Relativistic Corrections to the Dipole Sum Rule*†

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The summed oscillator strength is calculated to order $(v/c)^2$ for a Dirac electron in a central force field. The result $(1+T_{00})^{-1}$ is interpreted in terms of the electron's increase of mass due to its kinetic energy. (T_{00} is the expectation value of the kinetic energy, in units of mc^2.) This analytical result is in fair agreement with our earlier numerical result, and those of Brown *et al.* for a K electron of lead. We also calculate the bremsstrahlung-weighted cross section for a Dirac electron in a Coulomb field, and compare with our numerical result for lead.

I. INTRODUCTION

DISPERSION theory[1] relates the forward-scattering amplitude for a photon of one energy to the dispersion integral over all frequencies of the absorption cross section. In the case of very high photon energy, the forward-scattering amplitude is proportional to the integrated absorption cross section. If we *assume* that the high-energy forward-scattering amplitude for an electron bound in the atom is the Thomson value e^2/mc^2, then we find the integrated cross section for the atomic photoeffect for all multipoles with retardation to have precisely the Thomas-Reiche-Kuhn (TRK) value of $\sigma_{\text{int}}=2\pi^2e^2\hbar/mc$, or $\sum_n f_{0n}=1$ for the summed oscillator strength.[1] This derivation of the TRK sum-rule is more general than the usual method using closure with Schrödinger matrix elements for the nonrelativistic (NR) electric-dipole contribution to the cross section; but the derivation is based on the assumption above concerning the high-energy forward-scattering amplitude.

In this paper we shall examine relativistic corrections of order v^2/c^2 to the sum-rule derivation of the summed oscillator strength for an atomic system in which the central potential commutes with the position. In two previous papers[2,3] we have found the summed oscillator strength for the special case of one Dirac electron in the Coulomb field of a lead nucleus using a numerical approach: we calculated the oscillator strength for discrete transitions, and combined our results with calculations by others of the lead photoeffect. We found a summed oscillator strength of 0.86, appreciably different from the value unity given by the TRK sum-rule. (In reference 2, Eqs. (3) and (4), we omitted the term $j_2(kr)P_2(\cos\theta)$; thus overestimating the retardation correction. Including this term gives a summed oscillator strength of 0.87. Note that in reference 3 we take the difference $\sigma_{\text{P.E.}}-\sigma_{\text{P.P.}}$, where $\sigma_{\text{P.E.}}$ is the photoeffect cross section, and $\sigma_{\text{P.P.}}$ is the cross section for pair production in which the produced electron would have occupied the already filled K state.) We also used dispersion theory to evaluate the forward-scattering amplitudes calculated by a different method by Brown *et al.*[4] for scattering by a K electron of Hg at energies from 0.32 mc^2, to 2.56 mc^2. The numerical agreement between our values and Brown's strengthens our conclusion that the high-energy forward-scattering amplitude for a bound electron is smaller than that of a free electron.

Brown *et al.* have also used the second Born approximation for an estimate of corrections to the form-factor calculation of electron scattering. In the forward-scattering case their result reduces to a scattering amplitude proportional to the expectation value of $(E+|V|)^{-1}$, where E is the electron's total energy and V its potential energy. Their result is in agreement with our Eq. (14) below.

In the next section we shall calculate the v^2/c^2 correction to the TRK sum-rule (nonretarded electric-dipole interaction) for a relativistic Hamiltonian. In Sec. III we find other v^2/c^2 terms, and compare with our numerical result for the summed oscillator strength for the lead photoeffect. In Sec. IV we calculate the bremsstrahlung-weighted cross section $[\sigma_b=\int(\sigma/W)dW]$ for a Dirac electron, and compare with our numerical result for the lead photoeffect.

II. ELECTRIC DIPOLE TRANSITIONS

The NR calculation leading to the Thomas-Reiche-Kuhn (TRK) sum-rule for electric-dipole transitions (without retardation) can be written in the form[5]

$$\sum_n f_{0n}=-(m/\hbar^2)[[H,y],y]_{00}=m(\partial^2H/\partial p_y^2)_{00}, \quad (1)$$

where we have evaluated the double commutator in the momentum representation, to obtain the second partial derivative of the Hamiltonian H with respect to the momentum component p_y. (The electric field is assumed to be along the y axis.) Use of the Schrödinger $H=p^2/2m+V(r)$ immediately gives the TRK sum-rule of unity

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† Preliminary accounts were given by J. S. Levinger, Bull. Am. Phys. Soc. Ser II, 1, 269 (1956); and University of Chicago Photonuclear Conference, November, 1956 (unpublished).

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[2] W. B. Payne and J. S. Levinger, Phys. Rev. 101, 1020 (1956).

[3] J. S. Levinger and M. L. Rustgi, Phys. Rev. 103, 439 (1956).

[4] G. E. Brown and J. B. Woodward, Proc. Phys. Soc. (London) A65, 977 (1952); Brenner, Brown, and Woodward, Proc. Roy. Soc. (London) A227, 59 (1954); G. E. Brown and D. F. Mayers, Proc. Roy. Soc. (London) A234, 387 (1956), and G. E. Brown (private communications).

[5] R. G. Sachs and N. Austern, Phys. Rev. 81, 705 (1951).

for any potential function $V(r)$ that commutes with position.

If we use the Schrödinger Hamiltonian and evaluate the expectation value in Eq. (1) using Dirac wave functions, it is clear that we still get the TRK sum-rule. To obtain a different relativistic sum-rule we must change not only the wave functions used in evaluating the expectation value; but we must also change the operator whose expectation value we are evaluating. Substitution of the Dirac Hamiltonian into Eq. (1) gives a nonsensical answer of zero, since the Dirac Hamiltonian is linear in the momentum. This result of zero comes from cancellation of the positive terms by negative terms due to induced transitions to negative-energy states. In principle this cancellation could be avoided by using a projection operator in the derivation of Eq. (1) so that we include only transitions to positive-energy states. However, the projection operator for a Dirac electron in a Coulomb field is rather cumbersome; so we shall perform our calculation in a circuitous manner.

We can obtain a relativistic sum-rule by using what we call the Darwin Hamiltonian in Eq. (1). This Hamiltonian[6] is found by applying the Dirac Hamiltonian twice, expanding in powers of (v/c), and keeping terms including order $(v/c)^4$, giving

$$H=p^2/2m-p^4/8m^3c^2+V-(\hbar^2/4m^2c^2)(dV/dr)\partial/\partial r+(1/2m^2c^2r)(dV/dr)\mathbf{S}\cdot\mathbf{L}. \quad (2)$$

The second term in the Darwin Hamiltonian corresponds to the first mass correction of special relativity.[6] The last two terms, such as the spin-orbit coupling term $\mathbf{S}\cdot\mathbf{L}$ are linear in the momentum p_y, and, therefore,[7] do not change the answer found by evaluation of the second derivative in Eq. (1).

The first term in H gives just the TRK sum-rule, and the second term, $-p^4/8m^3c^2$, gives a negative correction. We have the correction

$$-m[(\partial^2/\partial p_y^2)(p_x^2+p_y^2+p_z^2)^2/8m^3c^2]_{00}=-(1/8m^2c^2)[12p_x^2+4p_y^2+4p_z^2]_{00}=-(5/3mc^2)(T)_{00}. \quad (3)$$

We have evaluated this correction term using spherically symmetric wave functions, so that $(p_x^2)_{00}=(p_y^2)_{00}=(p_z^2)_{00}=(2m/3c^2)(T)_{00}$, where T is the kinetic energy. Our relativistic analog to the TRK sum-rule is then

$$\sum_n f_{0n}=m(\partial^2H/\partial p_y^2)_{00}=1-(5/3mc^2)(T)_{00}+O(v^4/c^4). \quad (4)$$

We note that the terms we used in Eq. (2), namely $p^2/2m-p^4/8m^3c^2$, are generally valid for a relativistic Hamiltonian, such as that of the Klein-Gordon equation, evaluated to this order. We have emphasized use of the Dirac equation, since we shall compare with numerical results for lead based on that equation; but to the accuracy considered in this paper we use only the mass-correction term of special relativity, and no other features of the Dirac equation.

III. OTHER MULTIPOLES, AND RETARDATION

Jacobsohn[8] has evaluated the NR summed oscillator strength for electric-quadrupole transitions, and for the retardation correction to electric dipole transitions. Both these terms are $O(v^2/c^2)$. Jacobsohn also states that for a Dirac electron in a Coulomb field the summed magnetic-dipole oscillator strength is of a higher order in v/c. We have a slightly different result from Jacobsohn's for the summed electric-quadrupole oscillator strength, and agree with his results for the retardation correction and magnetic-dipole transitions. We shall sketch our derivations, but shall not give the details.

The electric-quadrupole oscillator strength is[9]

$$f_{0n}{}^Q=(m\omega^3/2c\hbar^2)(q_{0n})^2. \quad (5)$$

For a spherically symmetric ground state we can choose any special case for polarization and propagation directions; we shall use $q=zy$. The frequency ω is replaced by the operator id/dt. We find, using closure,

$$\begin{aligned}\sum_n f_{0n}{}^Q&=(im/4\hbar c^2)\sum_n[(\ddot{q})_{0n}(\dot{q})_{0n}+(\dot{q})_{0n}(\ddot{q})_{0n}]\\&=(im/4\hbar c^2)\{[\dot{q},\ddot{q}]\}_{00}\\&=-(1/4mc^2)[(2p_z^2/m+2p_y^2/m+z^2\partial^2V/\partial y^2+y^2\partial^2V/\partial z^2+2yz\partial^2V/\partial y\partial z+y\partial V/\partial y+z\partial V/\partial z]_{00}. \quad (6)\end{aligned}$$

For an S ground state, we perform averages over the solid angle, and obtain

$$\sum_n f_{0n}{}^Q=(2/3mc^2)(T)_{00}+(1/15mc^2)\times(r^2d^2V/dr^2+4rdV/dr)_{00}. \quad (7)$$

This expression agrees with Jacobsohn's Eq. (A.5), except that in Eq. (8) we change the sign of his last term involving the Laplacian of the potential, in agreement with a private communication from him. Jacobsohn's changed expression is

$$\sum_n f_{0n}{}^Q=(2/3mc^2)(T)_{00}+(1/60mc^2)\times[(\mathbf{r}\cdot\nabla)^2V+9(\mathbf{r}\cdot\nabla)V+3r^2\nabla^2V]_{00}. \quad (8)$$

(Jacobsohn's derivation and resulting expression is more general than ours since he did not assume a central potential.) The expressions (7) and (8) have been checked for the case of an isotropic simple harmonic oscillator, of natural frequency ω_0, for which direct evaluation of Eq. (5) gives a summed quadrupole oscillator strength of $\hbar\omega_0/mc^2$.

[6] For example, see L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), Eq. (44.8).

[7] S. Frankel, Phys. Rev. **99**, 169 (1955).

[8] B. Jacobsohn, Ph.D. thesis, University of Chicago, 1947 (unpublished); and private communication.

[9] Note that our definition of the quadrupole oscillator strength is different from that in reference 5 by an extra factor of the square of the photon energy.

The retardation correction f^R to electric-dipole transitions is found to $O(v^2/c^2)$ by the power-series expansion of $\exp(ikz)$, and gives,[10] for photon propagation along z and polarization along y,

$$f_{0n}{}^R = -(2m\omega/\hbar c^2)(yz^2)_{0n}(\dot{y})_{0n}. \quad (9)$$

Again we find the summed oscillator strength by replacing ω by id/dt, and applying closure. We find, for an S ground state,

$$\sum_n f_{0n}{}^R = -(1/mc^2)(z^2\partial^2 V/\partial y^2)_{00} = -(1/15mc^2)(r^2d^2V/dr^2+4rdV/dr)_{00}. \quad (10)$$

Our result is in agreement with Jacobsohn's more general Eq. (A.10):

$$\sum_n f_{0n}{}^R = -(1/15mc^2)[2r^2\nabla^2 V - (\mathbf{r}\cdot\nabla)^2 V+(\mathbf{r}\cdot\nabla)V]_{00}. \quad (11)$$

These expressions have been checked against the result $-\hbar\omega_0/2mc^2$ for an isotropic simple harmonic oscillator.

The magnetic dipole oscillator strength is

$$f_{0n}{}^M = (\hbar\omega/2mc^2)[(\mu_x)_{0n}]^2,$$

where μ_x is the magnetic dipole component in Bohr magnetons along the direction x of the incident magnetic field. Applying the same sum-rule techniques, we have for the summed magnetic dipole oscillator strength

$$\sum_n f_{0n}{}^M = -(1/4mc^2)\{[[H,\mu_x],\mu_x]\}_{00}. \quad (12)$$

The coefficient of the double commutator is of $O(v^2/c^2)$. A nonrelativistic central-force atomic Hamiltonian H commutes with the magnetic moment operator μ_x. Then the summed magnetic dipole oscillator strength can be neglected in this paper, where we stop at $O(v^2/c^2)$.

We now find the summed oscillator strength f^t to $O(v^2/c^2)$ by adding Eqs. (4), (7), and (10) for electric dipole, electric quadrupole, and retardation correction, respectively. We find the simple result

$$\sum_n (f^t)_{0n} = 1-(1/mc^2)(T)_{00}. \quad (13)$$

Since the terms involving V canceled, this result holds to order (v^2/c^2) for any ordinary central potential.

Equation (13) can be given a simple interpretation in terms of the relativistic change of mass of the bound particle. The forward-scattering amplitude F at very high frequencies is (e^2/mc^2) times the summed oscillator strength[1]:

$$F(\infty) = (e^2/mc^2)(1+T_{00}/mc^2)^{-1} = e^2/(mc^2+T_{00}). \quad (14)$$

[For our interpretation we have replaced $1-T_{00}/mc^2$ by $(1+T_{00}/mc^2)^{-1}$, which is the same to our order of accuracy.] The term T_{00} in the denominator of the last expression in Eq. (14) represents the increase in the mass energy of the charged particle due to the expectation value of its kinetic energy. We now interpret the fact that the potential energy V does not enter in our final expression, Eq. (13). We have been implicitly considering an infinitely massive source for the potential felt by the bound electron. When very high-frequency light is scattered by the bound electron, the electron acts as if it were more massive than a free electron, because of its kinetic energy. The negative potential energy of the system does not occur in this phenomenon, since the atom as a whole does not move. (If we measured the mass of the entire atom, as for example by a mass spectrometer, then the expectation value of V would have to be considered, and would decrease the atomic mass.)

Since expression (13) holds only to $O(v^2/c^2)$, we use a NR expression for T_{00} for a comparison with our numerical results for lead. We have $T_{00}/mc^2 = \frac{1}{2}(Z/137)^2 = 0.18$ for lead. Equation (13) then gives a summed total oscillator strength of 0.82 in rough agreement with our numerical value[3] of 0.87. We would not expect the agreement to be exact for lead, since the numerical values for f are not exact, and also in our sum-rule calculation the neglected terms of $O(v^4/c^4)$ are $O[(Z/137)^4]$ which is $O(0.13)$. [Note, for example, that we can obtain somewhat different numerical results for lead from Eq. (13) by rewriting it in the form of Eq. (14); or alternatively by using Dirac instead of Schrödinger wave functions in evaluation of T_{00}.] We therefore regard the agreement as satisfactory between our analytical work of this paper and our numerical work of previous papers. Further, Moss has shown recently[11] that the classical power absorption, integrated over all frequencies, is less for a relativistic oscillator than the NR classical value found by Van Vleck.[12]

IV. BREMSSTRAHLUNG-WEIGHTED CROSS SECTION

In this section we calculate the bremsstrahlung-weighted cross section $[\sigma_b = \int(\sigma/W)dW]$ for a Dirac electron in a Coulomb field. We shall compare our numerical result with our work on lead.[3] We shall also give two other moments for the $E2$ absorption cross section.

The bremsstrahlung-weighted cross section for $E1$ absorption, without retardation, is[13]

$$\sigma_b = (4\pi^2/3)\alpha\langle r^2\rangle_{00}, \quad (15)$$

where α is the fine-structure constant. As in the nuclear case, σ_b depends on the wave function of the ground state, but does not depend on the form of the Hamiltonian. If we evaluate the mean square radius $\langle r^2\rangle_{00}$ using Schrödinger wave functions, we obtain $3(a_0/Z)^2$, where a_0 is the Bohr radius. Substitution into Eq. (15) gives, for the case of lead, $\sigma_b = 1200$ barns. If we evaluate $\langle r^2\rangle_{00}$ using Dirac wave functions, we obtain the smaller

[10] Reference 8, Eq. (4.14).

[11] T. A. Moss and J. S. Levinger, Bull. Am. Phys. Soc. Ser. II, 2, 98 (1957); and T. A. Moss, M. S. thesis, Louisiana State University, January 1957 (unpublished).

[12] J. A. Van Vleck, Phys. Rev. 24, 347 (1924).

[13] J. S. Levinger and H. A. Bethe, Phys. Rev. 78, 115 (1950).

value

$$\langle r^2\rangle_{00}=3(a_0/Z)^2(\gamma+1)(2\gamma+1)/6. \quad (16)$$

For lead, $\gamma=(1-\alpha^2Z^2)^{\frac{1}{2}}=0.801$, so the mean square radius is reduced by a factor $(1.801)(2.602)/6=0.781$. [A consistent calculation to our order gives a factor $1-(7/12)(Z\alpha)^2=0.79$.] The numerical value for the bremsstrahlung-weighted cross section becomes $(1200)\times(0.781)=937$ barns.

We now consider the v^2/c^2 corrections to this value, due to $E2$ transitions and retardation effects in $E1$ transitions. The $E2$ oscillator strength $f_{0n}{}^Q$ from Eq. (5) gives us the minus-first moment

$$\begin{aligned}\mu_{-1}{}^Q&=\textstyle\sum_n f_{0n}{}^Q/W=(m/2\hbar^2c^2)\sum_n(\dot q_{0n})^2\\&=(m/2\hbar^2c^2)(\dot q^2)_{00}\\&=-(2/15mc^2)(r^2d^2/dr^2+4rd/dr)_{00}. \quad (17)\end{aligned}$$

(The quadrupole operator $q=zy$.)

The retardation-correction oscillator strength $f_{0n}{}^R$ of Eq. (9) gives us the minus-first moment

$$\begin{aligned}\mu_{-1}{}^R&=\textstyle\sum_n f_{0n}{}^R/W=-(2m/\hbar^2c^2)\sum_n(\dot yz^2)_{0n}(\dot y)_{0n}\\&=-(2m/\hbar^2c^2)(\dot y^2z^2)_{00}\\&=(2/15mc^2)(r^2d^2/dr^2+4rd/dr)_{00}. \quad (18)\end{aligned}$$

We see from Eqs. (17) and (18) that the $E2$ and retardation corrections to σ_b just cancel each other. (This cancellation can be seen more easily for the S ground-state wave function considered: for this case we can write $\dot q=2z\dot y$, since the magnetic-dipole operator $\dot zy-z\dot y$ gives zero for an S state.)

The expression, to order v^2/c^2, for σ_b is then given by Eq. (15), which gave a numerical value of 937 barns for Dirac wave functions for an electron in the Coulomb field of a lead nucleus. This sum-rule value is 7% larger than the numerical value of 874 barns found by numerical integration of the lead oscillator strength.[2,3] The 7% discrepancy should be due to errors in the oscillator strength taken from references 2 and 3, and to the neglected v^4/c^4 terms in the sum-rule calculation.

We give for reference sum-rule results for the minus-second[5] and minus-third moments of the NR $E2$ oscillator strength:

$$\begin{aligned}\mu_{-2}{}^Q&=\textstyle\sum_n f_{0n}{}^Q/W^2=(-m/\hbar^2)\{[[H,q],q]\}_{00}\\&=(1/6\hbar^2c^2)\langle r^2\rangle_{00}, \quad (19)\\\mu_{-3}{}^Q&=\textstyle\sum_n f_{0n}{}^Q/W^3=(m/2\hbar^4c^2)\sum_n(q_{0n})^2\\&=(m/30\hbar^4c^2)\langle r^4\rangle_{00}. \quad (20)\end{aligned}$$

All the sum-rules given in this paper are for a single charged particle in a potential that commutes with the particle's position. They will in general have to be modified for correlations among particles and also, as in the nuclear photoeffect, for terms involving the commutator of the potential energy with the particle position.

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