Recoil corrections in the hydrogen isoelectronic sequence

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(Received 21 December 2005; published 13 March 2006)

A version of the Bethe-Salpeter equation appropriate for calculating recoil corrections in highly charged hydrogenlike ions is presented. The nucleus is treated as a scalar particle of charge Z, and the electron treated relativistically. The known recoil corrections of order $m^2/M(Z\alpha)^4$ are derived in both this formalism and in NRQED.

DOI: 10.1103/PhysRevA.73.032505 PACS number(s): 31.30.Jv, 12.20.Ds

I. INTRODUCTION

Precision tests of QED in atoms were first carried out for hydrogen, and have been extended to other one-electron systems such as positronium and muonium, as well as helium [1], lithium [2], and even beryllium [3]. In all these cases the nuclear charge Z is low, so the basic expansion parameter of bound state QED, $Z\alpha$, is a small quantity. For this reason, techniques in which the smallness of this parameter is exploited have been refined in sophistication over the years, culminating in the present widespread use of effective field theories such as NRQED [4] and the effective Hamiltonian method [5]. However, at the same time experiments of increasing precision have been carried out on both highly charged hydrogenlike ions and also ions with more electrons, where as an example of the accuracy achieved at the highest Z we note the recent determination [6] of the $2p_{1/2}$-$2s_{1/2}$ transition energy in lithiumlike uranium,

$$E_{2p_{1/2}}-E_{2s_{1/2}} = 280.645(15)\ \text{eV}. \tag{1}$$

As the expansion parameter $Z\alpha$ is no longer small in this case, techniques in which an expansion in it is avoided are necessary. In the nonrecoil limit, in which the nuclear mass is taken to infinity, Furry representation QED [7] allows a systematic Feynman diagram based treatment of highly charged ions. A central structure in this approach is the electron propagator in a Coulomb field, the Dirac-Coulomb propagator, which satisfies the equation

$$\left[\left(E+\frac{Z\alpha}{|\vec{x}|}\right)\gamma_0 + i\vec{\gamma}\cdot\vec{\nabla} - m\right]S_F(\vec{x},\vec{y};E) = \delta^3(\vec{x}-\vec{y}). \tag{2}$$

As pointed out by Wichmann and Kroll [8] for the vacuum polarization, and by Brown, Langer and Schaefer [9] for the self-energy, treating this propagator exactly using numerical methods allows a determination of the Lamb shift that automatically accounts for all orders of an expansion in $Z\alpha$.

When applied to lithiumlike uranium, use of this propagator gives a one-loop Lamb shift contribution (including screening corrections) to the $2p_{1/2}$-$2s_{1/2}$ splitting of −41.793 eV, which when combined with the nonradiative energy shift of 322.231 eV leaves a 0.207 eV discrepancy with experiment. This can be used to infer the two-loop Lamb shift, which has recently been calculated for the ground state of hydrogenic ions [10], but before this can be done recoil terms, the subject we wish to address in this paper, must be reliably calculated.

Recoil effects have, of course, been treated for low-Z atoms, but again the techniques cannot be directly extended to high-Z ions. The general level of treatment of these small corrections in this latter case is to scale the overall energies by a factor of μ/m, where the reduced mass μ is defined in the usual way in terms of the electron mass m and the nuclear mass M,

$$\mu = \frac{mM}{m+M}. \tag{3}$$

This has a relatively small effect for the transition we are discussing, amounting to only −0.006 eV, below the experimental error. A larger effect comes from the mass-polarization operator

$$H_{\text{MP}} = \sum_{i<j}\frac{\vec{p}_i\cdot\vec{p}_j}{M}. \tag{4}$$

When this term is evaluated in a realistic potential it contributes −0.081 eV, for a total lowest order effect of −0.087 eV, 42% of the discrepancy. To accurately infer the two-loop Lamb shift, a more sophisticated treatment of recoil effects is clearly needed. The only such treatment we are aware of that has been applied to highly charged ions is that given by Shabaev [11] and collaborators [12] who, in fact, find significant corrections to the above result. We note, however, that the calculations of Pachucki and Grotch [13] and Eides and Grotch [14] described in the Appendix, while applied to hydrogen, are also all-orders methods that could, in principle, be applied to the high-Z case. The present paper is intended to lay the groundwork for an alternative approach. We will restrict our attention to the hydrogen isoelectronic sequence,

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and in addition restrict our attention to diagrams that contribute in the low-Z case to order $m^2(Z\alpha)^4/M$, leaving the treatment of a more complete set of diagrams, along with the treatment of the many-electron problem, for a later paper.

While considerable progress has been made in QED in recent years with the use of effective field theories, these rely on expanding around the nonrelativistic Schrödinger equation, which, as just discussed, is not appropriate for highly charged ions. However, the Bethe-Salpeter formalism [15], introduced first to treat the binding of the deuteron and shortly afterwards applied to the atomic problem by Salpeter [16], allows the problem to be treated in a systematic manner. However, this equation is famously difficult to apply, and most applications rely on expanding around the nonrelativistic limit, which we wish to avoid.

The treatment given by Shabaev is fairly complicated, and we wish to provide a cross check by introducing as simple a formalism as possible. This can be done by slightly modifying a formalism introduced by Lepage [17], and it is this approach we will now describe.

The plan of the paper is to set up in the following section a three-dimensional formalism equivalent in rigor to the Bethe-Salpeter equation. In the next section the one- and two-photon exchange diagrams that contribute to order $m^2(Z\alpha)^4/M$ will be evaluated in the Coulomb gauge, and their nonrelativistic limit will be taken. This will be followed by a NRQED treatment, and in the Conclusion we will describe how a calculation relevant to highly charged ions can be carried out. The Appendix describes in more detail the history of the calculation of recoil corrections in hydrogenic ions.

II. FORMALISM

It has been known for quite some time [18] that there is an arbitrary number of bound state equations equivalent in rigor to the original form of the Bethe-Salpeter equation, but that are effectively three-dimensional. Many practical calculations have used formulations that also incorporate the Schrödinger equation [19,20]. However, for the problem we are considering a relativistic approach is demanded. We note that a fairly detailed discussion of a number of notational and formal issues involved with the use of three-dimensional forms of the Bethe-Salpeter equation is given in Ref. [20], to which we refer to the reader interested in more detail.

The spectrum of many high-Z ions has been studied, and it would be impractical to consider the differing spins of each nucleus. For this reason we simply treat the nucleus as a spinless particle of charge $Z|e|$. The Feynman rules for the electrodynamics of a spin-0 particle involve the coupling $iZ|e|(p+p')_\mu$ for the one-photon vertex, and $2i(Ze)^2 g_{\mu\nu}$ for the seagull vertex. The $\mu=0$ component of the one-photon vertex for a nucleus close to a mass shell will then be dominated by the factor $2M$, where M is the mass of the nucleus. Hyperfine effects associated with nuclear spin can be treated separately. We can also model the finite size of the nucleus by replacing the nuclear charge Z with a form factor $Z(\vec{q}^2)$ if desired, but this will not be done in this paper.

We now consider the truncated two-particle Green's function for the scattering of an electron and nucleus. We define the initial and final electron three momenta as $\vec{k}$ and $\vec{l}$, respectively, and work in the center of mass so that the corresponding nuclear momenta are $-\vec{k}$ and $-\vec{l}$. For the fourth component of the momentum we choose E_1+k_0 and E_1+l_0 for the electron line and E_2-k_0 and E_2-l_0 for the nuclear line, where E_1 and E_2 will be chosen close to the electron and nuclear masses, and when the total center of mass energy $E=E_1+E_2$ is a bound state energy a pole will be present. The formalism to be described below in its simplest form leads to a perturbation expansion about $E_1=\epsilon$ and $E_2=M$, with ϵ equal to the Dirac bound state energy,

$$\epsilon = m\left[1+\left(\frac{Z\alpha}{n-(j+1/2)+\sqrt{(j+1/2)^2-(Z\alpha)^2}}\right)^2\right]^{-1/2} = m\left\{1-\frac{(Z\alpha)^2}{2n^2}-\frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{j+1/2}-\frac{3}{4n}\right)+O((Z\alpha)^6)\right\}, \tag{5}$$

giving a total bound state energy $E=M+\epsilon=M+m-m(Z\alpha)^2/2n^2+\cdots$. However, since this does not incorporate the known reduced mass dependence of the nonrelativistic binding energy, we will instead arrange the formalism so that $E_1=\mathcal{E}=\mu/m\epsilon$ and $E_2=M+m-\mu\equiv\tilde{M}$. We incorporate these energies into the four vectors $P_1=(\mathcal{E},\vec{0})$ and $P_2=(\tilde{M},\vec{0})$. If we also define four vectors $k=(k_0,\vec{k})$ and $l=(l_0,\vec{l})$, the initial electron and nuclear momenta are P_1+k, P_2-k, and the final momenta P_1+l, P_2-l. The truncated two-particle Green's function obeys the equation

$$\begin{aligned} G_T(P_1+k,P_2-k;P_1+l,P_2-l) &= iK(P_1+k,P_2-k;P_1+l,P_2-l) \\ &\quad + \int \frac{d^4q}{(2\pi)^4} K(P_1+k,P_2-k;P_1+q,P_2-q)S(q)G_T(P_1 \\ &\quad + q,P_2-q;P_1+l,P_2-l), \end{aligned} \tag{6}$$

where K represents all two-particle irreducible kernels and the spin-$\frac{1}{2}$-spin-0 two-particle propagator has the form

$$S(q) = \frac{i}{\gamma(P_1+q)-m+i\epsilon}\frac{i}{(P_2-q)^2-M^2+i\epsilon}. \tag{7}$$

For brevity in the following we will write the above as

$$G_T(k,l;E) = iK(k,l;E) + \int \frac{d^4q}{(2\pi)^4} K(k,q;E)S(q)G_T(q,l;E). \tag{8}$$

The main point of all simplifications of the Bethe-Salpeter formalism is that we can replace the relatively complicated two-particle propagator S with a simplified form S_0 and write

$$G_T(k,l;E) = i\bar{K}(k,l;E) + \int \frac{d^4q}{(2\pi)^4} \bar{K}(k,q;E)S_0(q)G_T(q,l;E), \tag{9}$$

which serves to define $\bar{K}$ through

$$\bar{K}(k,l;E) = K(k,l;E) + \int \frac{d^4q}{(2\pi)^4} K(k,q;E)[S(q) - S_0(q)]K(q,l;E) + \int \frac{d^4q}{(2\pi)^4} \int \frac{d^4p}{(2\pi)^4} K(k,q;E)[S(q) - S_0(q)] \times K(q,p;E)[S(p) - S_0(p)]K(p,l;E) + \cdots . \tag{10}$$

Our choice for $S_0(q)$ is

$$S_0(q) = \frac{\pi\delta(q_0)}{\tilde{M}} \frac{i}{\mathcal{E}\gamma_0 - \vec{\gamma}\cdot\vec{q} - \mu + i\epsilon} \equiv \frac{i\pi\delta(q_0)}{\tilde{M}} S_0(\vec{q}). \tag{11}$$

As mentioned above, we could have chosen another form with $\mathcal{E}$ and μ replaced with ϵ and m, which would lead to the Dirac equation with mass m in the $M\to\infty$ limit. Our method will lead to a Dirac equation with reduced mass μ in that limit. We note that this method of building in the reduced mass is relatively simple, in particular, requiring no rescaling of coupling constants. The δ function we have chosen differs from that of Ref. [17], in which a δ function that puts the nucleus on a mass shell is chosen. While the latter choice has a number of advantages when the Feynman gauge is used, we use Coulomb gauge in this calculation, and putting the nucleus on-shell is not needed. At this point we can go to a completely three-dimensional formalism by choosing $k_0 = l_0 = 0$, a choice that has no effect on the location of the bound state poles, and which allows us to replace the four vectors k and l with $\vec{k}$ and $\vec{l}$. In this case Eq. (9) takes the three-dimensional form

$$G_T(\vec{k},\vec{l};E) = i\bar{K}(\vec{k},\vec{l};E) + \frac{1}{2\tilde{M}} \int \frac{d^3q}{(2\pi)^3} i\bar{K}(\vec{k},\vec{q};E)S_0(\vec{q})G_T(\vec{q},\vec{l};E). \tag{12}$$

One gets to a bound state equation by creating an untruncated Green's function $\bar{G}(\vec{k},\vec{l};E)$ defined through

$$\bar{G}(\vec{k},\vec{l};E) = \frac{1}{2\tilde{M}} S_0(\vec{k})(2\pi)^3\delta^3(\vec{k}-\vec{l}) + \frac{1}{4\tilde{M}^2} S_0(\vec{k})G_T(\vec{k},\vec{l};E)S_0(\vec{l}) \tag{13}$$

that satisfies

$$\bar{G}(\vec{k},\vec{l};E) = \frac{1}{2\tilde{M}} S_0(\vec{k})(2\pi)^3\delta^3(\vec{k}-\vec{l}) + S_0(\vec{k})\frac{1}{2\tilde{M}} \int \frac{d^3q}{(2\pi)^3} i\bar{K}(\vec{k},\vec{q};E)\bar{G}(\vec{q},\vec{l};E). \tag{14}$$

While this function differs from the Bethe-Salpeter untruncated Green's function, it has poles at exactly the same total energy [21]. In order to obtain a solvable problem, we now introduce the simpler equation

$$G_0(\vec{k},\vec{l};E) = \frac{1}{2\tilde{M}} S_0(\vec{k})(2\pi)^3\delta^3(\vec{k}-\vec{l}) + S_0(\vec{k})\frac{1}{2\tilde{M}} \int \frac{d^3q}{(2\pi)^3} iK_{1C}(\vec{k},\vec{q};E)G_0(\vec{q},\vec{l};E), \tag{15}$$

which can be written, because the kernel K_{1C} for one-Coulomb-photon exchange is

$$K_{1C} = \frac{4\pi i Z\alpha}{|\vec{k}-\vec{q}|^2} 2\tilde{M}\gamma_0, \tag{16}$$

as

$$(\mathcal{E}\gamma_0 - \vec{\gamma}\cdot\vec{k} - \mu)G_0(\vec{k},\vec{l};E) = \frac{1}{2\tilde{M}}(2\pi)^3\delta^3(\vec{k}-\vec{l}) - 4\pi Z\alpha \int \frac{d^3q}{(2\pi)^3} \frac{1}{|\vec{k}-\vec{q}|^2} \gamma^0 \times G_0(\vec{q},\vec{l};E), \tag{17}$$

where we have multiplied by $S_0^{-1}(\vec{k})$.

In the following section we will discuss the effect of expanding $\bar{G}$ about G_0, but here we restrict our attention to the latter function, which, except for the factor of $1/2\tilde{M}$ multiplying the δ function, is precisely the momentum space form of Eq. (2) with the electron mass replaced with the reduced mass. It has the spectral representation

$$G_0(\vec{k},\vec{l};E) = \sum_n \frac{\psi_n(\vec{k})\bar{\psi}_n(\vec{l})}{\mathcal{E}-\mathcal{E}_n}, \tag{18}$$

where $\psi_n(\vec{l})$ is the solution to the Dirac equation with the usual normalization factor multiplied by $\sqrt{1/2\tilde{M}}$, and has poles when $E = \tilde{M} + \mathcal{E}_n \equiv E_0$. To illustrate, the ground state (g) wave function has energy

$$E_0{}^g = \tilde{M} + \mu\gamma \tag{19}$$

where $\gamma = \sqrt{1-(Z\alpha)^2}$, and the form

$$\psi_0{}^g(\vec{p}) = \sqrt{\frac{1}{2\tilde{M}}}(\mu Z\alpha)^{-3/2} \begin{pmatrix} g(p)\chi_{-1\mu}(\hat{p}) \\ \dfrac{\vec{\sigma}\cdot\vec{p}}{2\mu} f(p)\chi_{-1\mu}(\hat{p}) \end{pmatrix}, \tag{20}$$

where $g(p)$ and $f(p)$ can be expressed in terms of the dimensionless variable $q = p/(\mu Z\alpha)$,

$$g(p) = \frac{N}{2q}\sin[\theta(1+\gamma)][1+q^2]^{-(1+\gamma)/2},$$

$$f(p) = \frac{N}{q^3(1+\gamma)}\left[\frac{\sin(\gamma\theta)}{\gamma}\sqrt{1+q^2} - q\cos[\theta(1+\gamma)]\right] \times [1+q^2]^{-(1+\gamma)/2}. \quad (21)$$

Here $\theta \equiv \tan^{-1} q$ and the normalization factor N is

$$N = 2^{\gamma+3}\pi\Gamma(1+\gamma)\sqrt{\frac{(1+\gamma)}{\Gamma(1+2\gamma)}}. \quad (22)$$

The χ_κ's are two-component eigenfunctions of J^2, J_z, L^2, and S^2 and are labeled by $\kappa = \mp(j+1/2)$ for $j = \ell \pm 1/2$ and μ, the quantum number corresponding to J_z. The spherical spinors are normalized so that $\chi^\dagger\chi$, when integrated over a solid angle, gives 1. In the following we adopt the convention of working with Dirac wave functions with the usual normalization, which we account for by multiplying a factor $1/(2\tilde{M})$ into expressions for energy shifts, which always involve two Dirac wave functions. We note that in most three-dimensional formalisms a lowest order potential that differs from the one-Coulomb photon exchange kernel must be devised to obtain a Schrödinger or Dirac equation and it, in general, has energy dependence, which leads to derivative terms: neither complication appears in the present formalism. With this definition of our lowest order problem, we now turn to the calculation of corrections to the lowest order energy, $\tilde{M}+\mathcal{E}$.

III. PERTURBATION EXPANSION

Perturbative corrections to the lowest order energy can be derived by calculating the shift of the pole position in $\bar{G}$. To the order we are interested in here, the shift can be shown to be

$$E - E_0 \equiv \Delta E_1 = \frac{1}{2\tilde{M}}\int \frac{d^3k\, d^3l}{(2\pi)^6}\bar{\psi}(\vec{k})[i\bar{K}(\vec{k},\vec{l};E) - iK_{1C}(\vec{k},\vec{l},E)]\psi(\vec{l}). \quad (23)$$

Schematically we can write

$$\bar{K} = K_{1C} + K_{1T} + K_{CCX} + K_{CCs} + K_{1C}(S-S_0)K_{1C} + \cdots. \quad (24)$$

Here 1C and 1T refer to one-Coulomb- and one-transverse-photon exchange, CCX is the crossed ladder diagram with two Coulomb photons, CCs is the seagull diagram with two-Coulomb photons, and the last term is the leading part of the correction induced in the kernel by our change of propagators as given in Eq. (10). The term $K_{1C}SK_{1C}$ is an uncrossed ladder diagram, denoted K_{CC}, and it is easy to see that the term $-K_{1C}S_0K_{1C}$ is equivalent to $-K_{1C}$ when used to evaluate ΔE_1. The net effect, illustrated in Fig. 1, is that

$$\bar{K} = K_{1T} + K_{CC} + K_{CCX} + K_{CCs} + \cdots. \quad (25)$$

Only these four terms need be considered to obtain the corrections of order $m^2(Z\alpha)^4/M$, and we now turn to their evaluation.

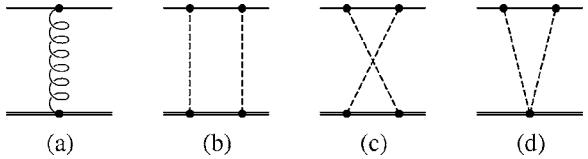

FIG. 1. Contributions to energy levels of hydrogenlike ions at order $m^2(Z\alpha)^2/M$. Initial and final wave functions are implicit. Vertices on the top (electron) line are the usual spin-$\frac{1}{2}$ QED factors $-ie\gamma_\mu$ (where $e=|e|$). Vertices on the bottom (nucleus) line are those appropriate for spin-0 QED: $iZe(p+p')_\mu$ for the one-photon vertex and $2i(Ze)^2 g_{\mu\nu}$ for the seagull vertex. Part (a) represents the exchange of a transverse photon; (b) represents the exchange of two Coulomb ladder photons; (c) represents the Coulomb-Coulomb crossed ladder; and (d) represents the Coulomb-Coulomb seagull.

A. One-transverse-photon exchange

The transverse-photon propagator with momentum q depends on both q_0 and $\vec{q}$. It simplifies in our formalism, which forces $q_0=0$, and K_{1T} gives the energy shift

$$\Delta E_{1T} = -\frac{4\pi Z\alpha}{2\tilde{M}}\int \frac{d^3k\, d^3l}{(2\pi)^6}\frac{1}{(\vec{q}^2)^2}[\vec{q}^2\psi^\dagger(\vec{k})\vec{\alpha}\cdot(\vec{k}+\vec{l})\psi(\vec{l}) - \vec{q}\cdot(\vec{k}+\vec{l})\psi^\dagger(\vec{k})\vec{\alpha}\cdot\vec{q}\psi(\vec{l})], \quad (26)$$

where $\vec{q}=\vec{k}-\vec{l}$. If we approximate the Dirac wave functions in terms of Schrödinger wave functions through

$$\psi(\vec{p}) = \begin{pmatrix} \phi_{NR}(p)\chi_{\kappa\mu}(\hat{p}) \\ \dfrac{\vec{\sigma}\cdot\vec{p}}{2\mu}\phi_{NR}(p)\chi_{\kappa\mu}(\hat{p}) \end{pmatrix}, \quad (27)$$

this simplifies to

$$\Delta E_{1T}(NR) = -\frac{4\pi Z\alpha}{4m\tilde{M}}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3l}{(2\pi)^3}\phi^\dagger_{NR}(k)\phi_{NR}(l) \times\left[\frac{|\vec{k}+\vec{l}|^2 + 2i\vec{\sigma}\cdot(\vec{k}\times\vec{l})}{q^2} - \frac{(k^2-l^2)^2}{q^4}\right]$$
$$= -\frac{4\pi Z\alpha}{m\tilde{M}}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3l}{(2\pi)^3}\phi^\dagger_{NR}(k)\phi_{NR}(l) \times\left[\frac{k^2l^2-(\vec{k}\cdot\vec{l})^2}{q^4} + \frac{i\vec{\sigma}\cdot(\vec{k}\times\vec{l})}{2q^2}\right], \quad (28)$$

where the spherical spinors are understood. This can be Fourier-transformed into coordinate space, leading to spin-independent and spin-dependent operators H_R and H_{SO},

$$H_R = -\frac{Z\alpha}{2\mu^2 r}(\delta_{ij}+\hat{x}_i\hat{x}_j)p_ip_j,$$

$$H_{SO} = \frac{Z\alpha}{4\mu^2 r^3}\vec{L}\cdot\vec{\sigma}. \quad (29)$$

After working out the expectation value of H_R one finds

$$\Delta E_T = \frac{m}{M} m(Z\alpha)^4 \left\{ \frac{1}{n^4} + \frac{\delta_{\ell,0}}{n^3} - \frac{3}{n^3(2\ell+1)} \right\} + \frac{m}{M}\langle 2H_{\rm SO}\rangle, \tag{30}$$

where

$$\langle H_{\rm SO}\rangle = \frac{\mu(Z\alpha)^4[j(j+1)-\ell(\ell+1)-3/4]}{2n^3\ell(\ell+1)(2\ell+1)}. \tag{31}$$

It is, of course, straightforward to simply use exact wave functions and evaluate the integral (26) numerically. The results of doing this for the ground state using the adaptive multidimensional integration program VEGAS [24] are shown in Fig. 2, where the exact result is compared with the NR approximation. As is also typical for the nonrecoil case, significant differences that would be poorly treated with an expansion in $Z\alpha$ arise at high Z. We note that a fit can be carried out, giving

$$\Delta E_{1\rm T}(1s) = \frac{m^2(Z\alpha)^4}{\tilde{M}}[-1-1.50(1)(Z\alpha)^2+\cdots] \tag{32}$$

consistent with the known $(Z\alpha)^6$ behavior.

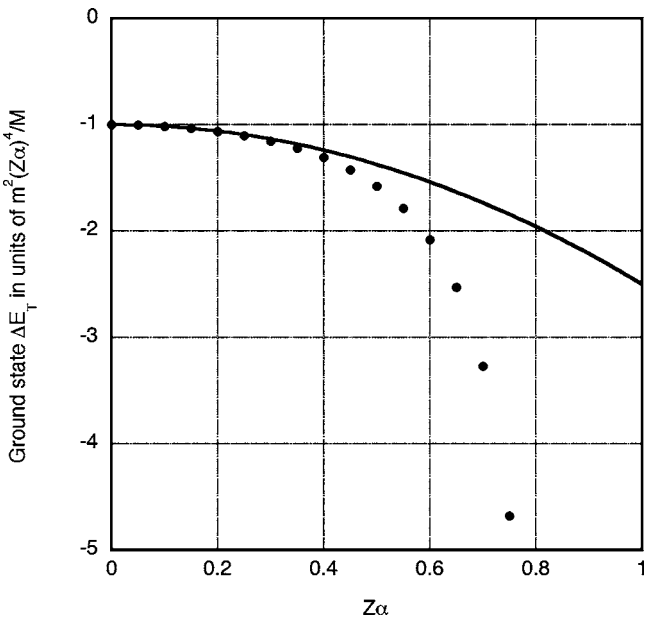

FIG. 2. Plot of ΔE_T for the ground state as a function of $Z\alpha$ in units of $m^2(Z\alpha)^4/M$. The data points represent the result of a numerical evaluation of (26) without approximation. The solid curve is the function $-1-(\frac{3}{2})(Z\alpha)^2$, which includes the first relativistic correction. We note that the expansion in $Z\alpha$ works well for small values of Z but fails badly for large Z.

B. Coulomb-Coulomb ladder

The diagram which requires the greatest care is the two-Coulomb photon ladder diagram, as it has a binding singularity. In addition, a new feature, present in a number of loop diagrams when the nucleus is treated as a scalar, is poor convergence in the integration over the fourth component of momentum, q_0, when Coulomb photons are present. Coulomb photon propagators, being independent of q_0, provide no convergence, and the remaining q_0 is nominally logarithmically divergent, though that divergence vanishes by symmetry. We regulate this near divergence by introducing a factor $\Lambda^2/(q_0^2+\Lambda^2)$ and subsequently taking Λ to infinity. This procedure introduces a term that will be shown to cancel when a gauge invariant set of graphs is considered. Including this factor into the diagram of Fig. 1(b) gives the energy shift

$$\Delta E_{\rm CC} = i\frac{(4\pi Z\alpha)^2}{2\tilde{M}}\int\frac{d^4q}{(2\pi)^4}\int\frac{d^3k\,d^3l}{(2\pi)^6}\frac{(2\tilde{M}-q_0)^2}{(\tilde{M}-q_0)^2-\vec{q}^2-M^2+i\delta}\frac{\Lambda^2}{\Lambda^2+q_0^2}\frac{1}{|\vec{k}-\vec{q}|^2|\vec{q}-\vec{l}|^2}\frac{\bar{\psi}(\vec{k})\gamma_0[(\mathcal{E}+q_0)\gamma_0-\vec{\gamma}\cdot\vec{q}+m]\gamma_0\psi(\vec{l})}{[(\mathcal{E}+q_0)^2-\vec{q}^2-m^2+i\delta]}. \tag{33}$$

The Dirac equation can be used to carry out the $\vec{k}$ and $\vec{l}$ integrations, leaving

$$\Delta E_{\rm CC} = \frac{i}{2\tilde{M}}\int\frac{d^4q}{(2\pi)^4}\frac{(2\tilde{M}-q_0)^2}{(\tilde{M}-q_0)^2-\Omega_q^2+i\delta}\frac{\Lambda^2}{\Lambda^2+q_0^2}\frac{\bar{\psi}(\vec{q})(\mathcal{E}\gamma_0-\vec{\gamma}\cdot\vec{q}-\mu)[(\mathcal{E}+q_0)\gamma_0-\vec{\gamma}\cdot\vec{q}+m](\mathcal{E}\gamma_0-\vec{\gamma}\cdot\vec{q}-\mu)\psi(\vec{q})}{[(\mathcal{E}+q_0)^2-\omega_q^2+i\delta]}, \tag{34}$$

where $\Omega_q=\sqrt{\vec{q}^2+M^2}$ and $\omega_q=\sqrt{\vec{q}^2+m^2}$. We note the "mismatch" in the numerator between terms with μ and with m: the former comes from the formalism, and the latter from the electron propagator in the diagram, which is not altered by the choice of formalism. We now carry out the q_0 integration by closing above with Cauchy's theorem: once this is done we are free to introduce a new four-vector $q=(\mathcal{E},\vec{q})$. Three terms result, with the simplest arising from the regulator,

$$\Delta E_{\rm CC1} = \frac{1}{4\tilde{M}}\int\frac{d^3q}{(2\pi)^3}\bar{\psi}(\vec{q})(\not{q}-\mu)\gamma_0(\not{q}-\mu)\psi(\vec{q}). \tag{35}$$

This term contributes in order $m^2(Z\alpha)^4/M$, but as it will be shown to cancel we do not evaluate it explicitly. The other two terms are both nonrecoil, with the most sensitive being

$$\Delta E_{\mathrm{CC2}} = \frac{1}{2\tilde{M}} \int \frac{d^3q}{(2\pi)^3} (\tilde{M}+\Omega_q)^2 \frac{1}{2\Omega_q} \times \frac{\bar{\psi}(\vec{q})(\not{q}-\mu)[(\mathcal{E}+\tilde{M}-\Omega_q)\gamma_0 - \vec{\gamma}\cdot\vec{q}+m](\not{q}-\mu)\psi(\vec{q})}{(\mathcal{E}+\tilde{M}-\Omega_q)^2-\omega_q^2}. \tag{36}$$

If we use the fact that

$$\frac{(\tilde{M}+\Omega_q)^2}{(2\tilde{M})(2\Omega_q)} = 1 + O(1/M^2) \tag{37}$$

this simplifies to

$$\Delta E_{\mathrm{CC2}} = \int \frac{d^3q}{(2\pi)^3} \frac{\bar{\psi}(\vec{q})(\not{q}-\mu)[(\mathcal{E}+\tilde{M}-\Omega_q)\gamma_0 - \vec{\gamma}\cdot\vec{q}+m](\not{q}-\mu)\psi(\vec{q})}{(\mathcal{E}+\tilde{M}-\Omega_q)^2-\omega_q^2}. \tag{38}$$

We proceed by rearranging the interior numerator in the above as follows:

$$\begin{aligned}
&\gamma^0(\mathcal{E}+\tilde{M}-\Omega_q) - \vec{\gamma}\cdot\vec{q} + m \\
&\quad = (\not{q}+\mu) + \gamma^0(\tilde{M}-\Omega_q) + (m-\mu) \\
&\quad = (\not{q}+\mu) + \frac{m}{M}\left\{\gamma^0\left(m - \frac{\vec{q}^2}{2m}\right) + m\right\} \\
&\quad = (\not{q}+\mu) + \frac{m}{M}\left\{\gamma^0\mathcal{E} + \gamma^0(m-\mathcal{E}) + m - \gamma^0\frac{\vec{q}^2}{2m}\right\} \\
&\quad = (\not{q}+\mu) + \frac{m}{M}\left\{(\not{q}+\mu) + \gamma^0(m-\mathcal{E}) + \vec{\gamma}\cdot\vec{q} - \gamma^0\frac{\vec{q}^2}{2m}\right\},
\end{aligned} \tag{39}$$

where in the last manipulation we have replaced m with μ, with the difference being higher order in $1/M$. If we now define $\kappa = q^2 - \mu^2$ and restore the factors $\not{q}-\mu$ on the left and right of the interior numerator we get

$$\kappa\left(1+\frac{m}{M}\right)(\not{q}-\mu) + \frac{m}{M}(\not{q}-\mu)\left[\gamma^0(m-\mathcal{E}) + \vec{\gamma}\cdot\vec{q} - \gamma^0\frac{\vec{q}^2}{2m}\right] \times (\not{q}-\mu). \tag{40}$$

We further make the expansion of the denominator

$$\begin{aligned}
&(\mathcal{E}+\tilde{M}-\Omega_q)^2 - \omega_q^2 \\
&\quad = (\mathcal{E}^2 - \vec{q}^2 - \mu^2) + 2\mathcal{E}(\tilde{M}-\Omega_q) - (m^2-\mu^2) + O(1/M^2) \\
&\quad = \kappa + \frac{\mathcal{E}}{M}(2m^2 - \vec{q}^2) - 2m^3/M + O(1/M^2) \\
&\quad = \kappa + \frac{1}{M}\{\mathcal{E}(\mathcal{E}^2 - \vec{q}^2 - m^2) - \mathcal{E}^3 + 3\mathcal{E}m^2 - 2m^3\} + \cdots \\
&\quad = \kappa + \frac{1}{M}\{\mathcal{E}\kappa - (m-\mathcal{E})^2(2m+\mathcal{E}) + \cdots\} \\
&\quad = \kappa\left[1 + \frac{\mathcal{E}}{M} - \frac{(m-\mathcal{E})^2(2m+\mathcal{E})}{M\kappa} + \cdots\right].
\end{aligned} \tag{41}$$

Combining these two forms then gives

$$\begin{aligned}
\Delta E_{\mathrm{CC2}} = \int \frac{d^3q}{(2\pi)^3}\bar{\psi}(\vec{q})(\not{q}-\mu)\Bigg\{1 &+ \frac{(m-\mathcal{E})}{M} \\
&+ \frac{(m-\mathcal{E})^2(2m+\mathcal{E})}{M\kappa} \\
&+ \frac{m}{M\kappa}\left(\gamma^0(m-\mathcal{E}) + \vec{\gamma}\cdot\vec{q} - \gamma^0\frac{\vec{q}^2}{2m}\right)(\not{q}-\mu)\Bigg\}\psi(\vec{q}).
\end{aligned} \tag{42}$$

If we label the terms in the curly brackets in (42) parts 1–6, the various contributions are

$$\Delta E_{\mathrm{CC21}} = \langle V\rangle_{\mathrm{Dirac}}, \tag{43}$$

$$\Delta E_{\mathrm{CC22}} = \frac{m}{M} m(Z\alpha)^4\left\{\frac{-1}{2n^4}\right\}, \tag{44}$$

$$\Delta E_{\mathrm{CC23}} = \frac{m}{M} m(Z\alpha)^4\left\{\frac{3}{8n^4}\right\}, \tag{45}$$

$$\Delta E_{\mathrm{CC24}} = \frac{m}{M} m(Z\alpha)^4\left\{\frac{-1}{4n^4}\right\}, \tag{46}$$

$$\Delta E_{\mathrm{CC25}} = \frac{m}{M} m(Z\alpha)^4\left\{\frac{-1}{2n^4} + \frac{2}{n^3(2\ell+1)} - \frac{\delta_{\ell,0}}{n^3}\right\} - \frac{m}{M}\langle 2H_{\mathrm{SO}}\rangle, \tag{47}$$

$$\Delta E_{\mathrm{CC26}} = \frac{m}{M} m (Z\alpha)^4 \left\{ \frac{-1}{4n^4} + \frac{1}{n^3(2\ell+1)} \right\}. \tag{48}$$

To cancel the factor of κ in the denominator, we note that its nonrelativistic limit is $-\vec{q}^2 - (\mu Z\alpha)^2/n^2$, so that the Schrödinger equation reads

$$\frac{-\kappa}{2\mu}\phi_{\mathrm{NR}}(\vec{q}) = 4\pi Z\alpha \int \frac{d^3p}{(2\pi)^3} \frac{1}{|\vec{q}-\vec{p}|^2}\phi_{\mathrm{NR}}(\vec{p}). \tag{49}$$

The strategy for the last three terms is then to "undo" the Dirac equation so that the Coulomb potential is explicitly present, take the nonrelativistic limit as in Eq. (27), and then use the Schrödinger equation. We illustrate this with ΔE_{CC25},

$$\begin{aligned}
\Delta E_{\mathrm{CC25}} &= \int \frac{d^3q}{(2\pi)^3} \frac{m}{M\kappa} \bar{\psi}(\vec{q})(\not{q}-\mu)\vec{\gamma}\cdot\vec{q}(\not{q}-\mu)\psi(\vec{q}) \\
&= \frac{(4\pi Z\alpha)^2}{(2\pi)^9} \int \frac{d^3k d^3q d^3l}{|\vec{k}-\vec{q}|^2|\vec{q}-\vec{l}|^2} \frac{m}{M\kappa} \bar{\psi}(\vec{k})\gamma_0\vec{\gamma}\cdot\vec{q}\gamma_0\psi(\vec{l}) \\
&\approx -\frac{(4\pi Z\alpha)^2}{(2\pi)^9} \int \frac{d^3k d^3q d^3l}{|\vec{k}-\vec{q}|^2|\vec{q}-\vec{l}|^2} \frac{m}{2M\kappa} \phi^{\dagger}{}_{\mathrm{NR}}(\vec{k}) \\
&\quad \times (\vec{\sigma}\cdot\vec{q}\vec{\sigma}\cdot\vec{l} + \vec{\sigma}\cdot\vec{k}\vec{\sigma}\cdot\vec{q})\phi_{\mathrm{NR}}(\vec{l}) \\
&\approx \frac{4\pi Z\alpha}{(2\pi)^6} \int \frac{d^3q d^3l}{|\vec{q}-\vec{l}|^2} \frac{1}{2mM} \phi^{\dagger}{}_{\mathrm{NR}}(\vec{q}) \\
&\quad \times [\vec{q}\cdot\vec{l} + i\vec{\sigma}\cdot(\vec{q}\times\vec{l})]\phi_{\mathrm{NR}}(\vec{l}).
\end{aligned} \tag{50}$$

The total contribution of term CC2 is then

$$\begin{aligned}
\Delta E_{\mathrm{CC2}} &= \langle V \rangle_{\mathrm{Dirac}} + \frac{m}{M} m (Z\alpha)^4 \left\{ \frac{-9}{8n^4} - \frac{\delta_{\ell,0}}{n^3} + \frac{3}{n^3(2\ell+1)} \right\} \\
&\quad - \frac{m}{M}\langle 2H_{\mathrm{SO}} \rangle,
\end{aligned} \tag{51}$$

where the formalism subtracts off the first, nonrecoil term. It is of interest that had we used the formalism with $\mathcal{E} \to \epsilon$, $\tilde{M} \to M$ mentioned above, the cancellation, while still removing the nonrecoil term, would leave a contribution that can be shown to start with the term $m^2(Z\alpha)^2/2Mn^2$, the standard reduced mass contribution to the nonrelativistic energy. As we have chosen to build this into our lowest order solution, the cancellation is finer, and leaves terms starting in order $m^2(Z\alpha)^4/M$.

The remaining part of the CC calculation involves closing around a negative energy electron pole, which, while leading to higher powers of $Z\alpha$ than when the nuclear pole is encircled, is also nonrecoil. Its full contribution is

$$\begin{aligned}
\Delta E_{\mathrm{CC3}} &= \frac{1}{2\tilde{M}} \int \frac{d^3q}{(2\pi)^3 2\omega_q} (2\tilde{M} + \mathcal{E} + \omega_q)^2 \\
&\quad \times \frac{\bar{\psi}(\vec{q})(\not{q}-\mu)[-\omega_q\gamma_0 - \vec{\gamma}\cdot\vec{q} + m](\not{q}-\mu)\psi(\vec{q})}{(\mathcal{E}+\tilde{M}+\omega_q)^2 - \Omega_q^2},
\end{aligned} \tag{52}$$

but we can approximate $\mathcal{E}=m$, $\omega_q=m$, and $\Omega_q=M$ in the nuclear propagator, leading to the simpler expression

$$\begin{aligned}
\Delta E_{\mathrm{CC3}} &= \frac{1}{2\tilde{M}} \int \frac{d^3q}{(2\pi)^3 2\omega_q} \frac{(2\tilde{M}+2m)^2}{(\tilde{M}+2m)^2 - M^2} \bar{\psi}(\vec{q})(\not{q}-\mu) \\
&\quad \times [-\omega_q\gamma_0 - \vec{\gamma}\cdot\vec{q} + m](\not{q}-\mu)\psi(\vec{q}).
\end{aligned} \tag{53}$$

We will show below that although this term is nonrecoil, starting in order $m(Z\alpha)^5$, the nonrecoil part cancels with a contribution from the crossed Coulomb ladder.

C. Crossed Coulomb diagram

The crossed ladder (CCX) diagram of Fig. 1(c) is given by

$$\begin{aligned}
\Delta E_{\mathrm{CCX}} &= i\frac{(4\pi Z\alpha)^2}{2\tilde{M}} \int \frac{d^4q}{(2\pi)^4} \int \frac{d^3k\, d^3l}{(2\pi)^6} \frac{(2\tilde{M}+q_0)^2}{(\tilde{M}+q_0)^2 - |\vec{q}-\vec{k}-\vec{l}|^2 - M^2 + i\delta} \\
&\quad \times \frac{\Lambda^2}{q_0^2+\Lambda^2} \frac{1}{|\vec{k}-\vec{q}|^2|\vec{q}-\vec{l}|^2} \frac{\bar{\psi}(\vec{k})\gamma_0[(\mathcal{E}+q_0)\gamma_0 - \vec{\gamma}\cdot\vec{q} + m]\gamma_0\psi(\vec{l})}{[(\mathcal{E}+q_0)^2 - \omega_q^2 + i\delta]}.
\end{aligned} \tag{54}$$

Taking a pole of the regulator term gives the same result as with the ladder, thus doubling ΔE_{CC1}. While the pole from the nuclear line enters in the entirely negligible order m^5/M^4, the electron pole contributes at the level of nonrecoil fine structure, and is

$$\Delta E_{\mathrm{CCX}} = \frac{(4\pi Z\alpha)^2}{2\tilde{M}} \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3k\, d^3l}{(2\pi)^6} \frac{(2\tilde{M}-\mathcal{E}-\omega_q)^2}{(\tilde{M}-\mathcal{E}-\omega_q)^2 - |\vec{q}-\vec{k}-\vec{l}|^2 - M^2} \frac{1}{2\omega_q} \frac{1}{|\vec{k}-\vec{q}|^2|\vec{q}-\vec{l}|^2} \bar{\psi}(\vec{k})\gamma_0[-\omega_q\gamma_0 - \vec{\gamma}\cdot\vec{q} + m]\gamma_0\psi(\vec{l}). \tag{55}$$

It is again legitimate to make the approximations $\mathcal{E}=m$, $\omega_q=m$, and $M^2+|\vec{q}-\vec{k}-\vec{l}|^2=M^2$, and further use of the Dirac equation gives the approximation

$$\Delta E_{\mathrm{CCX}}=\frac{1}{2\tilde{M}}\int\frac{d^3q}{(2\pi)^3 2\omega_q}\frac{(2\tilde{M}-2m)^2}{(\tilde{M}-2m)^2-M^2}\bar{\psi}(\vec{q})(\not{q}-\mu)\times[-\omega_q\gamma_0-\vec{\gamma}\cdot\vec{q}+m](\not{q}-\mu)\psi(\vec{q}). \tag{56}$$

This term can now be combined with the CC3 contribution, and the nonrecoil term can easily be seen to cancel. There remains a nonvanishing recoil term of order $m^2(Z\alpha)^5/M$,

$$\Delta E_{\mathrm{CC3}}+\Delta E_{\mathrm{CCX}}=\frac{1}{2\tilde{M}}\int\frac{d^3q}{(2\pi)^3 2\omega_q}\bar{\psi}(\vec{q})(\not{q}-\mu)\times[-\omega_q\gamma_0-\vec{\gamma}\cdot\vec{q}+m](\not{q}-\mu)\psi(\vec{q}), \tag{57}$$

which we keep, although beyond the order of interest we are considering here, as it has an interesting connection with the seagull diagram.

D. Seagull diagram

A different feature of our formalism is the presence of so-called seagull graphs. In the Coulomb gauge the seagull graph consists of a Coulomb-Coulomb (CC) term and a transverse-transverse term (TT), with the latter beyond our present order of interest. Again regularizing the q_0 integration, the CC seagull graph [see Fig. 1(d)] contributes

$$\Delta E_{\mathrm{CCs}}=-2i\frac{(4\pi Z\alpha)^2}{2\tilde{M}}\int\frac{d^4q}{(2\pi)^4}\int\frac{d^3k\,d^3l}{(2\pi)^6}\frac{\Lambda^2}{\Lambda^2+q_0^2}\frac{1}{|\vec{k}-\vec{q}|^2|\vec{q}-\vec{l}|^2}\frac{\bar{\psi}(\vec{k})\gamma_0[(\mathcal{E}+q_0)\gamma_0-\vec{\gamma}\cdot\vec{q}+m]\gamma_0\psi(\vec{l})}{[(\mathcal{E}+q_0)^2-\vec{q}^2-m^2+i\delta]}. \tag{58}$$

If we again close above to carry out the q_0 integration the regulator term contributes $-2\Delta E_{\mathrm{CC1}}$: as ΔE_{CC1} was doubled from the crossed Coulomb diagram, this completes the cancellation of contributions arising from the regulator term. The other pole picks up a negative energy electron contribution, and gives, using the Dirac equation,

$$\Delta E_{\mathrm{CCs}}=-2\frac{1}{2\tilde{M}}\int\frac{d^3q}{(2\pi)^3 2\omega_q}\bar{\psi}(\vec{q})(\not{q}-\mu)[-\omega_q\gamma_0-\vec{\gamma}\cdot\vec{q}+m]\times(\not{q}-\mu)\psi(\vec{q}). \tag{59}$$

The net result is that the only role of the seagull diagram to order $m^2(Z\alpha)^4/M$ is in canceling the regulator terms from the ladder and crossed ladder, and in addition it combines with $m^2(Z\alpha)^5/M$ terms coming from the negative energy pole terms in those diagrams.

IV. TOTAL AT ORDER $(Z\alpha)^4$

The combination of the CC, CCX, CCs, T, and C graphs gives

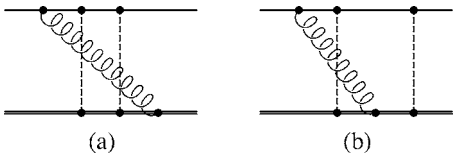

FIG. 3. Graphs contributing to the Salpeter correction of order $m^2(Z\alpha)^5/M$. In graph (a) a transverse photon crosses two-Coulomb photons. In graph (b) the transverse photon crosses a single-Coulomb photon, with a Coulomb ladder photon on the side. There are two graphs like (b) since the ladder photon can be on either side.

$$\Delta E=\frac{m}{M}m(Z\alpha)^4\left\{\frac{-1}{8n^4}\right\}. \tag{60}$$

In order to find the total recoil contribution at this order, one must combine this with the recoil contribution from $\mu[f(n,j)-1]$, which is $-(m^2/M)[f(n,j)-1]$, where $f(n,j)=\epsilon/m$ is defined through Eq. (5). The total recoil contribution through terms of order $(Z\alpha)^4$ is

$$\Delta E_{\mathrm{recoil}}=\frac{m^2}{M}\left\{-[f(n,j)-1]-\frac{(Z\alpha)^4}{8n^4}\right\}=\frac{m^2}{M}\left\{\frac{(Z\alpha)^2}{2n^2}+(Z\alpha)^4\left(\frac{-1}{2n^4}+\frac{1}{2n^3(j+1/2)}\right)\right\}. \tag{61}$$

This is the known Barker and Glover result [22] for the recoil contribution at this order.

V. SALPETER CORRECTION

One of the first accomplishments of a fully relativistic treatment of the two-body bound state problem was Salpeter's discovery [16] that corrections of order $\alpha m/M$ times fine structure were present in hydrogenlike atoms: use of the older formalism of the Breit equation had found no such contributions [23]. While we are not calculating all such terms here, we show how they arise from one and higher Coulomb exchanges that are crossed by a transverse photon, illustrating with the graph of Fig. 3(a). This gives rise to the somewhat complicated expression

$$\Delta E = -\frac{(4\pi Z\alpha)^3}{2M}\int\frac{d^4k}{(2\pi)^4}\int\frac{d^4l}{(2\pi)^4}\int\frac{d^3p\,d^3p'}{(2\pi)^6}\frac{(2M+2k_0-l_0)}{(M+k_0)^2-|\vec{k}-\vec{p}|^2-M^2+i\delta}$$
$$\times\frac{(2M+k_0-l_0)}{[(M+k_0-l_0)^2-|\vec{k}-\vec{l}|^2-M^2+i\delta]}\frac{(k-2p)_j(\delta_{ij}-k_ik_j/\vec{k}^2)}{k_0^2-\vec{k}^2+i\delta}\frac{1}{|\vec{l}-\vec{p}|^2}\frac{1}{|\vec{k}-\vec{l}+\vec{p}'|^2}$$
$$\times\bar{\psi}(\vec{p}')\gamma_i\frac{1}{(\mathcal{E}+k_0)\gamma_0-\vec{\gamma}\cdot(\vec{k}+\vec{p}')-m+i\delta}\gamma_0\frac{1}{(\mathcal{E}+l_0)\gamma_0-\vec{\gamma}\cdot\vec{l}-m+i\delta}\gamma_0\psi(\vec{p}). \tag{62}$$

We wish to show that this expression is dominated by a term that contains part of the Dirac-Coulomb propagator of Eq. (2). Specifically, if we expand the momentum space form of that equation in powers of the Coulomb potential, the term involving one potential is

$$S_F^{1C}(\vec{p}',\vec{p};E)=\frac{1}{E\gamma_0-\vec{\gamma}\cdot\vec{p}'-m}\frac{-4\pi Z\alpha}{|\vec{p}'-\vec{p}|^2}\gamma_0\frac{1}{E\gamma_0-\vec{\gamma}\cdot\vec{p}-m}, \tag{63}$$

where the distinction between m and μ is dropped in this section as the graph being considered has a factor m/M. To see how this arises from the graph of Fig. 3(a), we first close the k_0 contour above and take the transverse-photon pole to get

$$\Delta E = i\frac{(4\pi Z\alpha)^3}{4M}\int\frac{d^3k}{(2\pi)^3}\frac{1}{k}\int\frac{d^4l}{(2\pi)^4}\int\frac{d^3p\,d^3p'}{(2\pi)^6}\frac{(2M-2k-l_0)}{(M-k)^2-|\vec{k}-\vec{p}|^2-M^2}\frac{(2M-k-l_0)}{[(M-k-l_0)^2-|\vec{k}-\vec{l}|^2-M^2+i\delta]}(-2p)_j$$
$$\times\left(\delta_{ij}-\frac{k_ik_j}{\vec{k}^2}\right)\frac{1}{|\vec{l}-\vec{p}|^2}\frac{1}{|\vec{k}-\vec{l}+\vec{p}'|^2}\bar{\psi}(\vec{p}')\gamma_i\frac{1}{(\mathcal{E}-k)\gamma_0-\vec{\gamma}\cdot(\vec{k}+\vec{p}')-m}\gamma_0\frac{1}{(\mathcal{E}+l_0)\gamma_0-\vec{\gamma}\cdot\vec{l}-m+i\delta}\gamma_0\psi(\vec{p}). \tag{64}$$

Because we are dropping terms of order m^3/M^2, the first nuclear denominator simplifies to $-2Mk$, and further carrying out the l_0 integration by closing the above gives a term from the second nuclear denominator that forces $l_0=-k$, giving

$$\Delta E = -\frac{(4\pi Z\alpha)^3}{4M}\int\frac{d^3k}{(2\pi)^3}\frac{1}{k^2}\int\frac{d^3l}{(2\pi)^3}\int\frac{d^3p\,d^3p'}{(2\pi)^6}$$
$$\times(-2p)_j\left(\delta_{ij}-\frac{k_ik_j}{\vec{k}^2}\right)\frac{1}{|\vec{l}-\vec{p}|^2}\frac{1}{|\vec{k}-\vec{l}+\vec{p}'|^2}\bar{\psi}(\vec{p}')\gamma_i$$
$$\times\frac{1}{(\mathcal{E}-k)\gamma_0-\vec{\gamma}\cdot(\vec{k}+\vec{p}')-m}\gamma_0\frac{1}{(\mathcal{E}-k)\gamma_0-\vec{\gamma}\cdot\vec{l}-m}$$
$$\times\gamma_0\psi(\vec{p}). \tag{65}$$

Using Eq. (63) then allows us to write

$$\Delta E = \frac{(4\pi Z\alpha)^2}{4M}\int\frac{d^3k}{(2\pi)^3}\frac{1}{k^2}\int\frac{d^3l}{(2\pi)^3}\int\frac{d^3p\,d^3p'}{(2\pi)^6}(-2p)_j$$
$$\times\left(\delta_{ij}-\frac{k_ik_j}{\vec{k}^2}\right)\frac{1}{|\vec{l}-\vec{p}|^2}\bar{\psi}(\vec{p}')\gamma_iS_F^{1C}(\vec{p}'+\vec{k},\vec{l};\mathcal{E}-k)\gamma_0\psi(\vec{p}). \tag{66}$$

The same kinds of argument apply for any number of Coulomb exchanges, allowing the replacement of S_F^{1C} with S_F. Care is required, however, for the first term of the expansion of S_F, which requires an ultraviolet cutoff in the k integration because of the approximations we have made. However, this term is finite when simply treated as a one-loop diagram. The actual calculation of the Salpeter correction would involve evaluating the one-loop diagram without approximation and then evaluating the above expression and higher Coulomb exchanges by using S_F-S_0, a technique that is standard in self-energy calculations. Replacing S_F^{1C} in the above with the spectral representation of S_F then gives

$$\Delta E = \frac{(4\pi Z\alpha)^2}{4M}\int\frac{d^3k}{(2\pi)^3}\frac{1}{k^2}\int\frac{d^3l}{(2\pi)^3}$$
$$\times\int\frac{d^3p\,d^3p'}{(2\pi)^6}(-2p)_j\left(\delta_{ij}-\frac{k_ik_j}{\vec{k}^2}\right)\frac{1}{|\vec{l}-\vec{p}|^2}$$
$$\times\sum_m\frac{\bar{\psi}(\vec{p}')\gamma_i\psi_m(\vec{p}'+\vec{k})\bar{\psi}_m(\vec{l})\gamma_0\psi(\vec{p})}{\mathcal{E}-E_m-k}. \tag{67}$$

Replacing $-2p_j$ with $-2(p-l)_j$ leads to the integral

$$\int\frac{d^3p\,d^3l}{(2\pi)^6}(p-l)_j\frac{4\pi Z\alpha}{|\vec{l}-\vec{p}|^2}\bar{\psi}_m(\vec{l})\gamma_0\psi(\vec{p})$$
$$=-iZ\alpha\int d^3x\frac{x_j}{x^3}\bar{\psi}_m(\vec{x})\gamma_0\psi(\vec{x})=(\mathcal{E}-E_m)\langle m|p_j|0\rangle, \tag{68}$$

where $\mathcal{E}$ is the Dirac energy of the state ψ of interest, here taken to be the ground state. Equations (67) and (68) lead to the relativistic generalization of Salpeter's [16] Eq. (45). The replacement of $-2p_j$ by $-2(p-l)_j$ arises from consideration

of the reducible graph shown in Fig. 3(b), which comes from the formalism when the three-photon exchange is considered, as described in Ref. [25]. In this diagram there are two nuclear propagators that depend on l_0, with one of them leading to the replacement mentioned above, and the other to a bound state singularity canceled by the formalism.

VI. NRQED CALCULATION OF THE ENERGY SHIFT TO ORDER $(Z\alpha)^4$ INCLUDING RECOIL

We base our expression of NRQED on the work of Kinoshita and Nio [26]. The NRQED Lagrangian for a particle of spin-$\frac{1}{2}$ and one of spin-0 has the form

$$\mathcal{L}=\psi^\dagger\left\{iD_t+\frac{\vec{D}^2}{2m}+\frac{\vec{D}^4}{8m^3}+c_F\frac{e\vec{\sigma}\cdot\vec{B}}{2m}+c_D\frac{e(\vec{D}\cdot\vec{E}-\vec{E}\cdot\vec{D})}{8m^2}+c_S\frac{ie\vec{\sigma}\cdot(\vec{D}\times\vec{E}-\vec{E}\times\vec{D})}{8m^2}+\cdots\right\}\psi+\phi\left\{iD_t+\frac{\vec{D}^2}{2M}+\cdots\right\}\phi+\mathcal{L}_{\rm EM},\tag{69}$$

where $D_t=\partial_t+ieA^0$ and $\vec{D}=\vec{\partial}-ie\vec{A}$ for the electron, and similarly but with $e\to -Ze$ for the nucleus. Electromagnetism is described by the usual Lagrangian $\mathcal{L}_{\rm EM}=(-\frac{1}{4})F_{\mu\nu}F^{\mu\nu}$, and we use the Coulomb gauge in our calculations. In terms of Feynman rules, we build on those given by Kinoshita and Nio in their Fig. 3. The new rules include a Coulomb vertex for the nucleus $-Ze$, a dipole vertex for the nucleus $Ze(\vec{p}'+\vec{p})/(2M)$, and a propagator for the nucleus $[E-\vec{p}^2/(2M)+i\epsilon]^{-1}$. The rule is to multiply all propagators by i, all vertices by $-i$, and to include an overall factor of i when calculating energy shifts. Loop integrals are done over all momenta with the measure $d^4k/(2\pi)^4$. The Bethe-Salpeter equation for NRQED (with lowest order propagators and vertices) is exactly the Schrödinger-Coulomb equation with reduced mass, which is also described in Kinoshita and Nio. We use the symbol $\Psi(p)$ for the NRQED Bethe-Salpeter wave function. For example, the ground state wave function is

$$\Psi(p)=(2\pi)\delta(p_0)\psi(\vec{p}),\tag{70}$$

where

$$\psi(\vec{p})=\frac{16\pi\xi^{5/2}}{(\vec{p}^2+\xi^2)^2}\chi_{-1\mu}\tag{71}$$

with $\xi=\mu Z\alpha$ and, for example, $\chi^\dagger_{-1,1/2}=-1/\sqrt{4\pi}(1,0)$.

The relevant graphs for the calculation of energies up to $O((Z\alpha)^4)$ and including recoil (to first order: m/M) are shown in Fig. 4. In the calculation of bound state NRQED graphs we take the electron line to enter with momentum $(\mathcal{E}_0,\vec{p})$ and the nucleus with momentum $(0,-\vec{p})$, where $\mathcal{E}_0=-\mu(Z\alpha)^2/(2n^2)$ is the Bohr energy level.

The crossed Coulomb ladder [Fig. 4(a)] has the form

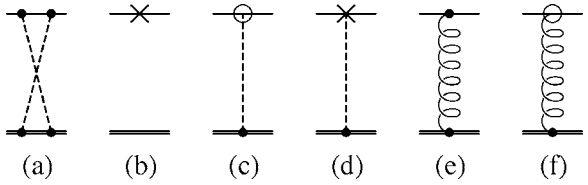

FIG. 4. NRQED contributions to energies at order $m^2(Z\alpha)^4/M$. Graph (a) is the two-Coulomb crossed ladder, (b) represents the p^4 relativistic kinetic energy correction to the electron line, (c) is the spin-orbit correction to the electron line (with Coulomb photon exchange), (d) is the Darwin correction to the electron line (with Coulomb photon exchange), (e) shows transverse photon exchange with dipole vertices on both electron and nuclear lines, and (f) represents transverse photon exchange with a Fermi vertex on the electron line and a dipole vertex on the nuclear line.

$$\Delta E_{\rm CCX}=i\int\frac{d^3q}{(2\pi)^3}\frac{d^4l}{(2\pi)^4}\frac{d^3p}{(2\pi)^3}\psi^\dagger(\vec{q})\times(-ie)\frac{i}{l_0+\mathcal{E}_0-\vec{l}^2/2m+i\epsilon}(-ie)\psi(\vec{p})\times\frac{i}{(\vec{q}-\vec{l})^2}\frac{i}{(\vec{l}-\vec{p})^2}(iZe)\frac{i}{l_0-[(\vec{l}-\vec{p}-\vec{q})^2]/2M+i\epsilon}\times(iZe).\tag{72}$$

The poles of the l_0 integral

$$\int\frac{dl_0}{2\pi i}\frac{1}{l_0+\mathcal{E}_0-\vec{l}^2/2m+i\epsilon}\frac{1}{l_0-[(\vec{l}-\vec{p}-\vec{q})^2]/2m+i\epsilon}=0.\tag{73}$$

are both on the same side of the real axis. It follows that the l_0 integral vanishes, as does the crossed Coulomb ladder contribution: $\Delta E_{\rm CCX}=0$.

The relativistic kinetic energy correction [Fig. 4(b)] is

$$\Delta E_K=i\int\frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})(-i)\left(\frac{-\vec{p}^4}{8m^3}\right)(2\pi)^3\delta(\vec{p}-\vec{q})\psi(\vec{p})=\left(\frac{\mu}{m}\right)^3\langle H_K\rangle\approx\left(1-\frac{3m}{M}\right)\langle H_K\rangle,\tag{74}$$

where

$$\langle H_K\rangle=\int\frac{d^3p}{(2\pi)^3}\psi^\dagger(\vec{p})\left(\frac{-\vec{p}^4}{8\mu^3}\right)\psi(\vec{p})=\mu(Z\alpha)^4\left(\frac{3}{8n^4}-\frac{1}{(2\ell+1)n^3}\right).\tag{75}$$

The spin-orbit correction to the electron line [Fig. 4(c)] is

$$\Delta E_{\rm SO} = i\int \frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})(-i)\frac{ie}{4m^2}(\vec{q}\times\vec{p})\cdot\vec{\sigma}\psi(\vec{p})\frac{i}{\vec{k}^2}(iZe)$$
$$= \frac{i}{4m^2}\int \frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})(\vec{q}\times\vec{p}\cdot\vec{\sigma})\psi(\vec{p})V_C(\vec{k})$$
$$= \left(\frac{\mu}{m}\right)^2\langle H_{\rm SO}\rangle \approx \left(1-\frac{2m}{M}\right)\langle H_{\rm SO}\rangle, \tag{76}$$

where $\vec{k}=\vec{q}-\vec{p}$ and

$$\langle H_{\rm SO}\rangle = \left\langle \frac{Z\alpha}{4\mu^2 r^3}\vec{L}\cdot\vec{\sigma}\right\rangle \tag{77}$$

as before.

The Darwin correction to the electron line [Fig. 4(d)] is

$$\Delta E_D = i\int \frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})\frac{ie}{8m^2}|\vec{q}-\vec{p}|^2\psi(\vec{p})\frac{i}{\vec{k}^2}(iZe)$$
$$= \left(\frac{\mu}{m}\right)^2\frac{4\pi Z\alpha}{8\mu^2}|\psi(0)|^2 \approx \left(1-\frac{2m}{M}\right)\langle H_D\rangle, \tag{78}$$

where

$$\langle H_D\rangle = \frac{4\pi Z\alpha}{8\mu^2}|\psi(0)|^2 = \mu(Z\alpha)^4\frac{\delta_{\ell,0}}{2n^3}. \tag{79}$$

The dipole-dipole transverse-photon exchange contribution [Fig. 4(e)] is

$$\Delta E_{\rm DD} = i\int \frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})\frac{ie}{2m}(p+q)^i\frac{i\delta^T_{ij}(\vec{k})}{-\vec{k}^2}$$
$$\times\psi(\vec{p})\frac{-iZe}{2M}(-p-q)^j$$
$$= \frac{-4\pi Z\alpha}{mM}\int \frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})\frac{\vec{p}^2\vec{q}^2-(\vec{p}\cdot\vec{q})^2}{\vec{k}^4}\psi(\vec{p})$$
$$= \frac{m}{M}\langle H_R\rangle, \tag{80}$$

just as in the relativistic calculation of one-transverse-photon exchange. We note that the expectation value $\langle H_R\rangle$ can be written as

$$\langle H_R\rangle = \left\{\frac{1}{n^4}+\frac{\delta_{\ell,0}}{n^3}-\frac{3}{n^3(2\ell+1)}\right\}\mu(Z\alpha)^4$$
$$= 3\langle H_K\rangle + 2\langle H_D\rangle - \frac{1}{8n^4}\mu(Z\alpha)^4. \tag{81}$$

Finally, the Fermi correction [Fig. 4(f)] is

$$\Delta E_F = \frac{-4\pi Z\alpha}{4mM}\int \frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})$$
$$\times\frac{-i\epsilon_{ijk}(q-p)_j\sigma_k\delta^T_{\rm in}(\vec{k})(p+q)_n}{\vec{k}^2}\psi(\vec{p})$$
$$= \frac{2i}{4mM}\int \frac{d^3q\,d^3p}{(2\pi)^6}\psi^\dagger(\vec{q})\vec{q}\times\vec{p}\cdot\vec{\sigma}\psi(\vec{p})V_C(\vec{k})$$
$$= \frac{m}{M}\left\langle \frac{Z\alpha}{2m^2r^3}\vec{L}\cdot\vec{\sigma}\right\rangle \approx \frac{m}{M}\langle 2H_{\rm SO}\rangle. \tag{82}$$

The sum of all contributions is

$$\Delta E = \Delta E_{\rm CCX}+\Delta E_K+\Delta E_{\rm SO}+\Delta E_D+\Delta E_{\rm DD}+\Delta E_F$$
$$= \left(1-\frac{3m}{M}\right)\langle H_K\rangle + \left(1-\frac{2m}{M}\right)\langle H_{\rm SO}\rangle + \left(1-\frac{2m}{M}\right)\langle H_D\rangle$$
$$+\frac{m}{M}\left(3\langle H_K\rangle + 2\langle H_D\rangle - \frac{1}{8n^4}\mu(Z\alpha)^4\right) + \frac{m}{M}\langle 2H_{\rm SO}\rangle$$
$$= \langle H_K + H_{\rm SO} + H_D\rangle - \frac{m^2}{M}\frac{(Z\alpha)^4}{8n^4}, \tag{83}$$

which again is the known Barker and Glover result for the fine structure with the recoil correction.

VII. CONCLUSIONS

A form of the Bethe-Salpeter equation of particular simplicity has been introduced that can be applied to the entire hydrogen isoelectronic sequence. We have shown that the power series expansion of the 1T kernel is nonperturbative at high Z, demonstrating the need for a complete numerical calculation for all kernels. Such a calculation has been done using a Green's function formalism by Shabaev and collaborators [11,12], but it is always desirable in QED to have checks on these complex calculations. We are presently calculating the remaining one-loop diagrams that enter in order $m^2/M(Z\alpha)^5$. As an indication of the numerical importance of these calculations for the transition discussed in the Introduction, we note that Ref. [12] finds a correction of −0.04 eV for the $2p_{1/2}$-$2s$ transition in hydrogenic uranium, to be compared to the 0.207 eV discrepancy presumably dominated by the two-loop Lamb shift. However, this is only part of the effect of recoil for lithiumlike uranium, and the question of relativistic corrections to mass polarization cannot be addressed in our formalism, which is strictly a two-body approach. We are presently investigating the relatively unexplored problem of forming many-particle generalizations of the Bethe-Salpeter equation that have the three-dimensional and relativistic aspects of the equation described in the present work.

ACKNOWLEDGMENTS

The work of J.S. was supported in part by NSF Grant No. PHY-0451842, and grateful thanks are given to K.T. Cheng and the hospitality of LLNL, where this work was started. Useful conversations with S. Morrison are also acknowledged.

APPENDIX

In this appendix we give a fuller description of the present status of the recoil problem, which has advanced well beyond the basically pedagogic example we have used to illustrate our method. As mentioned above, the first application of

the Bethe-Salpeter equation to atomic physics was made by Salpeter [16], who found the correction

$$E_S = \frac{m^2(Z\alpha)^5}{\pi M n^3}\left[-\frac{2}{3}\delta_{l0}\ln(Z\alpha) - \frac{8}{3}\ln k_0(n,l) - \frac{1}{9}\delta_{l0} - \frac{7}{3}a_n\right], \tag{A1}$$

where

$$a_n = -2\delta_{l0}\left[\ln\frac{2}{n} + 1 - \frac{1}{2n} + \sum_{i=1}^{n}\frac{1}{i}\right] + \frac{1-\delta_{l0}}{l(l+1)(2l+1)}, \tag{A2}$$

$\ln k_0(n,l)$ is the Bethe logarithm, and terms of order m^3/M^2 have been dropped. About ten years ago considerable activity was devoted to calculating higher order terms, which can be parametrized as

$$E_R = \frac{m^2(Z\alpha)^6}{Mn^3}D_{60}(n,l,Z\alpha). \tag{A3}$$

Some care is required with this definition, which depends on the formalism. For example, our formalism absorbs some terms of this order into the lowest order energy, but if that energy is defined with m rather than μ those terms would be part of D_{60}. Another source of formalism dependence is the fact that the Barker-Glover contribution of order $m^2/M(Z\alpha)^4$ treated in this paper can be treated as the first term in the $Z\alpha$ expansion of the expression

$$E_{\mathrm{BG}} = -\frac{m^2}{2M}[f(n,j) - 1]^2. \tag{A4}$$

In the following we will assume that terms of order $m^2/M(Z\alpha)^6$, arising from both these sources, have been incorporated into the formalism. The remaining contributions of this order are then associated with the function $D_{60}(n,l,Z\alpha)$. This function can be studied as an expansion in $Z\alpha$, or treated exactly, with our present method intended to provide the latter treatment. As mentioned above, exact results have been obtained by Shabaev *et al.* [11]. Somewhat before these all-order results appeared, Pachucki and Grotch [13], using a method valid for arbitrary Z but applied to the low-Z case, found the first term in the perturbative expansion of $D_{60}(n,l,Z\alpha)$ for s states,

$$D_{60}(n,0,0) = 4\ln 2 - \tfrac{7}{2}. \tag{A5}$$

This result was subsequently confirmed in Ref. [14]. Golosov *et al.* [27], Elkhovskii [28], and Jenschura and Pachucki [29] extended the results to non-s states, finding

$$D_{60}(n,l\neq 0,0) = \left[3 - \frac{l(l+1)}{n^2}\right]\frac{2}{(4l^2-1)(2l+3)}. \tag{A6}$$

However, while these results agree with Ref. [11], we note that different results have been obtained by Yelkhovsky [30], and no explanation for the discrepancy has been found. While generally agreement between the perturbative expansion and all-order methods is strong evidence of correctness, another check of the all-orders method that application of our technique will provide would be of interest. We note finally that further terms in the expansion of $D_{60}(n,0,Z\alpha)$ have been calculated [31], with the result

$$D_{60}(n,0,Z\alpha) = 4\ln 2 - \frac{7}{2} + \frac{11}{30\pi}(Z\alpha)\ln(Z\alpha). \tag{A7}$$

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