit, it differs from the standard hyperfine operator in two respects: the hermitization has been “forgotten”, and the dimensionless form has \( m^{-2} \) replaced by \( E^{-2} \).
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