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Weak-interaction effects in heavy atomic systems

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Effects of *P*-violating and *CP*-violating weak interactions in the heavy atoms Rb, Cs, Au, and Tl are calculated in a variety of potential models, including the relativistic Hartree-Fock model. Excitation energies and hyperfine constants are also calculated using these models and compared with experiment as a control. Values determined for the *P*-violating electric dipole matrix elements for $\mathrm{Cs}(6s_{1/2}\rightarrow 7s_{1/2})$ and $\mathrm{Tl}(6p_{1/2}\rightarrow 7p_{1/2})$ are in agreement with other similar calculations. The spread in values of the *P*- and *CP*-violating electric dipole matrix elements among the various models is found to be about 20%. A program is outlined for reducing this spread by systematically extending the present calculations to higher orders in the electron-electron interaction.

I. INTRODUCTION

This paper is the first in a planned series of papers devoted to a systematic investigation of the effects of *P*-violating and *CP*-violating weak interactions in heavy atoms. We will be concerned with two effects, each of which has to do with electric dipole matrix elements. The first effect is the induction of a nonvanishing off-diagonal electric dipole matrix element between two atomic states of the same parity caused by the exchange of a Z_0 boson between atomic electrons and the nucleus. The second is the induction of an enhanced atomic electric dipole moment caused by an intrinsic electron electric dipole moment.

The exchange of Z_0 bosons, which leads to *P* violation in the atom, is described by the Weinberg-Salam theory.[1] It leads to phenomena such as circular dichroism and optical rotation which have been used to detect *P* violation in Cs,[2-4] Tl,[5,6] Bi,[7] and Pb.[8] The present investigation is concerned only with atoms having a single valence electron so we will not be treating the interesting cases of Bi and Pb. While experimental determinations were at the 15% or worse level, relatively crude theoretical estimates sufficed to establish the existence of *P* violation. However, given the present possibility of an order of magnitude improvement in the measurements,[9] it now becomes imperative to see if atomic theory can be improved, so that a quantitative test of the Weinberg-Salam theory at very low energies comparable in accuracy to that achieved in high-energy tests can be made.

An intrinsic electron electric dipole moment d_e leads to *CP* violation in atoms and induces an atomic electric dipole moment. Measurements of this atomic dipole moment place limits on the intrinsic electric dipole moment of the electron. The present experimental limit on d_e, derived from measurements of the linear Stark effect in heavy atoms,[10] is $d_e < 2\times 10^{-24}$ e cm. Given the possibility for improving the measurements of atomic dipole moments by several orders of magnitude,[11] it should be possible to improve the present limit significantly, and ideally to detect and measure d_e. This in turn would have important consequences particularly for supersymmetric gauge theories, where predictions[12] presently range from $d_e = 10^{-25}$ to 10^{-30} e cm.

The purpose of the present paper is to lay groundwork for a systematic study of these two effects. The main difficulty encountered is not with the weak interactions, which can be treated in lowest-order perturbation theory, but with the electron-electron Coulomb interaction in the atom. This latter problem can be treated systematically in perturbation theory by breaking the full many-electron Hamiltonian into a part in which each electron moves in a central potential $V(r)$, and a perturbation consisting of the difference between the actual electron-electron Coulomb repulsion and the central potential. An atomic shell structure emerges already in the lowest approximation, from which one can readily construct a lowest-order atomic wave function useful for many practical calculations. In the present paper we are concerned with applications of this lowest-order approximation to *P* and *CP* violation. There is of course an infinite degree of flexibility in the choice of $V(r)$. A common choice is the Hartree-Fock potential, which has particular advantages in perturbation theory calculations, since higher-order terms become relatively simple. The corresponding drawback is that physical parameters such as excitation energies and hyperfine constants, calculated in lowest order with Hartree-Fock wave functions, do not compare as favorably with experiment as those calculated using a carefully chosen model potential. In the present study we consider in addition to the Hartree-Fock model three such parametric potentials, the Tietz potential,[13] the Green potential,[14] and the Norcross potential,[15] all of which have been applied previously to studies of *P* violation. It is our position that the use of several potentials is essential in a systematic study in order to gauge the reliability of the corresponding calculations. Calculations in the framework of one model may be more sensitive to higher-order effects than another, and may thus be misleading. However, if all evaluations of a quantity in different models give answers to within 10% of one another, then we could define that 10% to be a theoretical error estimate. In the present calculations the actual spread is found to be closer to 20%. What we hope is, that as we proceed to higher orders, the spread in values will be reduced to 1%. If this hope is realized we would be in a position to give theoretical predictions comparable in accuracy to the level expected from the next generation of experiments.

II. LOWEST-ORDER CALCULATION

To lowest order in the electron-electron interaction, each electron moves independently in a central potential $V(r)$. The orbital $u_a(\mathbf{r})$ of an electron with quantum numbers described collectively by the symbol a satisfies a one-electron Dirac equation,

$$[h_0+h_w+V(r)]u_a(\mathbf{r})=\epsilon_a u_a(\mathbf{r}) \; . \tag{1}$$

The quantity h_0 is the part of the Dirac Hamiltonian giving the electron kinetic energy and its interaction with the nucleus, while h_w is the part describing the weak interactions. We consider two forms for h_w:

$$h_w=\begin{cases} -\dfrac{G_F}{\sqrt{8}}Q_w\gamma_5\rho_{\text{nuc}}(\mathbf{r}) & \text{for } P \text{ violation} \\ 2i\dfrac{d_e}{e}\gamma_4\gamma_5\mathbf{p}^2 & \text{for } CP \text{ violation,} \end{cases} \tag{2}$$

where the second right-hand side follows from Ref. 16. The quantity G_F is the Fermi coupling constant and Q_w is the so-called weak charge, $Q_w=(1-4\sin^2\theta_W)Z-N$, where Z is the nuclear charge, N the neutron number, and θ_W is the Weinberg angle. In Eq. (2) we designate the normalized nuclear charge density by $\rho_{\text{nuc}}(\mathbf{r})$. The quantities γ_4 and γ_5 are Dirac matrices, and $\mathbf{p}$ is the electron momentum. Because of the presence of h_w in Eq. (1), the orbitals $u_a(\mathbf{r})$ will have mixed parity. We decompose $u_a(\mathbf{r})$ into a part $v_a(\mathbf{r})$ independent of h_w, and a second part $w_a(\mathbf{r})$, linear in h_w, which has parity opposite to $v_a(\mathbf{r})$ but the same angular momentum. For each orbital $u_a(\mathbf{r})$ we then have

$$[h_0+V(r)-\epsilon_a]v_a(\mathbf{r})=0 \; , \tag{3a}$$

$$[h_0+V(r)-\epsilon_a]w_a(\mathbf{r})=-h_w v_a(\mathbf{r}) \; . \tag{3b}$$

Equation (3a) is solved to give the lowest-order orbitals v_a, and Eq. (3b) is then solved to give the small perturbations induced by the weak interactions. In calculating atomic dipole matrix elements, contributions from the core orbitals vanish because of spherical symmetry and only those contributions from the valence electron remain. For the case of P violation we are interested in off-diagonal matrix elements of the electric dipole operator ez between two valence states, say 1 and 2,

$$D=\langle w_2 \,|\, ez \,|\, v_1\rangle+\langle v_2 \,|\, ez \,|\, w_1\rangle \; . \tag{4}$$

In the case of CP violation we are interested in the corresponding diagonal matrix element. Several comments are in order concerning the preceding equations.

(1) It may appear that, when solving Eq. (3b) for the perturbed valence orbital w_a, core contributions should be excluded because of the Pauli principle. Orthogonalization of the perturbed valence orbital to the core orbitals is in fact unnecessary and incorrect, since exclusion principle-violating contributions from the valence orbital precisely account for excitations of core orbitals into the unoccupied valence state.

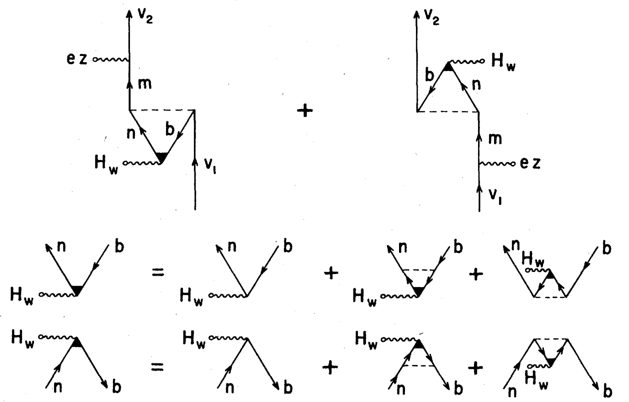

FIG. 1. The graphs in the first row show the terms in perturbation theory corresponding to $V_{\text{HF}}^{(1)}$ of Eq. (3b′). Those on the second and third rows define the dressed vertex occurring in the first row.

(2) When the Hartree-Fock model is used, Eq. (3b) should be modified to account for the fact that perturbations of the core orbitals induce a first-order correction $V_{\text{HF}}^{(1)}$, to the Hartree-Fock potential, viz.,

$$[h_0+V_{\text{HF}}(v_a,r)-\epsilon_a]w_a(\mathbf{r}) = -h_w v_a(\mathbf{r})-V_{\text{HF}}^{(1)}(v_a,w_a,r)v_a(\mathbf{r}) \; . \tag{3b′}$$

These coupled equations replace Eq. (3b) when the Hartree-Fock potential is used. Equations (3b′) are referred to as the parity-nonconserving-Hartree-Fock (PNC-HF) equations.[17] It is found that corrections to dipole moments of about 30% arise from the term $V_{\text{HF}}^{(1)}$. The corrections included in $V_{\text{HF}}^{(1)}$ are illustrated diagrammatically in Fig. 1.

III. LOWEST-ORDER RESULTS

In the present studies we employ four potential models as follows:

A. Tietz potential

To give a simple analytical approximation to the Fermi-Thomas model of the atom, Tietz[13] introduced the potential

$$V(r)=-(\alpha Z/r)\phi(x)$$

with

$$\phi(x)=1/[1+(\pi/8)^{2/3}x]^2 \; ,$$

where $x=rZ^{1/3}/\mu$ with $\mu=\frac{1}{2}(3\pi/4)^{2/3}\approx 0.8853\ldots$. Modifications of the Tietz potential were employed by Neuffer and Commins[18] to study P violation in Cs and Tl. We follow these authors and employ, as a first model, a modified Tietz potential of the form

$$V(r)=-\frac{\alpha}{r}\left[1+\frac{(Z-1)}{(1+tr)^2}e^{-\gamma r}\right] , \tag{5}$$

TABLE I. Comparison of theoretical excitation spectra from the potential models employed in this work and measured values. Energies are given in a.u.

State[a]	Tietz	Green	Norcross	Expt.[b]	HF
			Rubidium		
$5s$	0.154 14	0.153 48	0.153 45	0.153 51	0.139 29
$5p^*$	0.095 57	0.096 15	0.096 31	0.096 19	0.090 82
$5p$	0.093 98	0.094 80	0.094 94	0.095 11	0.089 99
$6s$	0.061 40	0.062 15	0.061 97	0.061 77	0.058 70
$6p^*$	0.045 05	0.045 70	0.045 56	0.045 45	0.043 89
$6p$	0.044 56	0.045 26	0.045 12	0.045 10	0.043 60
$7s$	0.033 45	0.033 82	0.033 72	0.033 62	0.032 44
			Cesium		
$6s$	0.143 43	0.143 09	0.143 01	0.143 10	0.127 37
$6p^*$	0.092 47	0.092 23	0.092 50	0.092 17	0.085 62
$6p$	0.088 92	0.089 15	0.089 28	0.089 64	0.083 79
$7s$	0.058 27	0.059 01	0.058 83	0.058 65	0.055 19
$7p^*$	0.043 79	0.044 24	0.044 10	0.043 93	0.042 02
$7p$	0.042 70	0.043 23	0.043 07	0.043 10	0.041 37
$8s$	0.032 13	0.032 51	0.032 40	0.032 30	0.030 95
			Gold		
$6s$	0.337 36	0.339 25	0.342 22	0.339 04	0.274 61
$6p^*$	0.174 87	0.166 04	0.167 91	0.168 82	0.133 79
$6p$	0.150 96	0.141 73	0.144 29	0.151 43	0.121 62
$7s$	0.090 50	0.087 56	0.090 29	0.090 79	0.083 22
$7p^*$	0.062 25	0.060 39	0.062 09	0.065 51	0.056 44
$7p$	0.058 05	0.056 29	0.057 80	0.062 34	0.053 35
$8s$	0.043 78	0.042 94	0.043 82	0.044 05	0.041 58
			Thallium		
$6p^*$	0.224 18	0.224 32	0.225 26	0.224 46	0.199 68
$6p$	0.185 43	0.184 84	0.187 96	0.188 96	0.166 93
$7s$	0.101 67	0.097 68	0.102 81	0.103 82	0.096 18
$7p^*$	0.069 02	0.066 41	0.069 38	0.068 82	0.065 05
$7p$	0.063 73	0.061 67	0.064 33	0.064 26	0.060 86
$8s$	0.047 25	0.046 00	0.047 69	0.047 92	0.045 75
$8p^*$	0.036 05	0.035 05	0.036 17	0.035 98	0.034 62

[a] $5p^* = 5p_{1/2}$, $5p = 5p_{3/2}$, etc.
[b] C. E. Moore, Ref. 19.

where t and γ are parameters adjusted to fit the low-lying spectra of the atoms under consideration. The values of t and γ used in the present study are

Atom	t	γ
Rb	1.9530	0.2700
Cs	2.0453	0.2445
Au	2.6660	0.2503
Tl	2.5937	0.2579

The excitation energies predicted by solving the Dirac equation in the Tietz potential are compared with experimental energies[19] in Table I. The comparison with experimental hyperfine integrals is given in Table II.

B. Green potential

A somewhat more sophisticated potential model was introduced by Green *et al.*[14] to reproduce Hartree-Fock

TABLE II. Ground-state hyperfine integrals: $2\int dr\, gf/r^2$, where g and f are large and small components of the radial two-component Dirac orbital for the valence electron.

State	Tietz	Green	Norcross	Expt.	HF
Rb $5s$	0.1162	0.1131	0.1114	0.1076	0.0683
Cs $6s$	0.1870	0.1872	0.1824	0.1799	0.1115
Au $6s$	1.4813	1.606	1.6254	1.8287	1.2644
Tl $6p$	-0.3772	-0.3749	-0.3653	-0.3730	-0.3092

eigenvalues and screening functions approximately throughout the periodic system, viz.,

$$V(r)=\frac{-\alpha}{r}\left[1+\frac{Z-1}{H(e^{r/d}-1)+1}\right], \tag{6}$$

where H was related to d by $H=d(Z-1)^{1/3}$ and, where d was treated as an adjustable parameter. A Green potential was used by Loving and Sandars[20] to study P violation in Cs. We employ this type of potential, where we treat both H and d as adjustable parameters, as our second model. The values of H and d used here were adjusted to the low-lying excitation spectra of the atoms being considered. We found

Atom	H	d
Rb	3.481 14	0.785 51
Cs	4.469 10	0.896 65
Au	8.143 70	1.022 40
Tl	11.2300	1.290 49

For Cs our values of H and d are somewhat different from those chosen by Loving and Sandars.[20]

C. Norcross potential

The most sophisticated potential used in the present study is one introduced by Norcross[15] to study the low-energy photoionization of Cs. This potential has been used previously by Bouchiat *et al.*[21] to study P violation in Cs. The Norcross potential can be written in the form

$$V_N(r)=V_{\mathrm{TF}}(\lambda,r)-\frac{\alpha}{2r^4}\alpha_d(1-e^{-(r/r_c)^6})$$
$$-\frac{\alpha}{2r^6}(\alpha_q-6\beta a_0)(1-e^{-(r/r_c)^{10}})\ . \tag{7}$$

The term $V_{\mathrm{TF}}(\lambda,r)$ is a version of the Thomas-Fermi potential determined according to a prescription set out by Eissner and Nussbaumer,[22] with λ taken as an adjustable parameter. The second and third terms in Eq. (7) are core-polarizability corrections; α_d is the dipole polarizability of the core, α_q is its quadrupole polarizability, and βa_0 is a dynamical correction to the quadrupole polarizability. The exponential factors in Eq. (7) are introduced to give a physically reasonable structure to the potential at small distances and the corresponding cutoff radius r_c is taken as a second adjustable parameter. The quantities α_d and α_q are determined from relativistic, coupled Hartree-Fock calculations[23] while βa_0 is estimated from the core-excitation energies. One significant difference between the potential used in the present work and that originally used by Norcross is that no adjustable spin-orbit interaction term is used here, since our potential is used in connection with the Dirac equation. A second difference is that only one r_c is used for all l. In our applications we adjust the two parameters λ and r_c to fit the low-lying spectra of the atoms under consideration. Our choices for the various parameters are given in Table III.

D. Relativistic Hartree-Fock potential

The fourth model potential used in the present study is a so-called $V(N-1)$ Hartree-Fock potential. The relativistic Hartree-Fock equations for the $N-1$ core electrons are first solved self-consistently and the Hartree-Fock equations for the valence electron or excited electron are subsequently solved in this fixed-core potential. This potential has been employed previously by Mårtensson-Pendrill[24] and by Dzuba *et al.*[25] to examine P violation in Cs. Since there are no adjustable parameters in the Hartree-Fock potential the corresponding excitation spectra which are listed in Table I compare less favorably with experiment than those from the other three potentials. However, higher-order corrections to Hartree-Fock energies and matrix elements are simpler to treat than the corresponding corrections in other models. There are no corrections to the Hartree-Fock excitation spectra in first-order perturbation theory. In order to obtain excitation spectra which agree with experiment as well as those given by the other models, second-order perturbation theory is required. Calculations by Dzuba *et al.*[26] for Cs in second-order perturbation theory based on $V(N-1)$ Hartree-Fock calculations give an excitation spectrum in excellent agreement with experiment.

IV. PARITY VIOLATION

Our studies of parity violation are limited to the following four special cases:

Atom (transition)	λ (Å)
$\mathrm{Rb}(5s_{1/2}\to 6s_{1/2})$	4967
$\mathrm{Cs}(6s_{1/2}\to 7s_{1/2})$	5395
$\mathrm{Au}(6s_{1/2}\to 7s_{1/2})$	1835
$\mathrm{Tl}(6p_{1/2}\to 7p_{1/2})$	2927

In each case the transition under consideration is an $M1$ transition with a small $E1$ admixture induced by the weak interaction. The cases of Cs and Tl have been studied extensively in previous works, and the techniques to evaluate the lowest-order result are well known. The cases of Rb and Au have not been investigated previously, but are potentially of experimental interest. We use an expli-

TABLE III. Parameters for the Norcross-type potentials used in the present work. The parameters λ and r_c are adjustable, while the remaining parameters are fixed. All parameters are given in a.u.

Atom	λ	r_c	α_d	α_q	β
Rb	0.99321	3.2318	9.076	35.41	4.41
Cs	1.06252	3.5461	15.81	86.40	7.90
Au	0.920	2.760	12.40	0.0	0.0
Tl	0.93985	3.2968	24.00	108.0	8.70

TABLE IV. Parity-violating dipole matrix elements $E1$-PV, in units of $iea_0(Q_w/N)\times 10^{-11}$, and Stark polarizabilities α and β, in units of a_0^3, calculated in various potential models.

	Tietz	Green	Norcross	PNC-HF	Expt.	Others	
Rubidium $5s \rightarrow 6s$ $A=85$ $R_{\text{nuc}}=5.480$ fm							
$E1$-PV	0.161	0.157	0.153	0.141			
α	-301	-272	-273	-285			
β	12.9	11.3	11.3	9.73			
Cesium $6s \rightarrow 7s$ $A=133$ $R_{\text{nuc}}=6.206$ fm							
$E1$-PV	1.04	1.04	1.02	0.912	0.93(16)[a] 1.00(8)[b]	0.880[c] 0.996[e] 0.886[g]	0.972[d] 1.06[f]
α	-342	-330	-330	-349	$-263.7(27)$[h]	-370.3[e]	-257.7[d]
β	36.7	32.9	33.9	29.3	26.6(4)	36.8	27.3
Gold $6s \rightarrow 7s$ $A=197$ $R_{\text{nuc}}=7.019$ fm							
$E1$-PV	5.11	4.92	5.09	6.84			
α	-80.1	-99.7	-92.0	-159			
β	15.4	17.5	16.6	20.3			
Thallium $6p^* \rightarrow 7p^*$ $A=205$ $R_{\text{nuc}}=7.079$ fm							
$E1$-PV	-9.54	-8.49	-9.20	-9.75	$-7.2(1.4)$[i]	-8.73[e]	-6.83[j]
α	385	372	445	448	232(12)[k]	385[e]	
β	-309	-321	-337	-379		-308	

[a] M. A. Bouchiat *et al.*, Ref. 4. Here $Q_w=-68.6$, $\beta=27a_0^3$.

[b] C. E. Wieman *et al.* (unpublished).

[c] V. A. Dzuba *et al.*, Ref. 24.

[d] C. Bouchiat, C. A. Piketty, and D. Pignon, Ref. 20.

[e] D. V. Neuffer and E. D. Commins, Ref. 18.

[f] B. P. Das, Ph.D. thesis, State University of New York at Albany, 1981.

[g] A.-M. Mårtensson-Pendrill (unpublished).

[h] S. L. Gilbert, R. N. Watts, and C. E. Wieman, Phys. Rev. A **29**, 137 (1984).

[i] P. Drell and E. D. Commins, Phys. Rev. Lett. **53**, 968 (1984). Here $Q_w=-112.7$, $\beta=195$.

[j] B. P. Das, J. Andriessen, M. Vajed-Samii, S. N. Ray, and T. P. Das, Phys. Rev. Lett. **49**, 32 (1982).

[k] E. D. Commins (private communication).

citly relativistic formalism, avoid saturation of the matrix elements by using accurate Green's-function techniques,[27] and take account of the finite size of the nucleus directly in the Dirac equation. This finite-size effect is treated assuming a uniform charge density, using nuclear radii given in Johnson and Soff.[28] Use of a Fermi distribution changed the results by several percent, and will be treated in the next paper of this series. In each case we calculate the induced $E1$ matrix element given in Eq. (4).

Table IV summarizes our results for each potential. In quoting experimental values in Table III we have assumed a value[29] of $\sin^2\theta_W=0.215$ to calculate the scaling factor Q_w/N. The values in the column labeled PNC-HF include the corrections arising when the first-order weak correction to the Hartree-Fock potential shown in Eq. (3b′) are included. The following several comments are in order concerning the values in Table IV.

(a) In the PNC-HF case we include the contribution from $V_{\text{HF}}^{(1)}$ in Eq. (3b′). In fact, without these corrections the value for Cs is[30] $E1=0.728i\times 10^{-11}$ (Q_w/N) ea_0, roughly 25% lower than PNC-HF.

(b) In the case of the Tietz potential, we obtain somewhat different results from Neuffer and Commins,[18] even though in the case of Tl the same t and γ were used. We attribute the discrepancy in Tl to our more accurate treatment of the wave functions at small distances: our exponential grid puts about 30 points inside the nucleus. Our Stark polarizabilities, which are insensitive to short distances, are in agreement with Ref. 18. For the Norcross potential in Cs, our results are slightly higher than Ref. 2, although agreement is not to be expected, since we did not include the effect of core polarizability on the dipole operator. This correction will arise naturally as a higher-order correction. The same remark applies to the Stark polarizabilities α and β also listed in Table IV.

(c) As a check on the reliability of the calculations, two evaluations were made. The matrix element involves the action of both the dipole operator and h_w: either operator can be used as the driving term in a differential equation for a perturbed orbital, with the other operator then sandwiched between this perturbed orbital and the unperturbed valence orbital. The methods agreed to six digits.

V. *CP* VIOLATION

The atomic dipole moment induced by the *CP*-violating interaction given in Eq. (2) is proportional to the intrinsic electric dipole moment d_e. The proportionality constant

TABLE V. Ground-state electric dipole moment enhancement factor, $R = D_{\mathrm{atom}}/d_e$ calculated using various potential models.

Atom	Tietz	Green	Norcross	PNC-HF	Other
Rb	34.0	29.7	30.0	26.7	24[a]
Cs	158	139	144	127	119[a]
Au	393	397	370	340	
Tl	−681	−675	−685	−1910	−700[b]

[a] P. G. H. Sandars, Ref. 31 (with shielding).

[b] P. G. H. Sandars and R. M. Sternheimer, Ref. 10.

R which shows the enhancement of this intrinsic moment in heavy polarizable atoms is given in Table V, where comparisons are made with previous calculations by Sandars[31] and by Sanders and Sternheimer[10] based on Hartree-Fock-Slater wave functions. As in the case of the P-violating electric dipole matrix element, the Hartree-Fock model values, omitting $V_{\mathrm{HF}}^{(1)}$, were found to be substantially smaller than the values from other potential models, and only the PNC-HF results are given. In the case of Tl, very large corrections due principally to excitation of the $6s_{1/2} \rightarrow p_{1/2}$ state arising from $V_{\mathrm{HF}}^{(1)}$ gave a factor of 3 increase in the size of the enhancement factor. This fact indicates that the choice of the Hartree-Fock ground state for the calculation of CP-violation effects in Tl may be unsuitable and possibly means that the perturbation theoretic approach will be unsuitable for this atom.

VI. HIGHER-ORDER PERTURBATION THEORY

The results presented in this paper, while numerically accurate to all digits displayed, cannot be directly compared to experiment as they stand. This is because they represent only the lowest-order term in the perturbation V_C, defined in terms of the decomposition of the full Hamiltonian of the system

$$H = \sum_i \left[\alpha_i \cdot \mathbf{p}_i + m\beta_i - \frac{Z\alpha}{r_i} \right] + \frac{1}{2} \sum_{i,j}{}' \frac{\alpha}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$\equiv H_0 + V_C \, , \tag{8}$$

with

$$H_0 \equiv \sum_i [\alpha_i \cdot \mathbf{p}_i + m\beta_i + V(r_i)] \, ,$$

$$V_C = \frac{1}{2} \sum_{i,j}{}' \frac{\alpha}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_i \left[V(r_i) + \frac{\alpha Z}{r_i} \right] .$$

In the case of a theory like quantum electrodynamics (QED), all perturbations come in with successively higher powers of a small parameter, viz., the fine-structure constant, and thus, barring extremely large coefficients of higher-order terms, each successive term provides about 100 times more accuracy. Here, however, no such parameter exists, and the smallness of higher-order terms is a sensitive function of the potential chosen to approximate the net effect of electron-electron interactions. Our way of approaching the problem of estimating the reliability of this kind of atomic physics calculation is to use several different potentials. If perturbation theory converges, then successively higher orders should give results that, while starting from a relatively wide range of potentials, give answers that cluster closer and closer to a final result that is to be taken as the correct physical answer. It is, of course, important to make sure that this method reproduces accurately measured atomic properties, such as valence energies and hyperfine splittings in order to ensure that no important classes of diagrams have been left out. In this way we introduce the idea of a "circle of convergence." Such a concept refers to a certain range of models of a heavy atom: regardless of the exact parametrization of $V(r)$, there should exist an infinite class of models that all converge to the true picture of the atom when sufficiently high orders of perturbations in V_C are taken into account. On the other hand, this leaves open the possibility that certain models may be outside this radius of convergence, and that perturbation theory in V_C does not converge. We consider it possible that the HF model of Tl may be an example of this. We wish to emphasize that this approach has not been tested, since the vast majority of higher-order calculations are in the HF framework, due to the simplicity of the perturbation series. We are presently in the process of setting up first- and second-order many-body perturbation theory for a general potential $V(r)$. While many of the higher-order terms can be treated with standard techniques, graphs such as those shown in Fig. 2 involve relativistic two-body Green's functions, which to our knowledge have not been previously employed in atomic calculations, though the nonrelativistic case has been treated.[32] We are presently developing numerical techniques to deal with such terms.

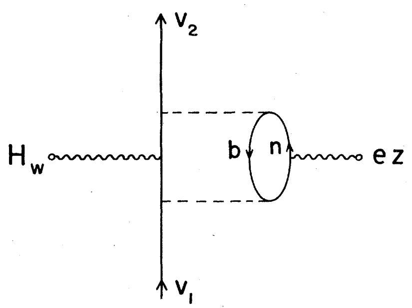

FIG. 2. A sample graph involving the relativistic two-body Green's function.

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