Nonperturbative Techniques for QED Bound States

Richard Hill†
Newman Laboratory of Nuclear Studies, Cornell University
Ithaca, NY 14853.

October 25, 2018

Abstract

Advantages of using a low-energy effective theory to study bound state properties are briefly discussed, and a nonperturbative implementation of such an effective theory is described within the context of nonrelativistic quantum mechanics. The hydrogen atom, in the approximation of a structureless, infinite-mass nucleus, but with the leading relativistic and radiative corrections included, is used to demonstrate the construction and solution of the effective theory. The resulting Hamiltonian incorporates a finite ultraviolet cutoff and can be solved nonperturbatively. An appendix lists explicit formulae for the various matrix elements necessary to diagonalize the Hamiltonian using gaussian basis sets.

1 Introduction

The study of QED bound states tests our understanding of nonperturbative field theory, and of the techniques used to study these nonperturbative phenomena. Comparison of theoretical predictions to precision experiments gives the best determination of various fundamental constants (e.g. \( R_\infty \) from hydrogen spectral lines, \( m_\mu \) from the muonium hyperfine splitting). Once all of the relevant constants are determined, a disagreement in the theory-experiment comparison can act as a signal to new physics.

Given these motivations to study precision bound state QED, there are some difficulties which must be addressed. Two of these difficulties are the complexity of relativistic formalisms, and the cumbersome nature of bound state perturbation theory.

Traditionally (although this tradition appears to be shifting), precision bound state calculations have been performed in relativistic formalisms, using the Bethe-Salpeter equation or one of its variants. A drawback of the integrated approach of such a formalism, which does not distinguish between low-momentum and high-momentum contributions (since this would violate relativistic invariance), is the difficulty in choosing an optimal gauge. For instance, Coulomb gauge could be most effective for parts of the calculation involving low momentum, but is cumbersome for high-momentum where Feynman gauge may be more appropriate. However in Feynman gauge, spurious low-order contributions appear which, though cancelling in the end, make it difficult to determine exactly which

---

*Talk presented at the MRST conference, University of Rochester, 8-9 May, 2000.
†electronic address: rjh@mail.lns.cornell.edu
Feynman diagrams must be evaluated to obtain a given accuracy. When a low energy effective theory is used to separate high- and low-momentum modes in a systematic way, the appropriate gauge can be chosen independently for both momentum regions. Technical simplifications of this sort result from the effective theory taking advantage of the essentially nonrelativistic character of the system.

Bound state perturbation theory involves nontrivial sums over intermediate states, and in high orders the terms to be evaluated increase in number and complexity. Another problem is the reliance on an unperturbed state which forms the basis for perturbations. This is not such a problem in the single particle case, where the familiar Schrödinger-Coulomb wavefunctions are an obvious choice, but for multiparticle systems such as helium no analytic unperturbed wavefunction is known. These difficulties can be overcome by solving the effective theory nonperturbatively.

In the rest of the talk, after mentioning some examples of low-energy effective theories, I demonstrate, in stages, the construction of an effective Hamiltonian for the hydrogen atom with leading relativistic and radiative corrections, in the approximation of a structureless, infinite mass nucleus. Ref. [2] gives a more modern application, to the decay rate of orthopositronium.

### 2 Low-Energy Effective Theories

An example of a low-energy effective theory is NRQED (nonrelativistic QED) field theory, described by the Lagrangian

\[
\mathcal{L}_{\text{eff}} = -\frac{1}{2}(E^2 - B^2) + \psi^\dagger \left(i\partial_t - e\phi + \frac{D^2}{2m}\right) \psi + c_1 \frac{D^4}{8m^3} + c_2 \frac{e}{2m} \sigma \cdot B + c_3 \frac{e}{8m^2} \nabla \cdot E + c_4 \frac{e}{8m^2} \left\{iD \cdot E \times \sigma\right\} + \cdots \psi + \psi \leftrightarrow \chi
\]

\[
+ \frac{d_1}{mM} \psi^\dagger \sigma \psi \cdot \chi^\dagger \sigma \chi + \frac{d_2}{mM} \psi^\dagger \psi \chi^\dagger \chi + \cdots
\]

together with a cutoff prescription, at momentum scale Λ. Here \(D = \nabla + ieA\) is the covariant derivative and \(\psi, \chi\) are Pauli spinor fields. \(c_1, c_2, \ldots, d_1, d_2, \ldots\) are renormalization constants which must be determined by matching the predictions of NRQED to those of QED. The local operators parameterized by \(d_1, d_2, \ldots\) account for the short-distance/high-momentum states which are excluded by the cutoff Λ.

Another, and familiar, example of a low-energy effective theory is nonrelativistic quantum mechanics, described by a Hamiltonian,

\[
H_{\text{eff}} = \frac{p^2}{2m} + V_{\text{long-range}}(r) + \frac{d_1}{m^2} \delta_3^3(r) + \frac{d_2}{m^4} (-\nabla^2 \delta_3^3(r)) + \frac{d_3}{m^4} \mathbf{p} \cdot \delta_3^3(r) \mathbf{p} + \cdots
\]

\(V_{\text{long-range}}(r)\) includes all long range interactions (the analogue of those operators parameterized by \(c_i\) in Eq. (1)). The remaining operators are the leading terms in an expansion of local operators. The structure of \(V_{\text{long-range}}(r)\) and the values of the coefficients \(d_i\) are determined by matching predictions

---

1. The low-energy effective theory will still be determined perturbatively, as an expansion in \(\alpha\) and the typical atomic velocity \(v\). It is the effective theory, and not QED itself, which will then be solved nonperturbatively.

2. The ideas here are in most cases a rewording, and in others a slight extension of the presentation in Ref. [1].
of the effective theory to those of the true theory (in the present case, QED). It is on the effective Hamiltonian which we will focus, and for which we will formulate our nonperturbative implementation.

3 The Schrödinger-Coulomb Problem

First, consider the Schrödinger-Coulomb problem, where the “true” theory has Hamiltonian

\[ H_{SC} = \frac{p^2}{2m} - \frac{(Z\alpha)}{r}. \]  

(3)

We will treat this as an example problem, to demonstrate the basic ideas in a familiar setting.

Our goal here is to build an effective Hamiltonian in the form of Eq.(2), which describes the theory defined by \( H_{SC} \). We first introduce a cutoff \( \Lambda \approx m \) which effectively removes states of momentum \( p > \sim \Lambda \) from the theory. This is reasonable, since for such large momenta, \( e^+e^- \) pair creation and other relativistic effects become important in QED.

The particular cutoff we choose is in the form of a gaussian multiplying the momentum space potential:

\[ \frac{1}{r} \rightarrow \left( \frac{1}{r} \right)_\Lambda \]  

(4)

\[ \frac{4\pi}{q^2} \rightarrow \frac{4\pi}{q^2} e^{-\frac{q^2}{2\Lambda^2}}, \]

where the second line is the Fourier transform of the first:

\[ \left( \frac{1}{r} \right)_\Lambda = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi}{q^2} e^{-\frac{q^2}{2\Lambda^2}} = \frac{1}{r} \text{erf}(\frac{\Lambda r}{\sqrt{2}}), \]  

(5)

with \( \text{erf}(x) \) the error function. Introducing the cutoff modifies the Coulomb potential at small distances \( r < \sim 1/\Lambda \). With this form of the cutoff, a natural choice for the local operator \( \delta^3_\Lambda(r) \) is:

\[ \delta^3_\Lambda(r) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} e^{-\frac{q^2}{2\Lambda^2}} = \frac{\Lambda^3}{(2\pi)^{3/2}} e^{-\frac{\Lambda^2 r^2}{2}} \]  

(6)

The other local operators in Eq.(2) are derived from \( \delta^3_\Lambda(r) \) by differentiation.

With our modified Hamiltonian, we no longer expect to solve the eigenvalue problem for the energies analytically; instead, we look for a numerical solution. Two approaches can be implemented easily:

(i) Differential Equation Integration: With \( H_{\text{eff}} \) expressed as a differential operator, the Schrödinger equation is:

\[ \left( -\frac{1}{2m} \nabla^2 + V(r) \right) \psi(r) = E\psi(r). \]  

(7)

Together with appropriate boundary conditions (\( \psi(r \rightarrow \infty) = 0, \psi(r \rightarrow 0) \) finite), this eigenvalue problem can be solved using standard numerical differential equation integration routines.

4 Alternatively, NRQED field theory could be used in an intermediate step: NRQED matched to QED, QM matched to NRQED.

4 It happens that \( H_{SC} \) is well defined without a UV cutoff, so that introducing one may seem artificial here. However, when relativistic corrections are included, a cutoff is essential. And even in the present case, there are numerical advantages to having the cutoff in place — for example, fewer basis functions are required in the matrix diagonalization.

5 Since an analytic solution takes the form of a series expansion in \( \alpha \), a numerical approach is more natural as a nonperturbative tool.
(ii) **Matrix Diagonalization**: This technique will be our main focus, it being more readily adaptable than the differential equation method when radiative corrections are introduced. Elements of a (linearly independent, but not necessarily orthogonal) basis are first chosen, for example:

\[
\Phi^{\text{lm}}_i(r) = Y^{\text{lm}}_{\theta,\phi}r^l e^{-\frac{r^2}{2R_i^2}}.
\]

where \(Y^{\text{lm}}_{\theta,\phi}\) is a spherical harmonic and \(R_i\) runs over an appropriate range of distance scales. We now take matrix elements of all operators involved: (for clarity, we replace the three indices \(i, l, m\) above by a single index)

\[
\langle \Phi^i | p^2 | \Phi^j \rangle \equiv (p^2)^{ij}
\]

\[
\langle \Phi^i | V | \Phi^j \rangle \equiv V^{ij}
\]

\[
\langle \Phi^i | \Phi^j \rangle \equiv W^{ij}.
\]

Now taking matrix elements of the Schrödinger equation, we obtain:

\[
\left(\frac{1}{2m}(p^2)^{ij} + V^{ij}\right)\psi_j = EW^{ij}\psi_j,
\]

or as matrices:

\[
\left(\frac{1}{2m}p^2 + V\right)\psi = EW\psi,
\]

where \(\Psi = \Phi^j\psi_j\), and repeated indices are summed over. Since we have not taken our basis elements to be orthonormal, \(W^{ij} \neq \delta^{ij}\). To recover a more standard form, define, as matrices,

\[
W^{-\frac{1}{2}}p^2W^{-\frac{1}{2}} \equiv \tilde{p}^2
\]

\[
W^{-\frac{1}{2}}VW^{-\frac{1}{2}} \equiv \tilde{V}
\]

\[
W^{\frac{1}{2}}\psi \equiv \tilde{\psi}.
\]

Then Eq.(11), upon multiplying both sides by \(W^{-\frac{1}{2}}\) becomes:

\[
\left(\frac{1}{2m}\tilde{p}^2 + \tilde{V}\right)\tilde{\psi} = E\tilde{\psi}.
\]

This matrix eigenvalue equation can be solved easily using standard matrix diagonalization routines\(^6\).

The long range potential of Eq.(2) is

\[
V_{\text{long-range}}(r) = -(Z\alpha) \left(\frac{1}{r}\right) \Lambda \equiv V_C.
\]

To complete the determination of \(H_{\text{eff}}\), we must evaluate the necessary local operator coefficients \(d_1, d_2, \ldots\). First, we should decide which coefficients must be evaluated, and to what accuracy. This is accomplished by noting that

\[
\langle \psi_0 | \frac{d_1}{m^2} \delta^3_{\Lambda}(r) | \psi_0 \rangle \approx \frac{d_1}{m^2} |\psi_0|^2 \approx d_1 m a^3.
\]

\(^6\) See for example Ref. [4]. For the relatively small computer time required for the problems treated here, a commercial program like “Maple” or “Mathematica” works fine.
So, to determine energy levels through, say, \( \mathcal{O}(ma^6) \), we need determine \( d_1 \) through \( \mathcal{O}(\alpha^3) \). Terms parameterized by \( d_2 \) and \( d_3 \) contain two more powers of \( p/m \approx \alpha \), and so contribute at \( \mathcal{O}(d_2ma^5) \), \( \mathcal{O}(d_3ma^5) \) to the energy.

We will implement the matching procedure between the true and effective theory by perturbative matching of scattering amplitudes for the process \( k \to l \). The lowest order scattering amplitude (the Born term) is simply the momentum space potential: (here \( q = l - k \) is the momentum transfer)

\[
|l \rangle \langle T | k \rangle = \left( \frac{-4\pi(Z\alpha)}{q^2} + \frac{d_1}{m^2} + \frac{d_2}{m^4}q^2 + \frac{d_3}{m^4} \cdot k \right) e^{-\frac{2\pi^2}{k^2}} \tag{16}
\]

The first term matches the \( \mathcal{O}(\alpha) \) result of the “true” Coulomb theory. Requiring the other terms to vanish, through \( \mathcal{O}(\alpha) \), gives:

\[
\begin{align*}
|l \rangle \langle T |^{(2)} k \rangle &= \int \frac{d^3p}{(2\pi)^3} \left[ \frac{-4\pi}{p^2} - 2m + \frac{4\pi}{p^2} \right] \\
\end{align*}
\]

Requiring this quantity to vanish yields:

\[
\begin{align*}
d_1^{(2)} &= \sqrt{\pi} \left( \frac{10}{3} \left( \frac{m}{\Lambda} \right)^3 - 20 \frac{d_2^{(1)}}{4\pi} \frac{\Lambda}{m} + 6 \left( \frac{d_2^{(1)}}{4\pi} \right)^2 \left( \frac{\Lambda}{m} \right)^5 \right) \\
&= -\frac{71\sqrt{\pi}}{96} \left( \frac{m}{\Lambda} \right)^3.
\end{align*}
\tag{21}
\]

By a similar calculation at \( \mathcal{O}(\alpha^3) \), with the above calculated values of \( d_2^{(1)} \) and \( d_1^{(2)} \),

\[
d_1^{(3)} = -\left( \frac{5\sqrt{3}}{72} + \frac{1633}{384} \right) \left( \frac{m}{\Lambda} \right)^4.
\tag{22}
\]

A comparison of the first few \( S \)-state energy levels calculated both with and without counterterms are shown in Table. As expected, with counterterms included the energy levels are in agreement with the Coulomb spectrum through \( \mathcal{O}(ma^6) \). This matching procedure can be extended systematically to higher orders.

---

5. Here we are using the relation \( T_{ik} = V_{ik} + V_{ik}G_p(E)T_{pk} \), where \( G_p(E) = (E - p^2/(2m) + i\epsilon)^{-1} \) is the nonrelativistic propagator and for the scattering state, \( E = k^2/(2m) \).

6. For energy levels correct through \( \mathcal{O}(ma^5) \), it would be sufficient to include only \( d_1^{(1)} \) and \( d_1^{(2)} \), with \( d_2 = 0 \). The value of \( d_1^{(2)} \) would then be given by Eq. (21) at \( d_2^{(1)} = 0 \).
| $n$ | $E/E_0$ | $E/E_0$ |
|-----|---------|---------|
| 1   | 0.99850 | 1.0000000035 |
| 2   | 0.24981 | 0.2499999996 |
| 3   | 0.11106 | 0.1111111109 |

Table 1: $S$-state energy levels at $\alpha = 0.02, \Lambda = m$. Here $E_0 = -m\alpha^2/2$ is the ground state Coulomb energy. In the first column, $d_1 = d_2 = 0$. In the second, these parameters take the values calculated in the text.

## 4 Relativistic Corrections

The leading relativistic corrections to the Schrödinger-Coulomb Hamiltonian take the form \[^5\]:

$$\delta H = -\frac{p^4}{8m^3} + \frac{\pi(Z\alpha)}{2m^2} \delta^3(r) + \frac{(Z\alpha) L \cdot \sigma}{4m^2 r^3}. \quad (23)$$

We can immediately see problems with these corrections as they stand, if we are to solve nonperturbatively. At high momentum, the $p^4$ term dominates over $p^2$, causing the Hamiltonian spectrum to be unbounded from below. Also, the $\delta$-function is too singular and all second- and higher order perturbations involving this term will be divergent. To remedy these problems, we introduce a cutoff:

$$\delta^3(r) \to \delta^3_{\Lambda}(r), \quad (24)$$

$$\frac{-1}{r^3} = \frac{1}{r} \left(\frac{1}{r}\right)' \to \frac{1}{r} \left(\frac{1}{r}\right)'_{\Lambda}, \quad (25)$$

giving the cutoff Darwin and spin-orbit potentials:

$$V_D = \frac{\pi(Z\alpha)}{2m^2} \delta^3_{\Lambda}(r)$$

$$V_{SO} = -\frac{(Z\alpha)}{4m^2} \frac{1}{r} \left(\frac{1}{r}\right)'_{\Lambda} L \cdot \sigma. \quad (27)$$

For the $p^4$ term, we choose to work with an equivalent form \[^9\] \[^1\]:

$$p^4 \to (2m)^2 (E - V)^2, \quad (28)$$

which defines our kinetic energy correction potential:

$$V_K(E) = -\frac{1}{2m} (E - V_C)^2, \quad (29)$$

where $V_C$ is the cutoff Coulomb potential.

Working through $O(m\alpha^5)$, the only counterterms necessary are $d_1^{(1)}$, which is given in Eq.(17), and $d_1^{(2)}$, which must be recalculated with the relativistic corrections in place:

$$d_1^{(2)} = \sqrt{\pi} \left( -\frac{10}{3} \left( \frac{m}{\Lambda} \right)^3 - \frac{m}{\Lambda} + \frac{1}{8m} \right). \quad (30)$$

\[^9\]Here we could also apply the cutoff directly to the $p^4$ operator, for example $p^4 \exp(-p^2/\Lambda^2)$. The other form happens to make evaluation of the counterterms more convenient since then only the free propagator $p^2/(2m)$ appears in scattering calculations.
This calculation is similar to that of Eq. (20), but with $T_{\text{true}}$ now referring to the scattering amplitude of QED in the external field approximation.

5 Radiative Corrections

It remains to include the effects of radiative corrections—in the language of Coulomb gauge, the effect of the transverse radiation field. Our analysis is complicated here by the fact that soft photons, of energy $E \sim m\alpha^2$, can no longer be described by instantaneous potentials in the electron’s Hamiltonian, since their characteristic propagation time ($\delta t \approx 1/E$) can be comparable to bound state timescales ($\delta t \approx 1/(ma^2)$). We can deal with this by expanding the state space to include two channels: one with just the electron, another with the electron and a transverse photon. The wavefunction now has components in both sectors:

$$\psi = \begin{pmatrix} \psi_e \\ \psi_{e\gamma} \end{pmatrix}.$$  \hspace{1cm} (31)

The new terms in the Hamiltonian which describe the coupling between channels are:

$$\delta H = H_\gamma - \frac{e}{m} p \cdot A(r),$$ \hspace{1cm} (32)

where

$$H_\gamma = \int \frac{d^3q}{(2\pi)^3} \sum_{\epsilon(q)} \omega_q a^\dagger_{q,\epsilon(q)} a_{q,\epsilon(q)}$$ \hspace{1cm} (33)

is the photon kinetic energy operator, and

$$A(r) = \int \frac{d^3q}{(2\pi)^3} \sum_{\epsilon(q)} \frac{1}{\sqrt{2 \omega_q}} \left( a_{q,\epsilon(q)} e^{iq \cdot r} + \text{h.c.} \right).$$ \hspace{1cm} (34)

For photons of momentum $q \ll m\alpha$ (i.e. $q \lesssim m\alpha^2$), the multipole expansion is valid:

$$A(r) = A(0) + r \cdot \nabla A(0) + \ldots$$ \hspace{1cm} (35)

For $q \gg m\alpha^2$ (i.e. $q \gtrsim m\alpha$), the photon propagation is effectively instantaneous, and can be described by instantaneous potentials in the electron Hamiltonian. So, denoting the potentials already present (Coulomb and relativistic corrections) by $V$, our coupled channel Hamiltonian takes the form:

$$H \approx \frac{p^2}{2m} + V + H_\gamma - \frac{e}{m} p \cdot A(0) + \ldots$$ \hspace{1cm} (36)

where the dots represent any new instantaneous potentials generated by interaction with the transverse photon sector.

The coupled channel problem can be reduced to an effective energy-dependent Hamiltonian acting only on the electron subspace. In general, if the coupled Schrödinger equation has the form:

$$\begin{pmatrix} H_e & H' \\ H'^\dagger & H_e + H_\gamma \end{pmatrix} \begin{pmatrix} \psi_e \\ \psi_{e\gamma} \end{pmatrix} = E \begin{pmatrix} \psi_e \\ \psi_{e\gamma} \end{pmatrix},$$ \hspace{1cm} (37)

then the effective Hamiltonian is

$$H = H_e + H'(E - H_e - H_\gamma)^{-1} H'^\dagger.$$

\hspace{1cm} \hspace{1cm} (38)
In the present case,

\[ H_e = \frac{p^2}{2m} + V \]  
\[ H' = -\frac{e}{m} \mathbf{p} \cdot \mathbf{A}(0), \]  

and \( H' \) is given by Eq. (33). Eq. (38) can be evaluated explicitly. Including radiative photon modes of momentum \( q \leq \Lambda_\gamma \approx m \), and assigning the photon a mass \( \lambda \) to control infrared divergences,

\[ H = H_e + \frac{\alpha}{\pi m^2} p^i \left[ -\int_0^{\Lambda_\gamma} dq \frac{q^2}{q^2 + \lambda^2} \left( \delta^{ij} - \frac{q^i q^j}{q^2} \right) \right. \]
\[ + \int_0^{\Lambda_\gamma} dq \frac{q^2}{q^2 + \lambda^2} \left( \delta^{ij} - \frac{q^i q^j}{q^2} \right) \left( \frac{q_{\lambda}}{E - H_e - q_{\lambda} + 1} \right) p^j, \]

with \( q_{\lambda} \equiv \sqrt{q^2 + \lambda^2} \).

The final step in our analysis is to compute any remaining instantaneous potentials, by comparing our effective theory to QED. We do this by examining the \( \mathcal{O}(\alpha) \) correction to the QED scattering amplitude, which can be written in terms of vertex form factors, and a vacuum polarization contribution:

\[ T_{\text{true}} = -\frac{4\pi(Z\alpha)}{q^2} F_1 + \frac{4\pi(Z\alpha)}{4m^2} \left( 1 - \frac{2i}{q^2} \mathbf{k} \cdot \mathbf{\sigma} \right) F_2 + \frac{4\pi(Z\alpha)}{q^2} \left( \frac{\alpha}{15\pi m^2} q^2 \right), \]  

with

\[ F_1 = 1 - \frac{\alpha}{3\pi m^2} q^2 \left( \ln \frac{m}{\lambda} - \frac{3}{8} + \mathcal{O}(\lambda) \right) + \mathcal{O}(q^4) \]  
\[ F_2 = \frac{\alpha}{2\pi} + \mathcal{O}(q^2) \]

To this we must compare the \( \mathcal{O}(\alpha) \) contribution coming from Eq. (40):

\[ T_{\text{eff}} = -\frac{4\pi(Z\alpha)}{q^2} \left[ -\frac{\alpha}{3\pi m^2} q^2 \left( \ln \frac{2\Lambda_\gamma}{\lambda} - \frac{5}{6} \right) \right]. \]

Comparing Eqs. (41) and (44), we see that potentials:

\[ V_{F_1} = \frac{4\alpha(Z\alpha)}{3m^2} \left( \ln \frac{m}{2\Lambda_\gamma} + \frac{11}{24} \right) \delta^3(r) \]  
\[ V_{F_2} = \frac{(Z\alpha)}{4m^2} \frac{\alpha}{2\pi} \left( 4\pi \delta^3(r) - \frac{2}{r} \left( \frac{1}{r} \right) ^{'} L \cdot \sigma \right) \]  
\[ V_{VP} = -\frac{4\alpha(Z\alpha)}{15m^2} \delta^3(r), \]

associated with \( F_1 \) and \( F_2 \) form factors, and vacuum polarization, respectively, must be added to our effective theory. Having determined these potentials, we now set \( \lambda = 0 \), and evaluate the \( \mathcal{O}(\alpha) \) piece

\[ ^{10} \text{Taking} \, \Lambda_\gamma \approx m \text{ instead of} \, \Lambda_\gamma \approx m_\alpha \text{ avoids the appearance of factors} \ln \alpha \text{ in higher order contact terms, but is not essential. The difference will be accounted for by the remaining instantaneous interactions—see Eq. (45).} \]

\[ ^{11} \text{Here wavefunction renormalization must be taken into account, since the potential is energy-dependent.} \]
of Eq. (40) \footnote{The first term in square brackets in Eq. (40) is absorbed by a mass renormalization. “LS” stands for “Lamb shift”, since this potential accounts for the dominant part of this effect. Note also that a cutoff in the form exp(−\(p^2/2\Lambda^2\)) has been included in \(V_{LS}\).}

\[
V_{LS}(E) = \frac{2\alpha}{3\pi m^2} e^{-\frac{m^2}{2\Lambda^2}} p^j \left( \frac{p^2}{2m} + V_C - E \right) \ln \frac{\Lambda}{\frac{m^2}{2m} + V_C - E} p^j e^{-\frac{p^2}{2\Lambda^2}}.
\] (48)

We can now present the complete effective Hamiltonian, including leading relativistic and radiative corrections:

\[
H_{\text{eff}} = \frac{p^2}{2m} + V_C + V_{\text{rel}} + V_{\text{rad}} + V_{\text{ct}},
\] (49)

where \(V_C\) is the cutoff Coulomb potential, \(V_{\text{rel}} = V_K(E) + V_D + V_{SO}\) incorporates relativistic corrections, \(V_{\text{rad}} = V_{LS}(E) + V_{F1} + V_{F2} + V_{FP}\) contains the radiative corrections, and \(V_{\text{ct}} = (d^{(1)}_1/m^2 + (Z\alpha)d^{(2)}_1/m^2)\delta^n(r)\) is the counterterm potential. For this application, we have (Eqs. (1)-(10))

\[
d^{(1)}_1 = -2\pi \frac{m^2}{\Lambda^2},
\]

\[
d^{(2)}_1 = \sqrt{\pi} \left( -\frac{10}{3} \left( \frac{m}{\Lambda} \right)^3 - \frac{m}{\Lambda} + \frac{1}{8} \frac{\Lambda}{m} \right).
\]

The spectrum of this Hamiltonian can be readily determined using matrix diagonalization \footnote{The necessary matrix elements of the various operators between gaussian basis functions are listed in the appendix.} and reproduces (Table 2) the well-known result through \(O(ma^5)\) \footnote{The necessary matrix elements of the various operators between gaussian basis functions are listed in the appendix.}:

\[
E(n, j, l) = -\frac{m(Z\alpha)^2}{2n^2} - \frac{m(Z\alpha)^4}{2n^3} \left( \frac{1}{j + 1/2} - \frac{3}{4n} \right) + \frac{ma(Z\alpha)^4}{\pi n^3} \left[ \delta_{l,0} \left( \frac{8}{3} \ln(Z\alpha) - \frac{10}{9} - \frac{4}{15} \right) + (1 - \delta_{l,0}) \left( \frac{j(j + 1) - l(l + 1) - 3/4}{2l(l + 1)(2l + 1)} - \frac{4}{3} \ln(k_0(n, l)) \right) \right].
\] (50)

It is worth noting that higher order terms, including ones containing \(\ln(\alpha)\), appear automatically when the theory is solved nonperturbatively. This can be important in high orders when the appearance of factors \((\ln \alpha)^n\), for large enough \(n\), causes poor convergence of series expansions.

| \(\alpha\) | \((E(1, 1/2, 0) - E'(1))/(4\alpha^5/3\pi n^3)\) | \((E(2, 1/2, 0) - E'(2))/(4\alpha^5/3\pi n^3)\) |
|---|---|---|
| 0.04 | 2.79656 | 2.51928 |
| 0.02 | 2.88486 | 2.65806 |
| 0.01 | 2.92986 | 2.72998 |

Table 2: \(S\)-state energy levels with relativistic and radiative corrections, at \(\Lambda = \Lambda_\gamma = m\). Here \(E'(n)/m = -(Z\alpha^2)/2n^2 - (Z\alpha)^4/2n^3(1 - 3/4n) + \alpha(Z\alpha)^4/\pi n^3(8/3\ln \alpha^{-1} + 10/9 - 4/15)\) is the part of Eq. (50) excluding \(\ln k_0\). At \(\alpha \to 0\) the second and third columns converge to \(\ln k_0(1, 0) = 2.98413\) and \(\ln k_0(2, 0) = 2.81177\), respectively.
Acknowledgements. The work presented here was done in collaboration with Peter Lepage. I also thank Jonathan Sapirstein for useful conversations, and Patrick Labelle for a proofreading of the manuscript.

References

[1] G.P. Lepage, “How to Renormalize the Schroedinger Equation,” in: Nuclear Physics, Proceedings of the VIII Jorge André Swieca Summer School, January, 1995, edited by C.A. Bertulani et. al. (World Scientific, Singapore, 1997), p. 135. [nucl-th/9706029]

[2] R. Hill, G.P. Lepage, to be published. [hep-ph/0003277]

[3] NRQED was introduced in W.E. Caswell, G.P. Lepage, Phys.Lett. 167B, 437 (1986). A more detailed description can be found in T. Kinoshita, M. Nio, Phys.Rev. D53 4909 (1996).

[4] W.H. Press, B.P. Flannery, S.A. Teukolsky and W.T. Vetterling, Numerical Recipes in C (Cambridge University Press, Cambridge, 1988).

[5] H.A. Bethe and E.E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Springer-Verlag, Berlin, 1957).

[6] J. Sapirstein and D.R. Yennie in: Quantum Electrodynamics, edited by T. Kinoshita (World Scientific, Singapore, 1990), p. 579.

Appendix: Matrix Elements for Gaussian Basis

Following is a list of matrix elements between basis functions

$$\Phi_{lm}^i(r) = Y_{lm}(\theta, \phi) r^l e^{-r^2/2r_i^2}. \quad (51)$$

It is convenient to define the quantity $R_{ij} = (R_i^{-2} + R_j^{-2})^{-1/2}$. Then the matrix elements are: (a factor $\delta_{m_i,m_j} \delta_{l_i,l_j}$ is suppressed)

$$[r^n]_{ij} = 2^{l+(n+1)/2} \Gamma \left( \frac{3}{2} + l + \frac{n}{2} \right) R_{ij}^{3+2l+n} \quad (52)$$

$$[p^2]_{ij} = \frac{l + 3/2}{R_{ij}^2} [r^0]_{ij} - \frac{1}{2} \left( \frac{1}{R_i^4} + \frac{1}{R_j^4} \right) [r^2]_{ij} \quad (53)$$

$$\left[ \frac{1}{r} \right]_{ij} = \frac{1}{\Lambda^{2(l+1)}} 2^l \left( - \frac{d}{da} \right) \left[ \frac{1}{a \sqrt{1 + a}} \right]_{a = 1/\Lambda^2 R_{ij}^2} \quad (54)$$

$$[\delta^3_{\Lambda}(r)]_{ij} = \frac{2^{l+1/2}}{4\pi \Lambda^{2l}} \sqrt{\frac{2}{\pi}} \Gamma \left( \frac{3}{2} + l \right) \frac{1}{\left( 1 + \frac{1}{\Lambda^2 R_{ij}^2} \right)^{l+3/2}} \quad (55)$$

$$\left[ -\nabla^2 \delta^3_{\Lambda}(r) \right]_{ij} = 3\Lambda^2 \left[ \delta^3_{\Lambda}(r) \right]_{ij} - \frac{2^{l+3/2}}{4\pi \Lambda^{2l-2}} \sqrt{\frac{2}{\pi}} \Gamma \left( \frac{5}{2} + l \right) \frac{1}{\left( 1 + \frac{1}{\Lambda^2 R_{ij}^2} \right)^{l+5/2}} \quad (56)$$
\[
\left[ \frac{1}{r} \left( \frac{1}{r} \right)_\Lambda \right]_{ij} = \frac{1}{\Lambda^{2l}} \left\{ -2l^{-1} \left( -\frac{d}{da} \right)^l \left[ \ln \frac{1+a+1}{\sqrt{1+a-1}} \right]_{a=1/(\Lambda^2 R^2_{ij})} + \frac{2l}{\sqrt{\pi}} \Gamma \left( l + \frac{1}{2} \right) \left( 1 + \frac{1}{\Lambda^2 R^2_{ij}} \right)^{l+1/2} \right\}
\]

Here, \( p^i \) is the operator appearing in \( V_{LS} \), and we concentrate on the ground state, with \( l = 0 \). To first order in \( V_{LS} \), we need only consider coupling between \( S \)- and \( P \)-states \((S \rightarrow P \rightarrow S)\) transitions. Here the sum over spherical harmonics results in the replacement \( \sum_i p^i(\cdots)p^i \rightarrow -(ip_r)(\cdots)(ip_r) \), where \( ip_r = d/dr \), and:

\[
[ip_r]_{ij} = \delta_{l_i,1}\delta_{l_j,0} \left( -\frac{[r^1]_{ij}}{R^2_{ij}} \right) + \delta_{l_i,0}\delta_{l_j,1} \left( \frac{[r^1]_{ji}}{R^2_{ij}} \right).
\]

Radially excited states \((l > 0)\) can be treated similarly; for instance \( l = 1 \) requires a sum over couplings between \( P \)- and \( S \)- and between \( P \)- and \( D \)-states.

The \( R_i \) should take values which cover the range from \( \sim 1/\Lambda \) to \( \sim 1/(m\alpha) \). For example, the values of Table I were generated using \( R_i = R_{\text{min}}(R_{\text{max}}/R_{\text{min}})^{i/N}, \) with \( i = 0..N, N = 60, R_{\text{min}} = 0.1/\Lambda, R_{\text{max}} = 100/(m\alpha) \) and \( \Lambda = m, \alpha = 0.02 \). For problems with more than one angular momentum channel, a separate set of basis functions should be used for both channels, e.g. \( N_S \) \( S \)-states and \( N_P \) \( P \)-states for the hydrogen atom problem with radiative corrections.

\[14\] Higher orders will introduce \( S \rightarrow P \rightarrow D \rightarrow P \rightarrow S \) transitions, but these are suppressed by several powers of \( \alpha \).