PHYSICAL REVIEW A VOLUME 33, NUMBER 4 APRIL 1986

Rapid Communications

The Rapid Communications section is intended for the accelerated publication of important new results. Since manuscripts submitted to this section are given priority treatment both in the editorial office and in production, authors should explain in their submittal letters why the work justifies this special handling. A Rapid Communication should be no longer than 3½ printed pages and must be accompanied by an abstract. Page proofs are sent to authors, but, because of the accelerated schedule, publication is not delayed for receipt of corrections unless requested by the author or noted by the editor.

Relativistic corrections to the Bethe sum rule

P. T. Leung* and M. L. Rustgi
Physics Department, State University of New York, Buffalo, New York 14260

S. A. T. Long
National Aeronautics and Space Administration, Langley Research Center, Hampton, Virginia 23665

(Received 26 November 1985)

Relativistic corrections to order α^2 to the Bethe sum rule have been obtained for a one-electron system employing the Foldy-Wouthuysen transformation. The results have wide applications in high-Z systems at large momentum transfers.

It is well known that the quantity known as the generalized oscillator strength $[f_n(q)]$ first introduced into atomic physics by Bethe[1] has important applications in photoeffect and inelastic charged-particle–atom collision problems. Conceptual generalizations of this can lead to applications in other areas too, such as in the treatment of charged-particle interactions with condensed phases in solid-state physics.[2] For an atom of charge Z making a transition from an initial state $|0\rangle$ (usually the ground state) of energy E_0 to a final state $|n\rangle$ of energy E_n, $f_n(q)$ is defined as

$$f_n(q)=\left|\left\langle n\left|\sum_{j=1}^{Z} e^{i\mathbf{q}\cdot\mathbf{r}_j}\right|0\right\rangle\right|^2 (E_n-E_0) \ , \tag{1}$$

where $\mathbf{q}$ is the momentum transferred to the atom. In the long-wavelength limit with the wavelength of the transferred quanta much larger than the size of the atom, $f_n(q)$ reduces back to the ordinary dipole oscillator strength which satisfies the well-known Thomas-Reiche-Kuhn (TRK) sum rule

$$\sum_n \left|\left\langle n\left|\sum_{j=1}^{Z} \mathbf{r}_j\right|0\right\rangle\right|^2 (E_n-E_0)=\frac{3\hbar^2 Z}{2m} \ , \tag{2}$$

where $\sum_n$ implies summation over both discrete and continuum states. Furthermore, it is also well known that $f_n(q)$ defined in Eq. (1) also satisfies a similar sum rule known as the Bethe sum rule:[1]

$$S\equiv\sum_n f_n(q)=\frac{\hbar^2 Z q^2}{2m} \ . \tag{3}$$

Note that both of the results (2) and (3) are known as nonrelativistic sum rules in the sense that the atom is assumed to be described by nonrelativistic wave functions satisfying the Schrödinger equation. Indeed, it is a remarkable fact that within this description, both the dipole and the generalized oscillator strengths satisfy identical sum rules as can be seen from Eqs. (2) and (3).[3] It is also interesting to note that within this nonrelativistic limit, the interference terms, arising from summing over the different pairs of electrons, have no contribution to the final sum.[4] However, in many situations, especially in those involving heavy atoms, the relativistic nature of the atomic electrons plays a very important role in both the determination of the atomic properties and the analysis of scattering results;[5] therefore, a relativistic generalization of the sum rules, Eqs. (2) and (3), is desirable. The attempt to generalize the TRK sum rule [Eq. (2)] to relativistic cases has a long history[6–10] starting from the earliest work by Levinger, Rustgi, and Okamoto. It is the purpose of this paper to present the relativistic generalizations of the Bethe sum rule [Eq. (3)] which is a much more general result than the dipole (TRK) sum rule. In the following, we shall first derive the relativistic sum assuming completeness by employing the Dirac Hamiltonian and then present a semirelativistic approach to order v^2/c^2 following the Foldy-Wouthuysen scheme to exclude the contributions from the negative-energy states. We shall limit ourselves to one-electron systems as in the previous works quoted above.[6–10]

Consider a Dirac electron in a central field described by the Hamiltonian

$$H=-ic\hbar\boldsymbol{\alpha}\cdot\nabla+\beta mc^2+V(r) \ . \tag{4}$$

Let the operator A be defined as

$$A=e^{i\mathbf{q}\cdot\mathbf{r}} \ ; \tag{5}$$

then the Bethe sum rule may be found from[3]

$$S=\sum_n |\langle n|A|0\rangle|^2 (E_n-E_0)=\langle 0|A^\dagger[H,A]|0\rangle \ , \tag{6}$$

where $[,]$ denotes the usual commutator. Equation (6) holds as long as we assume that $|n\rangle$ forms a complete set

of eigenfunctions for H. Hence, for a Dirac electron, the sum S in Eq. (6) will include both the sets of positive- and negative-energy states.

Since $\boldsymbol{\alpha}$ and $\mathbf{r}$ commute, from Eqs. (4) and (5), we have

$$[H,A]=c\hbar\boldsymbol{\alpha}\cdot\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}} \ . \tag{7}$$

Substitute Eq. (7) into Eq. (6) and we obtain

$$S=c\hbar\langle 0|\boldsymbol{\alpha}\cdot\mathbf{q}|0\rangle=0 \ . \tag{8}$$

This result is consistent with the previous results obtained by Levinger *et al.*[6] and others.[9] As before, the null result for S is again due to the exact cancellation between the contributions from positive- and negative-energy states to the sum. However, this result is not useful for treating atomic problems in general since, in such cases, only transitions between positive-energy atomic states will be involved. In the following, we shall attempt a semirelativistic treatment to get rid of the negative-energy states and still maintain completeness for the set of atomic states.

For a Dirac particle moving in a central field, a semirelativistic description of the stationary states in the Foldy-Wouthuysen (FW) representation[11] is given by the following eigenvalue equation:

$$H_{\mathrm{FW}}\Psi_{\mathrm{FW}}=E\Psi_{\mathrm{FW}} \ , \tag{9}$$

where

$$H_{\mathrm{FW}}=\frac{\mathbf{P}^2}{2m}+eV-\frac{\mathbf{P}^4}{8m^3c^2}+\frac{e\hbar}{4m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\boldsymbol{\sigma}\cdot\mathbf{L}+\frac{e\hbar^2}{8m^2c^2}\nabla^2V \ , \tag{10}$$

and the eigenfunction Ψ_{FW} forms a complete set of two-spinor wave functions.[12] The potential V in Eq. (10) for a hydrogenlike system with a nuclear charge Ze is given by

$$V=\frac{Ze}{r} \ . \tag{11}$$

To calculate the Bethe sum rule, we substitute Eq. (10) into Eq. (6) and obtain

$$S=\langle 0|A^{\dagger}[H_{\mathrm{FW}},A]|0\rangle \ , \tag{12}$$

with A as in Eq. (5). Thus, from Eqs. (10) and (12), we see that only the $\mathbf{P}^4$ term and the spin-orbit term contribute to the correction to S. Employing[3]

$$[\mathbf{P}^2,A]=\hbar^2e^{i\mathbf{q}\cdot\mathbf{r}}(q^2-2i\mathbf{q}\cdot\nabla) \ ,$$

one obtains

$$[\mathbf{P}^4,A]=\hbar^4e^{i\mathbf{q}\cdot\mathbf{r}}[q^4-2q^2\nabla^2-4(\mathbf{q}\cdot\nabla)^2-4iq^2\mathbf{q}\cdot\nabla+4i(\mathbf{q}\cdot\nabla)\nabla^2] \ . \tag{13}$$

For the correction due to the spin-orbit term, we have to calculate

$$[f(r)\boldsymbol{\sigma}\cdot\mathbf{L},A]=-f(r)e^{i\mathbf{q}\cdot\mathbf{r}}\boldsymbol{\sigma}\cdot\mathbf{r}\times\mathbf{q} \ , \tag{14}$$

where

$$f(r)=\frac{e\hbar}{4m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r} \ .$$

Substituting Eqs. (13) and (14) into Eq. (12), we obtain the relativistic correction to order v^2/c^2 to the Bethe sum rule given by

$$\Delta S=-\frac{\hbar^4}{8m^3c^2}\left[\int\Psi_0^*[q^4-2q^2\nabla^2-4(\mathbf{q}\cdot\nabla)^2-4iq^2\mathbf{q}\cdot\nabla+4i(\mathbf{q}\cdot\nabla)\nabla^2]\Psi_0d\tau-\int\Psi_0^*f(r)\boldsymbol{\sigma}\cdot\mathbf{r}\times\mathbf{q}\Psi_0d\tau\right] \ . \tag{15}$$

To calculate further, we have to know the ground-state wave function of a hydrogenlike system described by the Foldy-Wouthuysen Hamiltonian H_{FW}. This was first obtained by Berestetskii and Landau[13] and is given by

$$\Psi_0(r)=\left(1-\frac{\hbar^2}{8m^2c^2}\nabla^2\right)\phi_0^D(r) \ , \tag{16}$$

where $\phi_0^D(r)$ is the large component of the exact Dirac wave function which can be written as[14]

$$\phi_0^D(r)=N'r^{\gamma-1}\phi_0^S(r)\chi_{\pm} \ , \tag{17}$$

where $\phi_0^S(r)$ is the ordinary Schrödinger wave function, N' is the normalization constant, and $\chi_+=\binom{1}{0}$ and $\chi_-=\binom{0}{1}$ are the up and down spinors, respectively. γ in Eq. (17) is defined as

$$\gamma=[1-(Z\alpha)^2]^{1/2} \tag{18}$$

with α being the fine-structure constant. On substituting Eqs. (16) and (17) into Eq. (15), it is not difficult to see that the contribution from the spin-orbit term vanishes, and hence, the only correction to S comes from the relativistic correction to the kinetic energy of the electron. In the first integral in Eq. (15), the two imaginary terms must vanish since ΔS must be a real quantity. To show this explicitly, we first note that Ψ_0 as given in Eqs. (16) and (17) is real, and the term involving $q^2\mathbf{q}\cdot\nabla$ vanishes as shown by Bethe.[3] The other imaginary term involving $(\mathbf{q}\cdot\nabla)\nabla^2$ can also be shown to vanish by employing Green's theorem in the form

$$\int_V[\Psi_0\nabla^2(\partial_i\Psi_0)-(\partial_i\Psi_0)\nabla^2\Psi_0]d\tau=\oint_S[\Psi_0\nabla(\partial_i\Psi_0)-\partial_i\Psi_0\nabla\Psi_0]\cdot\mathbf{n}da=0 \ . \tag{19}$$

With these results, Eq. (15) finally reduces to

$$\Delta S=-\frac{\hbar^4}{8m^3c^2}\int\Psi_0[q^4-2q^2\nabla^2-4(\mathbf{q}\cdot\nabla)^2]\Psi_0d\tau \ , \tag{20}$$

where Ψ_0 is given in Eq. (16). However, it is not difficult to see that the term involving ∇^2 in Eq. (16), when substituted into Eq. (20), will yield results of order v^4/c^4 which we have been neglecting all through; therefore, we can safely drop it, and our final normalized $\Psi_0(r)$ takes the form[14]

$$\Psi_0(r)=N\,r^{\gamma-1}e^{-Zr/a} \ ,$$

with

$$N=2^{\gamma-1/2}[\pi\Gamma(2\gamma+1)]^{-1/2}\left(\frac{Z}{a}\right)^{\gamma+1/2} \ . \tag{21}$$

Since $\Psi_0(r)$ is spherical symmetric, Eq. (23) can finally be written as

$$\Delta S=-\frac{\hbar^4}{8m^3c^2}\left[q^4-\frac{10q^2}{3}\int\Psi_0\nabla^2\Psi_0d\tau\right] \ . \tag{22}$$

By making use of $\Psi_0(r)$ in Eq. (21), we finally obtain

$$\Delta S = -\frac{\hbar^4}{8m^3c^2}\left[q^4+\frac{10}{3}\frac{q^2Z^2}{a^2}\frac{1}{(2\gamma-1)}\right] . \quad (23)$$

For systems with small nuclear charge, $Z\alpha \ll 1$ and $\gamma \approx 1$, the result reduces to

$$\Delta S = -\frac{\hbar^4}{8m^3c^2}\left[q^4+\frac{10}{3}\frac{q^2}{a^2}Z^2\right] , \quad (24)$$

which is the same result if one had used the Schrödinger wave function for Ψ_0 in Eq. (22) to do the calculation. For systems with large nuclear charge, so that $Z\alpha \approx 1$, the result in Eq. (23) will differ appreciably from that of Eq. (24). As an example, let us consider a highly ionized lead atom with $Z=82$, $\gamma \approx 0.8$. Equation (23) gives

$$\Delta S = -\frac{\hbar^4}{8m^3c^2}\left[q^4+1.67\left(\frac{10}{3}\right)q^2\frac{Z^2}{a^2}\right] . \quad (25)$$

Note also that in the long-wavelength limit, when $q \ll 1/a$, the result in Eq. (24) gives back the result for the relativistic correction of the TRK sum rule obtained previously,[6,8,10] but Eq. (25) gives a result 1.67 times that of the previous result.

Thus, in general, for a highly ionized one-electron system such as those often found in space plasmas or in stellar interiors, the relativistic corrections to the Bethe sum rule to order v^2/c^2 are given by the result obtained in Eq. (23). This result should therefore be applicable to the analysis of inelastic scattering data from such systems. Furthermore, since the nonrelativisitic Bethe sum rule has been widely applied in the theory of the stopping number and shell correction of atomic K electrons,[15] the result of Eq. (23) should be useful in seeking relativistic corrections to the above theory due to the relativistic nature of the K electrons for heavy target elements. Finally, in order to generalize the result to the case of a many-electron system, we must have the correct semirelativistic Hamiltonian for the system and must face the additional complications caused by those interference terms from summing over different pairs of electrons. It is possible that the effective Hamiltonians obtained by Sucher[16] will be applicable in this case or, alternatively, one may approach the problem by employing the field-theoretic technique.[17] The investigation of the relativistic correction of the Bethe sum rule for many-electron systems will be left for future investigation.

This work was partially supported by the National Aeronautics and Space Administration under Grant No. NAG1442.

*On leave from Physics Department, Tamkang University, Tamsui, Taiwan 251, Republic of China.

[1]H. A. Bethe, Ann. Phys. (Leipzig) **5**, 325 (1930).

[2]For a review of the importance of the generalized oscillator strength see, M. Inokuti, Rev. Mod. Phys. **43**, 297 (1971).

[3]H. A. Bethe and R. W. Jackiw, *Intermediate Quantum Mechanics*, 2nd ed. (Benjamin, New York, 1968), p. 304.

[4]This is in contrast to the sum of inelastic form factors in many nuclear physics problems in which the interference terms play a very important role via the two-proton density function. See, e.g., T. de Forest, Jr. and J. D. Walecka, Adv. Phys. **15**, 1 (1966).

[5]See, e.g., J. Sucher, in *Relativistic Effects in Atoms, Molecules, and Solids*, edited by G. L. Malli, NATO Advanced Study Institute, Series B, Physics, Vol. 87 (Plenum, New York, 1983).

[6]J. S. Levinger, M. L. Rustgi, and K. Okamoto, Phys. Rev. **106**, 1191 (1957).

[7]T. Matsuura and K. Yazaki, Phys. Lett. **46B**, 17 (1973).

[8]J. L. Friar and S. Fallieros, Phys. Rev. C **11**, 274 (1975).

[9]S. P. Goldman and G. W. F. Drake, Phys. Rev. A **25**, 2877 (1982).

[10]K. M. Schmitt and H. Arenhövel, Z. Phys. A **320**, 311 (1985).

[11]L. L. Foldy and S. A. Wouthysen, Phys. Rev. **78**, 29 (1950).

[12]Note that the rest energy can always be absorbed into the phase of the eigenfunction. See, e.g., V. B. Beresteskii, E. M. Lifshitz, and L. P. Pitaevskii, *Quantum Electrodynamics* (Pergamon, New York, 1982).

[13]V. B. Beresteskii and L. D. Landau, Zh. Eksp. Teor. Fiz. **19**, 673 (1949).

[14]See, e.g., J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964).

[15]L. M. Brown, Phys. Rev. **79**, 297 (1950); M. C. Walske, *ibid.* **88**, 1283 (1952).

[16]J. Sucher, Phys. Rev. A **22**, 348 (1980).

[17]See, e.g., J. D. Walecka, Nucl. Phys. **A399**, 387 (1983); T. de Forest Jr., Phys. Lett. **152B**, 151 (1985).