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Bound-state self-energy calculation using partial-wave renormalization

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A rigorous method to calculate the first-order self-energy in a model potential is presented. An alternative straightforward way of renormalization is introduced to avoid the commonly used potential expansion implying a large number of diagrams in higher-order QED effects. The divergent mass term is defined in coordinate space and decomposed into a sum over finite partial-wave (l) contributions. The unrenormalized bound self-energy is similarly decomposed into a partial-wave sum and the renormalization is performed for each partial wave. The renormalized sum converges fairly rapidly (the asymptotic behavior is l^{-3}). The method is applied to lithiumlike uranium, for which the electron self-energy in the potential of a point nucleus, as well as the effects of the finite nucleus and of the screening by the remaining electrons on the self-energy, are obtained with an accuracy better than 0.1 eV. The results are in very good agreement with experiment and with calculations recently performed using other techniques.

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I. INTRODUCTION

The precise measurement of transition energies in highly charged heavy ions, for instance the $2p_{1/2}$-$2s_{1/2}$ transition in lithiumlike uranium, recently performed by Schweppe *et al.* [1], has stimulated new efforts to improve the accuracy of QED calculations for such systems [2–5]. Since QED effects scale strongly with Z they are comparable to correlation effects in these heavy systems. To further improve the accuracy on these systems it is necessary to include higher-order QED effects. The usual renormalization scheme would then be quite complicated when considering, for instance, diagrams of the two-photon self-energy type. It is therefore of great interest to see if the standard methods of renormalization can be changed or improved to also yield a realizable calculation scheme for higher-order effects. In this paper we show that the mass-renormalization scheme can be simplified for first-order self-energy, which is the dominant QED contribution. We are now working on extending the procedure to evaluate higher-order contributions [6].

The first-order self-energy for a free electron in a momentum state p is described as the emission and reabsorption of the same virtual photon. This interaction (δm) is already included in the observable mass of the electron $m_{\rm obs} = m_{\rm bare} + \delta m$. For a bound electron the self-energy also gives rise to an additional observable shift. The use of $m_{\rm obs}$ instead of $m_{\rm bare}$ in the equations leads to divergences. By subtracting off a mass term, one corrects for the use of $m_{\rm obs}$ and the equations become renormalized.

The early relativistic self-energy calculations [7,8] were based on an expansion in ($Z\alpha$) of the interaction with the external field, a technique obviously restricted to low or medium-high Z values. A method for computing the bound-state self-energy to all orders in $Z\alpha$ was introduced by Brown, Langer, and Schaefer in 1959 [9,10], and Desiderio and Johnson [11] implemented the method for local potentials. The method was based on a potential expansion of the intermediate bound state into divergent zero-potential and one-potential terms and a convergent many-potential term (Fig. 1). The method suffers, however, from a slow asymptotic behavior (l^{-2}) and is in practice applicable only to high Z ($Z \geq 70$).

By using an analytic variant of the potential expansion, Mohr [12–14] developed a method yielding a high accuracy for Coulomb potentials. In 1991 Blundell and Snyderman [15,16] presented an alternative way of evaluating the self-energy for local potentials. The finite contributions (F1+F2 in Fig. 1) from the zero- and one-potential terms were evaluated analytically and the convergent many-potential term was successfully treated numerically with basis-set techniques, and a comparably rapid partial-wave convergence (l^{-3}) was obtained.

In this Rapid Communication we report an alternative way of calculating the electron self-energy based on a direct renormalization without employing the standard potential expansion [17]. The basic idea is to decompose both the unrenormalized bound-state self-energy and the mass term into divergent sums over finite partial-wave contributions. The renormalization subtraction is then performed at the partial-wave level and a convergent renormalized bound-state self-energy is obtained.

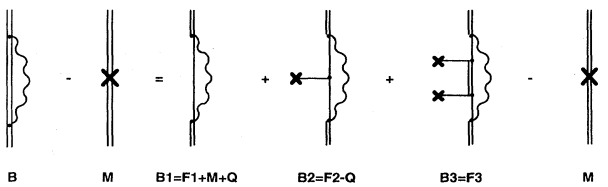

FIG. 1. The renormalized bound-state self-energy (B−M) decomposed into a zero-potential (B1) term, a one-potential (B2) term, and a many-potential (B3) term. M is the mass term and Q a charge divergency which is introduced in this potential expansion. (B−M) can also be written as (F1+F2+F3).

No regularization procedure is needed, since even before the renormalization each partial-wave contribution is finite. The asymptotic behavior in terms of partial waves is proportional to l^{-3}.

II. THEORY

The unrenormalized bound term (B in Fig. 1) can be written as (units where $m_e = c = \hbar = 1$ are used)

$$E_{\rm bound}(a) = \alpha 2\pi \int d^3x_2 d^3x_1 \int \frac{d^3k}{(2\pi)^3}\frac{1}{k}\sum_m \frac{\psi_a^\dagger(\mathbf{x}_2)e^{i\mathbf{k}\cdot\mathbf{x}_2}\alpha_\mu\psi_m(\mathbf{x}_2)\psi_m^\dagger(\mathbf{x}_1)\alpha^\mu e^{-i\mathbf{k}\cdot\mathbf{x}_1}\psi_a(\mathbf{x}_1)}{E_a - E_m - \mathrm{sgn}(E_m)k}$$
$$= \alpha\frac{1}{4\pi^2}\int d^3k\frac{1}{k}\sum_m \frac{\langle a|\alpha_\mu e^{i\mathbf{k}\cdot\mathbf{x}_2}|m\rangle\langle m|e^{-i\mathbf{k}\cdot\mathbf{x}_1}\alpha^\mu|a\rangle}{E_a - E_m - \mathrm{sgn}(E_m)k}, \tag{1}$$

where the sum over m denotes a summation over positive- and negative-energy states. The bound state $\psi_a(\mathbf{x})$ is a solution of the Dirac equation with a potential V, and $\mathbf{k}$ is the virtual photon momentum. By performing the angular part of the $\mathbf{k}$ integration and using a standard spherical wave expansion,

$$E_{\rm bound}(a) = \frac{\alpha}{\pi}\sum_{l=0}^{\infty}(2l+1)\int dk\,k\sum_m \frac{\langle a|\alpha_\mu j_l(kr_2)\mathbf{C}^l|m\rangle\langle m|j_l(kr_1)\mathbf{C}^l\alpha^\mu|a\rangle}{E_a - E_m - \mathrm{sgn}(E_m)k} \tag{2}$$

is obtained, where $\mathbf{C}^l$ are angular tensors proportional to the spherical harmonics. There is an implicit dot product between the angular tensors. At this stage we make an important observation. Equation (1) looks linearly divergent in k but is actually reduced to a logarithmic divergency because of a cancellation between positive- and negative-energy states in the m sum. In Eq. (2) the divergency is moved from the k integration to the outer sum over partial waves. For each l value the k integration is convergent. The partial-wave expansion thus serves as an effective cutoff in k space.

The mass term M (Fig. 1) is defined as the free-electron self-energy with a momentum distribution determined by the bound state $|a\rangle$. The standard way of treating the mass term is to introduce photon regulators which cut off high-energy photon momenta,

$$M(a) = \lim_{\Lambda\to\infty}\int d^3p\int d^3p'\langle a|p\rangle\langle p|\Sigma^\Lambda(p)|p'\rangle\langle p'|a\rangle$$
$$= \lim_{\Lambda\to\infty}\delta m(\Lambda)\langle a|\beta|a\rangle$$
$$= \lim_{\Lambda\to\infty}\frac{\alpha}{\pi}\left(\frac{3\ln\Lambda^2}{4}+\frac{3}{8}\right)\langle a|\beta|a\rangle, \tag{3}$$

where $\Sigma(p)$ is the free-electron self-energy operator and the integration over momenta includes summation over spinor components. In our approach we express the mass term in partial waves, in analogy with Eq. (2)

$$M(a) = \frac{\alpha}{\pi}\sum_{l=0}^{\infty}(2l+1)\int d^3p\int d^3p'\int d^3q\int dk\,k\langle a|p\rangle\frac{\langle p|\alpha_\mu j_l(kr_2)\mathbf{C}^l|q\rangle\langle q|j_l(kr_1)\mathbf{C}^l\alpha^\mu|p'\rangle}{E_p - E_q - \mathrm{sgn}(E_q)k}\langle p'|a\rangle. \tag{4}$$

No regulator is required since everything is finite for each partial wave. This mass term looks similar to the one used by French and Weisskopf [7]. Note that the zero-potential term (B1 in Fig. 1) differs from this term in the energy denominator where E_p should be replaced by E_a. In the renormalization procedure we employ the difference between Eqs. (2) and (4) is taken for each partial wave, and then the summation is performed.

The improvement in the convergence compared to earlier methods arises, since we, instead of calculating separate finite contributions (F1 $\propto l^{-2}$, F2 $\propto l^{-2}$, and F3 $\propto l^{-3}$ in Fig. 1) obtained by the potential expansion, calculate the sum of these terms [(B−M) $\propto l^{-3}$ in Fig. 1] for each partial wave.

It should be pointed out that the covariant mass term defined in Eq. (3) is logarithmically divergent in the four-dimensional k space. The only practical procedure for cancelling out this mass term is to make a potential expansion of the unrenormalized bound-state self-energy. When using the partial-wave form of the mass term [Eq. (4)] every subtraction is made in the three-dimensional k space.

III. NUMERICAL APPROACH

In order to generate the bound-state orbitals we use a numerical finite basis-set approach developed by Salomonson and Öster [18]. The mass term can be calculated in two different ways. One way is to use a complete numerical basis set that is generated using the bound-state method in the limit $Z \to 0$. The ultimate reason for calculating the mass term completely numerically is to take advantage of the strong cancellations that appear when the renormalization is performed. By performing the integrations in the bound and the mass terms in exactly the same way we can make extensive use of the similarities between the two terms to get a stable difference.

The radial free-electron matrix element can also be evaluated analytically in an infinite continuous space, as suggested by Quiney and Grant [19]. This leads to triangular conditions for the momenta. An advantage of this technique is that no poles appear in the mass term due to the exact triangular conditions that are valid in the infinite space (but not in a finite box). A disadvantage

TABLE I. Electronic screening of the self-energy in Li-like uranium (in eV).

Model potential	$2s_{1/2}$	$2p_{1/2}$	$2p_{1/2}$-$2s$
Optimized local potential (OHFS)	−2.51(3)	−0.84(3)	1.67(3)
DF, direct part	−2.77(3)	−0.99(3)	1.78(3)
DF with Coul. exchange	−2.41(3)	−0.79(3)	1.62(3)
DF with Coul. and Breit exchange	−2.61(3)	−1.05(3)	1.56(3)

is that one cannot utilize the cancellations between the mass term and the bound term for each grid. The most beneficial way is a combination of both methods. By subtracting a completely numerical zero-potential term (a dummy term that scales as N^3) from the unrenormalized bound term, we use the similarities in the high-energy region to get a stable difference. We then add a partly analytical zero-potential term, which is very accurate. This gives a stable high-energy behavior to the bound term, and after subtracting the partly analytical mass term, the renormalized value will become very accurate.

IV. NUMERICAL RESULTS

The self-energy has been evaluated for the $2s$ and $2p_{1/2}$ states of lithiumlike uranium. The partial-wave renormalization was performed up to $l_{\max}$=20. Since the contributions for each partial wave decrease as l^{-3}, the l tail was estimated with good accuracy. We have as a test of our procedure tried to reproduce Mohr's hydrogenic point-nucleus results for uranium [20]. We obtain 66.28(3) eV for $2s$ and 9.62(3) eV for $2p_{1/2}$, which should be compared with the values 66.295 and 9.625 eV of Mohr. By comparing the results for the point-nucleus hydrogenic system to the extended nucleus results in the same r and k grids, an accurate estimate of the nuclear-size effect is obtained. This difference is more accurate than the individual results and they agree well with those of Blundell [4, 21]. For the extended nucleus, a uniform charge distribution, with the rms value (deduced from experiment) of 5.8625 fm [22], is used. The effect of the nuclear structure for the given rms lies within our limits of error.

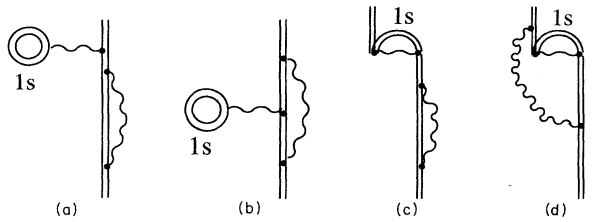

FIG. 2. Diagrams representing the lowest-order electron screening of the self-energy. These diagrams are included, together with similar higher-order diagrams, by using orbitals generated in a $1s^2$ core potential. Diagrams (a) and (b) represent the direct part and (c) and (d) the exchange part of the interaction with the core.

TABLE II. Self-energy of $2s$ and $2p_{1/2}$ in Li-like U (eV).

Phys. effect	$2s$	Others	$2p_{1/2}$	Others
Hydrogenic, point nuc.	66.28(3)	66.295[a]	9.62(3)	9.625[a]
Nuclear size effect	−0.87(3)	−0.90(6)[b]	−0.07(2)	−0.10(5)[b]
Screening				
(direct)	−2.77(3)	−2.75(2)[b]	−0.99(3)	−0.97(2)[b]
(exchange)	0.21(5)		0.04(4)	
Total self-energy	62.85(8)		8.60(8)	

[a]Mohr [20].
[b]Blundell [4, 21].

The effect of the electronic screening has been evaluated using four different central potentials: (a) a local potential OHFS (optimized Hartree-Fock-Slater) [23, 24], which reproduces the Dirac-Fock results very well; (b) the direct part of the Dirac-Fock potential; (c) the full Dirac-Fock (DF) potential with exchange; and (d) the DF potential. with the Breit exchange The results obtained for the electronic screening with the different potentials relative to a hydrogenic system with the same finite nucleus are given in Table I. The self-energy procedure we use is technically—in contrast to the earlier methods—easily applicable to nonlocal potentials also. There are, however, conceptual theoretical problems for such potentials. For instance, the use of a nonlocal potential violates the

TABLE III. Transition energy for the $2p_{1/2}$-$2s_{1/2}$ transition in Li-like uranium (in eV).

Physical effect	This work	Blundell
Relativistic MBPT	322.29(15)[a]	322.41[a]
Valence self-energy, direct	−54.07(3)	−54.09
Valence self-energy, exchange	−0.17(5)[b]	0.36[b]
Core self-energy	−0.08(8)[b,c]	−0.51(2)[b]
Vacuum polarization	12.56(1)[d]	12.56(1)
Nuclear recoil and polarization	0.10[e]	0.10
Higher-order effects		0.01(4)
Total transition energy	280.63(20)	280.83(10)
Experimental	280.59(9)[f]	

[a]The difference is mainly due to the inclusion of more than one Breit interaction in our calculation, through the use of Breit perturbed orbitals.
[b]Not directly comparable (see text).
[c]Our result was obtained using OHFS potentials for $1s^2 2s$ and $1s^2 2p_{1/2}$, respectively. Using potentials defined as the direct interaction with one $1s$ and one valence electron, ($2s$,$2p_{1/2}$) 0.21 eV was obtained. This is in good agreement with Blundell's result for the direct interaction (0.23 eV).
[d]Blundell [4, 21].
[e]We have used −0.08(8) eV for nuclear recoil [4] and 0.18(5) eV for nuclear polarization [30].
[f]Schweppe *et al.* [1].

gauge invariance, since an incomplete set of higher-order diagrams is indirectly included in the potential. However, we think it is worth reporting our results. The DF potential with exchange gives the same result as the local OHFS potential within 0.1 eV. The results for the direct electronic screening [Figs. 2(a) and 2(b)] agree well with those of Blundell. Our exchange effects [Figs. 2(c) and 2(d)] are not directly comparable to those of Blundell. We have included the exchange effects in the potential affecting both the internal and external lines, while Blundell only modifies external lines perturbatively. In Table II we have collected the results for the self-energy of the two states. The values used for the electronic screening is some weighted average of the results with different potentials. The errors assigned include not only the numerical uncertainty for a given potential but also an estimate of the uncertainty due to the choice of potential. In order to compare the self-energy results with the experimental value for the $2s$-$2p_{1/2}$ transition, a good estimate of the non-QED part, i.e., the DF value and the many-body contribution is needed. We have repeated and extended the calculation done by Blundell, Johnson, and Sapirstein [25] using the GRASP code of Grant and co-workers [26] combined with our coupled-cluster code [18, 27–29] (Table III). The many-body result differs somewhat, since we have included the Breit interaction self-consistently in the orbitals. Therefore our result contains certain higher-order Breit interactions, which are not included in the calculation by Blundell. The agreement between the calculated and experimental transition energies is good, considering the fact that higher-order effects are included only in an approximate way. The valence self-energy, including the nuclear-size effect and the direct part of the electronic screening, is accurate, and the agreement between different calculations is very good. The exchange part of the screening is a true many-body effect and has to be calculated in a more rigorous way in order to reduce the large uncertainty. This is also true for the core self-energy, which is hard to estimate accurately.

From the numerical results reported here we can draw the conclusion that the simple renormalization scheme we have introduced works well for the first-order self-energy. It is now our intention to apply a similar procedure to evaluate higher-order QED contributions.

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