Relativistic Ritz approach to hydrogenic atoms

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The Rydberg formula along with the Ritz quantum defect ansatz has been a standard theoretical tool used in atomic physics since before the advent of quantum mechanics, yet the theory has remained limited by its non-relativistic foundation. Here I present a relativistic theory that effectively describes hydrogenic systems with arbitrary mass ratios. Requiring the theory’s predictions to match those of bound-state QED reveals nonlinear consistency relations within the QED results that relate higher-order corrections to those at lower order, providing guideposts for future perturbative calculations. I also describe insights into the asymptotic behavior of Bethe logarithms.

Applications of the approach include fitting to atomic spectroscopic data, opening the possibility to determine fundamental constants and check for internal consistency of spectral data sets.

I. INTRODUCTION

The Standard Model of particle physics is an impressive scientific achievement, but is unlikely to be the final chapter in our quest to describe nature at a fundamental level. Several outstanding issues have been identified that appear to require physics beyond the Standard Model, including the observed matter/anti-matter asymmetry of the Universe and the many observations supporting the dark matter hypothesis. Accelerator laboratories have been used for nearly a century to perform particle physics experiments at increasingly higher energies, pushing the limits of our knowledge. However, in recent decades it has become more feasible to seek new frontiers through the precision study of atoms and molecules.

Improving the precision of the theoretical description of atoms within bound-state quantum electrodynamics (BSQED) is increasingly difficult (see, e.g.,) and, at the same time, spectroscopic experiments can be subject to unanticipated sources of error. Having an effective theory of atoms and molecules could be of use in guiding future progress on both theoretical and experimental fronts. The idea behind an effective theory is simple but profound: nature has for many physical systems allowed us to describe phenomena at long-distances without necessarily knowing the details of the short-ranged interactions. Such an approach is at least as old as Rayleigh’s explanation for the blueness of the sky, but the ideas of effective field theory have had much contemporary use in particle physics and cosmology; see, e.g.,

Here I apply the effective approach to the quantum mechanics of hydrogenic atoms. No system is purely Coulombic, even for a pair of (hypothetical) point-like scalar particles. In addition to the possible effects of finite particle size and spin coupling, field-theoretic effects like vacuum polarization and self energy corrections are always present. However, for single-electron atoms, all of these effects have a characteristic length scale less than or equal to the inverse of the electron mass, \( r_{\text{QED}} = m_e^{-1} \). If the atom has a nuclear charge \( Z \) and is bound with a particle of charge \( -e \), the characteristic atomic orbital radius is \( r_{\text{atom}} = n^2/(m_{\text{red}} Z \alpha) \), where \( m_{\text{red}} \) is the reduced mass and \( \alpha = e^2/(4\pi) \) is the fine-structure constant. It is hence plausible for a long-range effective theory to have validity if the ratio of these length scales,

\[
\frac{r_{\text{QED}}}{r_{\text{atom}}} = \frac{m_{\text{red}} Z \alpha}{m_e n^2},
\]

is small. For regular electronic hydrogen, deuterium, or positronium, this is true for the ground state. For other systems, such as muonic hydrogen or multi-electron atoms, we should expect that \( n \gg 1 \) would be necessary to make reliable predictions.

Quantum defect theory would be the most obvious thing to try first as an effective theory in this context; it has been vital for the description of Rydberg states of multi-electron atoms. With that approach, the Rydberg formula is used to parameterize the energy levels of an atom composed of particles with masses \( m_1 \) and \( m_2 \):

\[
E = -\frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} \frac{(Z \alpha)^2}{(n - \delta)^2},
\]

where the quantum defect, \( \delta \) effectively parametrizes deviations from the Coulomb potential at short distance and is generally assumed to obey a Ritz-type series expansion in energy. However, this theory cannot properly account for all relativistic effects. This is a problem for hydrogenic atoms wherein kinetic relativistic corrections are of the same order of magnitude as the short-ranged relativistic corrections, such as spin-orbit coupling. Attempts to construct a relativistic quantum defect theory for the Dirac-Coulomb system may be found

\footnote{Here the unit choice \( \hbar = c = 1 \) is used except for data analysis.}
in the literature, e.g. Ref. [11], which is the unphysical case of an electron bound to an infinitely massive atomic core. In Ref. [12] I presented a relativistic defect theory for positronium, and the generalization of that work constitutes the present article.

What follows in Section II is the derivation of a relativistic effective theory for hydrogenic atoms with arbitrary mass ratios. In Section III a matching between this effective theory and the asymptotic predictions of BSQED is performed, revealing non-trivial consistency relations within BSQED. In Section IV implications for BSQED is performed, revealing non-trivial consistency conditions for positronium, and the generalization of that work constitutes the present article.

II. MODEL SUMMARY

Following the procedure first explored in [12], let us seek an effective time-independent Schrödinger equation that describes the long distance interaction of two charged particles, namely

\[ (\hat{\epsilon}_1 - m_1 + \hat{\epsilon}_2 - m_2 + U_{\text{eff}}(r)) \psi = E\psi, \quad (3) \]

where \( r \) is the relative separation of the two particles, \( \hat{p} \equiv \hat{p}_1 = -\hat{p}_2 \) is the conjugate momentum operator for the center-of-momentum motion, and \( E \) is the energy of the system less the two masses. The relativistic energy operators

\[ \hat{\epsilon}_i = \sqrt{\hat{p}_i^2 + m_i^2}, \quad (4) \]

could, in principle, be implemented by expanding to any desired order in the quantities \( \hat{p}_i^2/m_i^2 \).

By matching the calculation of the differential scattering cross section of the two particles using (a) the field-theoretical method and (b) the Born approximation to scattering with [13], we may obtain the effective potential, \( U_{\text{eff}}(r) \). Following [12], the field theoretic calculation of the differential elastic scattering cross section yields

\[ \frac{d\sigma}{d\Omega} = \frac{1}{64\pi^2 (\epsilon_1 + \epsilon_2)^2} |M_{fi}|^2. \quad (5) \]

where the c-numbers \( \epsilon_1 \) and \( \epsilon_2 \) are relativistic energies of particle 1 and 2, respectively. Computation of the scattering amplitude, \( M_{fi} \), for two distinguishable spin-\( \frac{1}{2} \) particles with electric charges \( e_1 \) and \( e_2 \) that scatter elastically with momentum transfer

\[ \hat{q} \equiv \hat{p}_2 - \hat{p}_1 \quad (6) \]

has a lowest order amplitude, due to a single photon exchange,

\[ M_{fi} = e_1 e_2 (\bar{u}'_1 \gamma^\mu u_1) D_{\mu\nu}(q) (\bar{u}'_2 \gamma^\nu u_2), \quad (7) \]

where \( \bar{u}'_i = \bar{u}(\hat{p}_i, m_i) \). The photon propagator in the Feynman (standard) gauge is

\[ D_{\mu\nu}(q) = \frac{4\pi}{q^2} g_{\mu\nu}, \quad (8) \]

and the square of the virtual photon four-momentum,

\[ q^2 = \omega^2 - \bar{q}^2, \quad (9) \]

is consistent with the metric convention \((+, −, −, −)\). As \( \bar{q} \rightarrow 0 \) limit is taken,

\[ \bar{u}'_1 \gamma^\mu u_1 = 2p_1^\mu + \mathcal{O}(\bar{q}), \quad (10) \]

which, at leading order, neglects any spin-dependent effects. Temporarily reintroducing factors of \( h \), loop diagrams that give relative corrections to \( \bar{q} \) must, for dimensional reasons, scale as some positive power of \( \frac{\bar{q}}{E_{\text{light}}} \), i.e.,

\[ M_{fi} = \frac{16\pi e_1 e_2}{q^2} (\epsilon_1 \epsilon_2 + \bar{p}^2) \left( 1 + \mathcal{O}\left( \frac{h |\bar{q}|}{E_{\text{light}}} \right) \right), \quad (11) \]

where \( E_{\text{light}} \) is the smallest relevant energy scale. In the context of the Standard Model, \( E_{\text{light}} \) is no less than \( m_e \). In dropping the correction terms in \( \mathcal{O} \), we omit all loop corrections as well as those terms that correspond to the well-known fine and hyperfine structure corrections. All such terms diminish in the real-space potential with distance faster than \( r^{-1} \). To re-iterate, here we have only assumed QED to be valid for very low momentum-exchange scattering, i.e. at very large spatial separation.

Omission of the terms described above has a very important simplifying consequence for the analyses that follow. Two propositions are made which we confirm below. First, we assume \( U_{\text{eff}}(r) \propto r^{-1} \) at leading order, which is plausibly true given equation (11). Second, we suppose that [3] will yield an equation that displays the long distance behavior

\[ \bar{p}^2 \psi \sim \left( C_0 + \frac{C_1}{r} \right) \psi, \quad (12) \]

for some c-numbers, \( C_0 \) and \( C_1 \). This means that the commutation relation

\[ [\bar{p}^2, U_{\text{eff}}(r)] \psi = 0 \quad (\text{effectively}), \quad (13) \]

may be used because the terms omitted in (13) decay with distance faster than \( r^{-2} \psi \) and are therefore subdominant at long distance to each term in the commutator.

To use (3) for the analysis of a scattering event in the long-distance limit, we assume the two incoming particles to have momenta \( \hat{k} \) and \( -\hat{k} \), and make the identifications

\[ E \equiv \epsilon_1 + \epsilon_2 - m_1 - m_2 \]
\[ \epsilon_i \equiv \sqrt{k_i^2 + m_i^2}. \quad (14) \]

Equation (13) allows us to use purely algebraic means to solve (3) for \( \bar{p}^2 \psi : \)

\[ \bar{p}^2 \psi = \left[ k^2 - \frac{2\epsilon_1 \epsilon_2}{\epsilon_1 + \epsilon_2} U_{\text{eff}}(r) + \mathcal{O}(U_{\text{eff}}^2) \right] \psi. \quad (15) \]
A first-order scattering analysis then yields

\[
\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2} \left( \frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \right)^2 |\tilde{U}_{\text{eff}}(q)|^2 ,
\]

where \( \tilde{U}_{\text{eff}}(q) \) is the Fourier transform of \( U_{\text{eff}}(r) \), and the factor \( \varepsilon_1 \varepsilon_2 / (\varepsilon_1 + \varepsilon_2) \) can be interpreted as a relativistic generalization of the reduced mass.

Finally, by using (11) to match (5) with (16), we find the effective potential in Fourier space to be

\[
\tilde{U}_{\text{eff}}(q) = -\frac{4\pi\varepsilon_1 \varepsilon_2}{q^2} \left( 1 + \frac{\tilde{\rho}^2}{\varepsilon_1 \varepsilon_2} \right) ,
\]

where this choice of sign is consistent with the known nonrelativistic behavior of the electric potential energy between two charged particles.

Let us now specialize to the case of \( \varepsilon_1 = -\varepsilon \), and \( \varepsilon_2 = +Z \varepsilon \) for some positive integer, \( Z \). The \( q^2 \) in the denominator of (17) makes a Fourier transform to real space somewhat complicated, but the end result is that working in the long-distance limit \( (r \to \infty) \) is equivalent to setting \( \omega = 0 \), leading to

\[
U_{\text{eff}}(r) = -\frac{Z \alpha}{r} \left( 1 + \frac{\tilde{\rho}^2}{\varepsilon_1 \varepsilon_2} \right) ,
\]

which is fully justified in Appendix A. Again, because of the effective commutation relation \( [\hat{\rho}, \hat{\rho}] = \frac{\alpha^2}{r^2} \), we may rearrange (3) algebraically to yield

\[
\tilde{\rho}^2 \psi = \left( -q^2 + \frac{2\tilde{m} Z \alpha}{r} + \frac{\mathcal{O}(\alpha^2)}{r^2} \right) \psi ,
\]

which is superficially identical to the canonical Schrodinger-Coulomb equation. However, here

\[
q^2 = -\frac{E (E + 2m_1)(E + 2m_2)(E + 2m_1 + 2m_2)}{4 (E + m_1 + m_2)^2} ,
\]

and

\[
\tilde{m} = \frac{E^2 + 2m_1 m_2 + 2E (m_1 + m_2)}{2 (E + m_1 + m_2)} .
\]

The radial solutions to the Schrodinger-Coulomb equation involve the superposition of two independent (regular and irregular) confluent hypergeometric functions. Here we focus exclusively on bound states \( (E < 0) \), for which the normalizeal,\(^3\) radial solutions are

\[
R(r) = e^{-qr} r^\ell U \left( 1 + \hat{\ell} - \frac{\tilde{m} Z \alpha}{q}, 2(\hat{\ell} + 1), 2qr \right) ,
\]

where \( U(a, c, x) \) is Tricomi’s confluent hypergeometric function,

\[
\hat{\ell} = \ell + \frac{\mathcal{O}(\alpha^2)}{2\ell + 1} ,
\]

and

\[
q = \frac{\tilde{m} Z \alpha}{n_*} ,
\]

where \( n_* \) is the effective quantum number. Two remarks are here warranted. Firstly, because the quantity \( 1 + \hat{\ell} - \frac{\tilde{m} Z \alpha}{q} \) will never be exactly equal to a negative integer in a real system, the regular radial solution diverges exponentially at large \( r \) and cannot be normalized, therefore it has been discarded. Secondly, the singular behavior of the solution involving the (irregular) Tricomi function near \( r = 0 \) is not a concern with this approach because we would not, for example, try to normalize wavefunctions on the entire domain \( 0 \leq r < \infty \). Instead, we imagine a boundary at a finite, but arbitrary, value of \( r \) on which boundary conditions encode information about interactions in the vicinity of the origin \( [14] \).

The solutions here are nevertheless thought to be in some sense near to their “pure relativistic Coulomb” forms, which are regular at \( r = 0 \), and for which \( n_* \) is equal to a positive integer, \( n \). As is standard, we write

\[
n_* = n - \delta ,
\]

where the quantum defect, \( \delta \), accounts for the short-ranged interactions that have not been modeled explicitly \([3, 14, 16]\). From equations (20) and (24) it follows that the physical energy eigenvalues are

\[
E = \sqrt{\frac{m_1^2 + m_2^2 + \frac{2m_1 m_2}{\sqrt{1 + \frac{Z \alpha}{n_*}}}}{2}} - \left( m_1 + m_2 \right) ,
\]

which is the central result\(^3\) of this article and upon which all subsequent results are based.

To see that these energies are plausible, a Taylor expansion of (26) in small \( Z \alpha / n_* \) yields a series whose first term is the standard Rydberg-Ritz term with a reduced mass, followed by a relativistic kinetic correction term,

\[^3\] During manuscript preparation I became aware of the unpublished article by J.H. Connell \( [17] \) in which a very similar “two-body Sommerfeld” formula appears. However, the markedly different derivation attempted in that work and a subsequent unpublished article \( [18] \) was incomplete by Prof. Connell’s admission. Furthermore, in that approach no connection is made to quantum defect theory or long-distance effective theories, in general.
\[ E = -\frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} \left( \frac{Z\alpha}{n^*_s} \right)^2 \left( 1 - \frac{3m_1^2 + 5m_1 m_2 + 3m_2^2}{4(m_1 + m_2)^2} \left( \frac{Z\alpha}{n^*_s} \right)^2 \right) + \mathcal{O} \left( \frac{Z\alpha}{n^*_s} \right)^6. \] (27)

In the limit \( m_1/m_2 \to 0 \),
\[ E = m_1 \left( \frac{1}{\sqrt{1 + \left( \frac{Z\alpha}{n^*_s} \right)^2}} - 1 \right), \] (28)

which are equal to the canonical Dirac-Coulomb energy levels when the quantum defect is set equal to

\[ \delta = (j + 1/2) - \sqrt{(j + 1/2)^2 - (Z\alpha)^2}. \] (29)

In the case of \( m_1 = m_2 = m \), equation (28) is consistent with the results of [12], namely
\[ E = m \left( \frac{2}{\sqrt{1 + \left( \frac{Z\alpha}{n^*_s} \right)^2}} - 2 \right), \] (30)

Finally, we must consider the form of the quantum defect. In a previous article concerning the special case of postronium [12], a Ritz-like expansion was posited, namely a series expansion in which the energies are assumed to be small relative to some high energy scale, \( \Lambda \):
\[ \delta_{\ell sj} = \delta_{(0)\ell sj} + \lambda_{(1)\ell sj} \frac{E}{\Lambda} + \lambda_{(2)\ell sj} \left( \frac{E}{\Lambda} \right)^2 + \ldots, \] (31)

where, for a non-annihilating system, the defect parameters, \( \delta_{(0)\ell sj}, \lambda_{(1)\ell sj}, \lambda_{(2)\ell sj}, \ldots \) are real and should depend on the orbital \( \ell \), total spin \( s \), and total \( j \) angular momentum of the state. Analyzing the asymptotic (large \( n \)) behavior of (26), it may be verified that the following modified ansatz is equivalent and is significantly easier to use for data fitting,
\[ \delta_{\ell sj} = \delta_{(0)\ell sj} + \frac{\lambda_{(1)\ell sj}}{\Lambda} \frac{E}{\Lambda} + \frac{\lambda_{(2)\ell sj}}{\Lambda^2} \left( \frac{E}{\Lambda} \right)^2 + \ldots. \] (32)

Ritz appears to have been the first to propose (what was later understood to be) an energy dependence of the quantum defect [13]. Given that it has a proper relativistic foundation, the method presented above will here be referred to as the relativistic Ritz approach.

### III. INSIGHTS INTO BOUND-STATE QED

Here we consider exclusively non-annihilating systems, hence the energies are taken to be real\(^4\). Let \( m \) and...
and $m_{\text{nucl}}$ be the mass of the lighter and heavier particles, respectively, the ratio

$$r_N = \frac{m}{m_{\text{nucl}}},$$

and

$$\mu = (1 + r_N)^{-1}.$$ (34)

The BSQED perturbative expressions for the energy levels may be written in following the asymptotic (large $n$) form,

$$E \sim \sum_{A,N=2}^{\infty} C_{A,N} \frac{\mu m (Z \alpha)^2}{n^N},$$

where the $C_{A,N}$ may contain logarithms of $\alpha$ and/or powers of $Z$. Using the known BSQED results

$$C_{A,2} = 0 \quad (A > 2)$$ (36)

$$C_{2,N} = 0 \quad (N > 2)$$ (37)

$$C_{3,N} = 0 \quad (\text{for all } N)$$ (38)

$$C_{4,N} = 0 \quad (N > 4)$$ (39)

$$C_{6,N} = 0 \quad (N > 6),$$ (40)

we can match the BSQED and relativistic Ritz results, term by term in a double expansion in small $\alpha$ and $n^{-1}$. Suppressing angular momentum indices for clarity, we find

$$\delta_{(0)} = - (Z \alpha)^2 \left( C_{4,3} + (Z \alpha) C_{5,3} + \mathcal{O}(Z \alpha)^2 \right)$$ (41)

and other defect parameters that are given in Appendix A. The matching does not work unless the following relations are also true:

$$C_{2,2} = - \frac{1}{2}$$ (42)

$$C_{4,4} = \frac{3}{8} (3 - \mu + \mu^2)$$ (43)

$$C_{5,N} = 0 \quad \text{(even } N)$$ (44)

$$C_{6,4} = - \frac{3}{2} C_{4,3}$$ (45)

$$C_{6,6} = \frac{3}{16} (-5 + 3\mu - 4\mu^2 + 2\mu^3 - \mu^4)$$ (46)

$$C_{7,4} = -3 C_{4,3} C_{5,3}$$ (47)

$$C_{7,6} = -5 C_{4,3} C_{5,5}$$ (48)

$$C_{7,8} = -7 C_{4,3} C_{5,7}$$ (49)

$$C_{7,10} = -9 C_{4,3} C_{5,9}$$ (50)

and additional relations up to $A = 10$ and $N = 10$ are given in Appendix A.

It appears that all even-$N$ terms obey an asymptotic consistency relation 3 to odd-$N$ terms that is, remarkably, exact to all orders in the mass ratio $r_N$. Equation (43) and (46) may be readily checked in two special cases: (a) when $m_{\text{nucl}} \to \infty$ it follows that $C_{44} = 3/8$ and $C_{66} = -5/16$; (b) when $m_{\text{nucl}} = m$ it follows that $C_{44} = 11/32$ and $C_{66} = -69/256$. At intermediate mass ratios, these results are consistent up to $O(r_N)$ with 20, whose results are based off of [21]. All terms up to $O(\alpha^4)$ are confirmed, including the non-linear relation 14. Equations (43) and (17) through (50) have implications for the so-called Bethe logarithms which we consider below.

IV. IMPLICATIONS FOR BETHE LOGARITHMS

The results from the previous section have implications for the asymptotic behavior of Bethe logarithms, the nonrelativistic or “normal” version typically denoted $\ln k_0(n, \ell)$. They result from one-loop self-energy corrections computed in BSQED (see, e.g., [22] or [21]), and appear in terms proportional to

$$\frac{m \alpha^5}{n^3} \ln k_0(n, \ell).$$ (55)

There is currently no known analytic method to compute the $\ln k_0(n, \ell)$, so they must be computed numerically for a given $n$ and $\ell$. Investigations have demonstrated that they asymptote to an $l$-dependent constant as $n \to \infty$, and may be fit with a series expansion in inverse powers of $n$ 23, i.e.,

$$\ln k_0(n, \ell) \sim \ln k_0(\infty, \ell) + \frac{\beta^{(1)}}{n} + \frac{\beta^{(2)}}{n^2} + \frac{\beta^{(3)}}{n^3} + \ldots$$ (56)

However, as they appear in terms like [55], in light of equation (14), Bethe logarithms are predicted by this analysis to admit an asymptotic expansion in only inverse

5 This even-odd correspondence is similar to that found by G.W.F. Drake in a non-relativistic context [13].
even powers of \( n \). Using the numerical results of Ref. [23] for \( n = 190 \) through \( n = 200 \), some of which are reproduced in Table I, we can fit for the parameters indicated in the general fit equation (46) as well as in the even-only fit in which the restriction \( \beta_k (i = \text{odd}) = 0 \) is made.

### Table I. Numerically computed values of the Bethe logarithm from Ref. [23]

| \( \ln k_0(n, \ell) \) | \( \ell = 0 \) | \( \ell = 1 \) |
|--------------------------|------------|------------|
| \( n = 190 \) | 2.72266958 & -0.049048944 |
| \( n = 191 \) | 2.72266942 & -0.049040025 |
| \( n = 192 \) | 2.72266927 & -0.049040596 |
| \( n = 193 \) | 2.72266911 & -0.049041159 |
| \( n = 194 \) | 2.72266896 & -0.049041713 |
| \( n = 195 \) | 2.72266881 & -0.049042258 |
| \( n = 196 \) | 2.72266867 & -0.049042796 |
| \( n = 197 \) | 2.72266852 & -0.049043325 |
| \( n = 198 \) | 2.72266838 & -0.049043846 |
| \( n = 199 \) | 2.72266824 & -0.049044360 |
| \( n = 200 \) | 2.72266810 & -0.049044865 |

In Tables II and III, the best-fit parameters are shown, as well as a comparison of the second-order Akaike Information Criterion (AICc) of each fit, computed using Mathematica. Ref. [24] contains an excellent discussion of the use of AICc for comparing the goodness-of-fit of various models to data. This criterion is defined by

\[
\text{AICc}_i = -2 \log \mathcal{L}(\hat{\theta}) + 2K \left( \frac{n}{n - K - 1} \right),
\]

(57)

where \( \mathcal{L}(\hat{\theta}) \) is the maximum likelihood for the set of best-fit model parameters, \( \hat{\theta} \), \( n \) is the sample size, and \( K \) is the number of model parameters. The “best” model has the minimum value of AICc. AICc, as opposed to AIC, is used according to the rule of thumb that the former should be used whenever \( n/K < 40 \) [24].

Given the substantially lower value of the AICc, it is clear that a series of even inverse powers of \( n \) is a superior model compared to a general series of inverse powers, for large values of \( n \). It is also noteworthy that the asymptotic even-only fit parameters are in very good agreement with the numerical values \( \ln k_0(\infty, 0) = 2.722654335 \) and \( \ln k_0(\infty, 1) = -0.049054544 \) reported in Ref. [23]. Similar results have been obtained for \( \ell = 2 \). However, the even-only fits described here give inferior fits for smaller values of \( n \), for example, the set of values for \( 1 \leq n \leq 20 \) computed and tabulated in Ref. [23]. This should not surprise us because the analyses discussed here are based on an asymptotic expansion around \( n \to \infty \).

For \( \mathcal{O}(\alpha^7) \), equations (47) through (50) indicate a relationship between the \( \mathcal{O}(\alpha^5) \) Bethe logarithms and the higher order “relativistic Bethe logarithms”, which is discussed, e.g., in Ref. [26] and [27]. However, this relationship has not been confirmed because the asymptotic behavior of the higher order Bethe logarithms are difficult to extrapolate; to my knowledge they have thus far only been computed for excited states from \( n = 2 \) to \( n = 8 \) [27].

### Table II. Numerical fits of the \( \ell = 0 \) Bethe logarithm using data found in Table I

| \( \ln k_0(\infty, 0) \) | General fit | Even-only fit |
|--------------------------|------------|------------|
| \( \rho_0^{(1)} \) | 2.7093(3) | 2.722654335(9) |
| \( \rho_0^{(2)} \) | 10.4(2) | - |
| \( \rho_0^{(3)} \) | -3.03(3) \times 10^3 | 0.56(6) |
| \( \rho_0^{(4)} \) | 3.94(2) \times 10^5 | - |
| \( \rho_0^{(4)} \) | -1.9(3.0) \times 10^7 | -232(1230) |

### Table III. Numerical fits of the \( \ell = 1 \) Bethe logarithm using data found in Table I

| \( \ln k_0(\infty, 1) \) | General fit | Even-only fit |
|--------------------------|------------|------------|
| \( \rho_1^{(1)} \) | -0.0458474(3) | -0.04905452(1) |
| \( \rho_1^{(2)} \) | -0.242(2) | - |
| \( \rho_1^{(3)} \) | 70.9(3) | 0.2020(8) |
| \( \rho_1^{(3)} \) | -9187(22) | - |
| \( \rho_1^{(4)} \) | 4.473147(5) \times 10^5 | -24(15) |
| \( \text{AICc} \) | -472.6 | -489.0 |

At \( \mathcal{O}(\alpha^7) \), equations (47) through (50) indicate a relationship between the \( \mathcal{O}(\alpha^5) \) Bethe logarithms and the higher order “relativistic Bethe logarithms”, which is discussed, e.g., in Ref. [26] and [27]. However, this relationship has not been confirmed because the asymptotic behavior of the higher order Bethe logarithms are difficult to extrapolate; to my knowledge they have thus far only been computed for excited states from \( n = 2 \) to \( n = 8 \) [27].

### V. DISCUSSION

Here I have derived a relativistic long-distance effective theory of hydrogenic atoms, dubbed the relativistic Ritz approach, and explored some of its consequences in the context of bound-state QED (BSQED). Consistency relations within BSQED have been discovered that illuminate additional structure in the theory which may aid theorists in advancing its predictive accuracy. By these same arguments, any short-ranged (or high-energy) beyond-QED effects should obey similar relations. Elsewhere, I will apply this approach to atomic hydrogen transition data [28].

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Appendix A: Theory Details

1. Effective Potential in Real Space

To justify the leap between the momentum-space potential \(17\) and the real space potential \(18\) note that, given the definition
\[
\vec{q} \equiv \vec{p}_1' - \vec{p}_1 ,
\]
the energy of the virtual photon obeys
\[
\lim_{\vec{q} \to 0} \omega = \frac{\vec{p} \cdot \vec{q}}{2\varepsilon_1 \varepsilon_2} (\varepsilon_2 - \varepsilon_1) . \tag{A1}
\]
In this limit, its square four-momentum is
\[
\vec{q}^2 = (\vec{p} \cdot \vec{q})^2 \left( \frac{(\varepsilon_2 - \varepsilon_1)}{2\varepsilon_1 \varepsilon_2} \right)^2 - \vec{q}^2 , \tag{A2}
\]
and from \(17\) it follows that
\[
\vec{U}_{\text{eff}}(\vec{q}) = \frac{4\pi Z_{\alpha}}{\vec{q}^2} \left( \frac{1 + \varepsilon_1 \varepsilon_2}{\varepsilon_1 \varepsilon_2} \right) \left( \frac{1}{1 - \left( \frac{(\vec{p} \cdot \vec{q})^2}{\vec{q}^2} \right) \left( \frac{(\varepsilon_2 - \varepsilon_1)}{2\varepsilon_1 \varepsilon_2} \right)^2} \right) . \tag{A3}
\]
When \(\vec{p}\) is treated as a c-number, the following inequality is obeyed
\[
\frac{(\vec{p} \cdot \vec{q})^2}{\vec{q}^2} \left( \frac{(\varepsilon_2 - \varepsilon_1)}{2\varepsilon_1 \varepsilon_2} \right)^2 \leq \frac{1}{4} , \tag{A4}
\]
which means that \(A3\) may be written as a geometric series
\[
\vec{U}_{\text{eff}}(\vec{q}) = -\frac{4\pi Z_{\alpha}}{\vec{q}^2} \left( \frac{1 + \varepsilon_1 \varepsilon_2}{\varepsilon_1 \varepsilon_2} \right) \times \sum_{n=0}^{\infty} \left( \frac{(\vec{p} \cdot \vec{q})^2}{\vec{q}^2} \left( \frac{(\varepsilon_2 - \varepsilon_1)}{2\varepsilon_1 \varepsilon_2} \right)^2 \right)^n . \tag{A5}
\]
For the special case in which \(m_1 = m_2\), considered in \(12\), only the \(n = 0\) term is non-zero and gives a Coulomb-like result. For the general case all terms must be considered, requiring the Fourier transforms
\[
I^{(n)} = \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q} \cdot \vec{r}} \frac{1}{\vec{q}^2} \left( \frac{(\vec{p} \cdot \vec{q})^2}{\vec{q}^2} \right)^n . \tag{A6}
\]
For \(n = 1\),
\[
I^{(1)} = \frac{1}{8\pi^2} \left( \vec{p}^2 - \frac{\vec{p} \cdot (\vec{r} \times \vec{p})}{r^2} \right) , \tag{A7}
\]
a result found readily in the literature, e.g., \(13\). Consider that \(\vec{p}^2 = -\partial_r^2 - \frac{1}{r^2} \partial_r + \vec{r} \cdot \nabla \Omega\) and \(\vec{r} \cdot (\vec{r} \times \vec{p}) = -r^2 \partial_r^2\). This means that the \(n = 1\) term acting on \(\psi\) scales as
\[
\mathcal{O} \left( \frac{1}{r^2} \partial_r \psi \right) \quad \text{or} \quad \mathcal{O} \left( \frac{1}{r^3} \psi \right) . \tag{A8}
\]
For arbitrary integer \(n\), discussed below, a different tack is taken, but the conclusion is that all \(n \neq 0\) terms acting on \(\psi\) fall off with distance faster than \(r^{-1}\psi\) and therefore may be discarded when compared to the leading Coulomb-like term. Choosing coordinates such that \(\vec{r}\) is aligned with the \(z\)-axis so that \(\vec{q} \cdot \vec{r} = qr \cos \theta\), let \(w = qr\) and \(x = \cos \theta\) and write equation \(A6\) as
\[
I^{(n)} = \frac{1}{(2\pi)^3 r} \int_0^\infty dw \int_0^{2\pi} d\phi \int_{-1}^1 dx e^{iwx} (\vec{q} \cdot \vec{p})^{2n} , \tag{A9}
\]
where \(\vec{q}\) is a unit vector in the direction of \(\vec{q}\). If equation \(A9\) is to decay with distance no faster than \(r^{-1}\) when acting on the wave function \(\psi\), given equation \(12\), the integral must contain a term proportional to \(p_r^{2n} = p_r^{2n+ \ldots}\). This requires the following contribution to \(A9\) to be nonzero
\[
I_n = \frac{1}{4\pi^2 r} \int_0^\infty dw \int_{-1}^1 dx e^{iwx} (\vec{q}_r)^{2n} \tag{A10}
\]
where the substitution \(\vec{q}_r = x \cos \theta = x\) has been made and the symmetry of the \(x\) integral has been exploited. A series representation of the cosine may be used to show that
\[
\int_{-1}^1 dx e^{iwx} x^{2n} = \frac{1}{n+1/2} \times 1 F_2 \left[ n+1/2, 1/2; n+3/2; -w^2/4 \right] , \tag{A11}
\]
where \(1 F_2\) is a hypergeometric function. With the variable substitution \(\chi = \frac{x^2}{4}\), it follows that
\[
I_n = \frac{1}{4\pi^2 r} \int_0^\infty d\chi \frac{1}{n+1/2} \times 1 F_2 \left[ n+1/2, 1/2; n+3/2; -\chi \right] = \frac{1/2}{\mu \rightarrow 0^+} \lim_{\mu \rightarrow 0^+} \mu^{n/2} \left( n+1/2 \right) = \frac{1/2}{\mu \rightarrow 0^+} \lim_{\mu \rightarrow 0^+} \mu^{n} \Gamma \left( n+1/2 \right) \tag{A12}
\]
where, in the second line, a known integral \(29\) was used in conjunction with the series representation of the incomplete gamma function, \(\gamma(a, x)\), and in the third line use was made of the limiting behavior
\[
\lim_{\mu \rightarrow 0^+} \gamma \left( n+1/2, 1/2 \right) \sim \Gamma \left( n+1/2 \right) + O \left( e^{-1/\mu} \mu^{1/2-n} \right) . \tag{A13}
\]
Therefore, \(I_0 = 1 / (4\pi r)\), while \(I_{n \neq 0} = 0\), thereby justifying \(13\),
\[
U_{\text{eff}}(r) = -\frac{Z_{\alpha}}{r} \left( 1 + \frac{\vec{p}^2}{\varepsilon_1 \varepsilon_2} \right) .
\]
As a final comment, note that the term in parentheses in (18) obeys the classical relationship,

\[ 1 + \frac{\vec{p}^2}{\varepsilon_1 \varepsilon_2} = \frac{|\vec{p}|}{\varepsilon_2 c_{T_{\text{rel}}}} , \]  

(A14)

where the (relativistic) relative velocity for the parallel motion of two particles,

\[ v_{\text{rel}} = \frac{|\vec{v}_1 - \vec{v}_2|}{1 - \vec{v}_1 \cdot \vec{v}_2} . \]  

(A15)

Appendix B: Lessons for QED

1. Details of QED matching

Letting

\[ f_1(\mu) = 3 - \mu + \mu^2 \]  

(B1)

and

\[ f_2(\mu) = -3 + 3\mu - 2\mu^2 - 2\mu^3 + \mu^4 , \]  

(B2)

it may be verified that the matching described in Section III results in the following values for the defect parameters

\[ \delta_{(0)} = -(Z\alpha)^2 \left( C_{4,3} + (Z\alpha) C_{5,3} + (Z\alpha)^2 C_{6,3} + (Z\alpha)^3 C_{7,3} \right) + \mathcal{O}(Z\alpha)^6 , \]  

(B3)

\[ \delta_{(2)} = \frac{(Z\alpha)^2}{2} f_1(\mu) \delta_{(0)} - (Z\alpha)^3 \left( C_{5,5} + (Z\alpha) C_{6,5} + (Z\alpha)^2 C_{7,5} + \mathcal{O}(Z\alpha)^3 \right) \]  

(B4)

\[ \delta_{(4)} = -(Z\alpha)^3 \left( C_{5,7} + (Z\alpha)^2 \left( C_{7,7} + \frac{1}{2} f_1(\mu) C_{5,5} \right) \right) + \mathcal{O}(Z\alpha)^6 , \]  

(B5)

and

\[ \delta_{(6)} = -(Z\alpha)^3 \left( C_{5,9} + (Z\alpha)^2 \left( C_{7,9} + \frac{1}{2} f_1(\mu) C_{5,7} \right) \right) + \mathcal{O}(Z\alpha)^6 . \]  

(B6)

The remaining consistency relations up to order \( \mathcal{O}(Z\alpha)^{10} \) are

\[ C_{9,4} = -3 \left( C_{6,3} C_{5,3} + C_{4,3} C_{7,3} \right) \]  

(B7)

\[ C_{9,6} = -5 \left( C_{6,3} C_{5,5} + C_{4,3} C_{7,5} + C_{6,3} C_{5,3} + \frac{1}{2} f_1(\mu) C_{4,3} C_{5,3} \right) \]  

(B8)

\[ C_{9,8} = -7 \left( C_{6,3} C_{5,7} + C_{4,3} C_{7,7} + C_{6,5} C_{5,5} + \frac{1}{2} f_1(\mu) C_{4,3} C_{5,5} \right) \]  

(B9)

\[ C_{9,10} = -9 \left( C_{6,3} C_{5,9} + C_{4,3} C_{7,9} + C_{6,5} C_{5,7} + \frac{1}{2} f_1(\mu) C_{4,3} C_{5,7} \right) \]  

(B10)

\[ C_{10,4} = -3 \left( C_{4,3} C_{8,3} + C_{5,3} C_{7,3} + \frac{1}{2} C_{6,3} \right) \]  

(B11)

\[ C_{10,6} = -5 \left( C_{4,3} C_{8,5} + C_{5,3} C_{7,5} + C_{6,3} C_{6,5} + C_{7,3} C_{5,5} - \frac{3}{2} C_{4,3} + \frac{1}{4} f_1(\mu) C_{5,3}^2 + \frac{1}{2} f_1(\mu) C_{4,3} C_{6,3} \right) \]  

(B12)

\[ C_{10,8} = -7 \left( C_{4,3} C_{8,7} + C_{5,3} C_{7,7} + \frac{1}{2} C_{6,5}^2 + C_{7,3} C_{5,7} + C_{5,5} C_{7,5} + \frac{1}{2} f_1(\mu) (C_{5,3} C_{5,5} + C_{4,3} C_{6,3}) \right) \]  

+ \frac{7}{16} C_{4,3}^2 f_2(\mu)  

(B13)

\[ C_{10,10} = \frac{1}{256} \left( -63 + 65\mu - 122\mu^2 + 144\mu^3 - 154\mu^4 + 118\mu^5 - 72\mu^6 + 28\mu^7 - 7\mu^8 \right) \]  

- \frac{9}{4} f_1(\mu) \left( C_{5,5}^2 + 2 C_{5,3} C_{5,7} \right) - 9 \left( C_{5,9} C_{7,3} + C_{5,7} C_{7,5} + C_{5,5} C_{7,7} + C_{5,3} C_{7,9} + C_{4,3} C_{8,9} \right) . \]  

(B14)
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