COMMENTS

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Comment on "Relativistic correction of the generalized oscillator strength sum rules"

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Romero and Aucar [Phys. Rev. A **57**, 2212 (1998)] have found a vanishing result for the relativistic correction to the dipole sum rule ΔS_1 for a one-electron system. They have given a result for the dipole sum rule ΔS_2 as well. We argue that these results are both incorrect and show explicitly that their approach yields a nonvanishing result for ΔS_1. The corrected result is in agreement with that which we have obtained in a recent paper, in which we present explicit expressions for ΔS_1, ΔS_2, and several other more general sum rules. [S1050-2947(99)06805-5]

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Romero and Aucar [1] have calculated various atomic sum rules, and presented explicit results for the relativistic dipole sum rules, S_1 and S_2, for a one-electron system. They find that

$$S_1 = S_1^{NR}, \tag{1}$$

thus concluding that ΔS_1, the relativistic correction to S_1, vanishes. They also find

$$S_2 = S_2^{NR} - \frac{\hbar^2}{2m^4c^2}\langle\alpha|p^4|\alpha\rangle. \tag{2}$$

The quantity ΔS_1 has been calculated by a number of authors with the consensus being that it is nonzero, so Eq. (1) would be of considerable interest if it is correct. We will show below that while Eq. (1) is formally correct, the quantity which these authors denote as S_1^{NR} is *not* the nonrelativistic result. Instead, this quantity also contains precisely the relativistic correction found by others [2,3]. We argue that Eq. (2) is incorrect as well, and refer the reader to our paper [3] for these and other sum rule calculations.

In Ref. [1], it is argued that S_1 may be derived from $S_1(\mathbf{q})$ in the limit of small q, where

$$(\hbar^2 q^2/2m) S_1(\mathbf{q}) = S_1^{LL}(\mathbf{q}) + S_1^{LS}(\mathbf{q}) + S_1^{SL}(\mathbf{q}) + S_1^{SS}(\mathbf{q}). \tag{3}$$

Expressions for each of the terms on the right-hand side of this equation are given in Eqs. (8) of [1]. Romero and Aucar find that for the dipole case, $S_1^{LL}+S_1^{LS}+S_1^{SL}=S_1^{NR}$, and then conclude incorrectly that $\Delta S_1=0$. To see that ΔS_1 is in fact nonzero, we now show that S_1^{NR}, as defined in [1], is not equal to the result obtained using the Schrödinger states and energies.

Inserting the lowest-order term in the expansion [4] of $K(p)$ into Eq. (8a), and using the replacements Eq. (12) of [1], S_1^{NR} is obtained as

$$S_1^{NR} = (2m/\hbar^2)\sum_{\alpha,m} \{\langle\alpha|x[V+p^2/2m]|m\rangle\langle m|x|\alpha\rangle - \langle\alpha|x|m\rangle\langle m|x[V+p^2/2m]|\alpha\rangle\}. \tag{4}$$

In [1], the passage from Eq. (8a) to Eq. (14a) is done through the use of the closure relation, Eq. (13). Doing this in Eq. (4), above, immediately leads to

$$S_1^{NR} = (1/\hbar^2)\sum_{\alpha} \{\langle\alpha|xp^2x|\alpha\rangle - \langle\alpha|x^2p^2|\alpha\rangle\}, \tag{5}$$

which yields the correct nonrelativistic result if the state $|\alpha\rangle$, which is the large component of the Dirac spinor, is normalized.

Unfortunately, only in the strict Schrodinger limit are the large components normalized. As a consequence, Eq. (13) of [1] is also only correct in this limit. For example, in the case of a positive-energy-free Dirac electron, the large component is

$$\langle\mathbf{r}|m\rangle = \frac{1}{\sqrt{\mathcal{V}}}\left(\frac{E_m+mc^2}{2E_m}\right)^{1/2}\chi_\pm e^{i\mathbf{p}_m\cdot\mathbf{r}/\hbar}, \tag{6}$$

with E_m the energy, and $\mathbf{p}_m$ the momentum of the electron in the state m, and χ_+ (χ_-) is the two-component spinor with spin up (down). This is normalized only in the limit of infinite mass. Since the calculations of [1] begin with the full Dirac spinors, the full spinor normalizations (e.g., the quantity preceding χ in Eq. (6) above, for the free electron case)

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will carry through the remainder of their paper. For finite mass, there will, therefore, be corrections to the closure relation, Eq. (13) of [1], and care must also be taken to include all corrections arising from the normalization in calculating matrix elements such as those in Eq. (5), above. Equation (13) of [1] is correct only when used with terms that are already $O(m^{-2})$, the limit of accuracy of the present calculations. For S_1^{NR}, on the other hand, one is taking the matrix element of an operator which is $O(m^0)$. Therefore, S_1^{NR} cannot be calculated by using the closure relation without corrections, and we have not found a way to do this calculation explicitly in the general case. We can, however, show that it is not simply equal to the nonrelativistic result. In so doing, we obtain a strong indication that our Eq. (4) leads to the same relativistic correction as found by others [2,3].

Our argument begins by noting that if $\Delta S_1 = 0$ for arbitrary potential, V—as is claimed in [1]—then this result must also hold in the specific case of $V=0$. In this case the sum over states $|m\rangle$ in Eq. (4) may be easily done. Inserting Eq. (6) into Eq. (4) above, the configuration space integrals lead to Dirac delta functions. The sum is then immediate, and for the one-particle case and states $|\alpha\rangle$ having definite parity, we obtain

$$\Delta S_1 = -\frac{5}{6m^2c^2}\langle \alpha | p^2 | \alpha \rangle. \tag{7}$$

This result is precisely that obtained for *arbitrary* potential V using other approaches [2,3]. Thus we see that ΔS_1 is nonzero and, at least in the free-electron limit, in agreement with previous calculations. Furthermore, it may be shown that the approach of Romero and Aucar leads to results for the Bethe sum rule, $S_1(\mathbf{q})$, which are also in agreement with those found by others [3,5].

In the calculation of S_2, Eqs. (16)–(18) of [1], the same error has been made. In writing Eq. (16a), the closure relation has been mistakenly used, giving an incorrect form for S_2^{NR}. We have not calculated S_2^{NR} for the free particle case, as we expect from our own results [3] that for $V=0$, it will be equal to the correct nonrelativistic result. For arbitrary potentials, however, Eq. (18) will have additional relativistic corrections if S_2^{NR} is calculated correctly [3]. Furthermore, the use of the closure relation leading to the other terms in Eqs. (16) is correct to $O(m^{-2})$, only. As discussed above, the use of this relation implies that higher-order contributions have been neglected. Therefore, the result given in Eq. (18) of [1] neglects other terms of the same order as their final result, explaining why it disagrees with the results we have obtained in [3].

Toward the end of their paper, Romero and Aucar conclude that the results for the Bethe sum rule $S_1(\mathbf{q})$, given in their Eq. (11), cannot be directly compared to the corresponding results of Leung, Rustgi, and Long [5], who calculated this quantity using a different approach. As is the case for the dipole sum rule S_1, for which direct comparisons to other works have been made, $S_1(\mathbf{q})$ is a mathematically well-defined object. It must, therefore, have a unique value, irrespective of the approach taken to find it. As we have stated above, it can be shown that the two approaches do agree with each other.

It is also argued in Ref. [1] that, due to the relativistic invariance of the nonrelativistic value for S_1 (it is equal to N, the number of electrons), one might expect that the relativistic corrections to this result must be zero. However, when calculating S_1 for the nonrelativistic case, use is made of the Schrodinger Hamiltonian, which is not itself relativistically invariant. There is no reason, therefore, to expect this result to also be correct in the relativistic regime.

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[1] R. Romero and G. A. Aucar, Phys. Rev. A **57**, 2212 (1998).

[2] J. S. Levinger, M. L. Rustgi, and K. Okamoto, Phys. Rev. **106**, 1191 (1957); H. O. Dogliani and W. F. Bailey, J. Quant. Spectrosc. Radiat. Transf. **9**, 1643 (1969); T. Matsuura and K. Yazaki, Phys. Lett. **46B**, 17 (1973); J. L. Friar and S. Fallieros, Phys. Rev. C **11**, 274 (1975); K.-M. Schmitt and H. Arenhövel, Z. Phys. A **320**, 311 (1985).

[3] S. M. Cohen and P. T. Leung, Phys. Rev. A. **57**, 4994 (1998).

[4] It should be noted that care must be taken in using the expression, Eq. (9) of [1], which is correct for the free particle case, only. We do not believe, however, that this will alter any of their results, unless extended beyond $O(m^{-2})$.

[5] P. T. Leung, M. L. Rustgi, and S. A. T. Long, Phys. Rev. A **33**, 2827 (1986). Note that in Eq. (23) of this paper, the factor $1/(2\gamma-1)$ should be unity [See P. T. Leung, *ibid.* **40**, 5417 (1989)], and that the q^4 term should be multiplied by two (see Ref. [3]).