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

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We have recently calculated corrections to the S_1 and S_2 generalized oscillator strength sum rules [Phys. Rev. A **57**, 2212 (1998)]. In a recent Comment, Cohen and Leung have pointed out the need of taking into account the normalization of the large component of Dirac wave functions. We agree on that and, although this will change the final results presented in the original paper, it is shown that, by including the normalization for the large components in a general way, the method of analysis remains valid and general.
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In their Comment [1] on our paper [2], Cohen and Leung make the objection that our use of the closure relation $\Sigma_n|n^L\rangle\langle n^L|=1-|\chi^L\rangle\langle\chi^L|$ for large components of Dirac eigenstates is wrong. The summation which runs over both occupied $|\chi\rangle$ and vacant $|n\rangle$ states is equal to unity only for normalized large components. The authors also claim that, "We have not found a way to do this calculation explicitly [to correct the closure relation] in the general case." We agree that this lack of normalization does change some parts of the calculation involving the S_1^{LL} term [the others remain unchanged because of their order $(v/c)^2$] and, hence, the final results of [2]. However, we would like to point out that the method of calculation remains both rigorous and general and that the normalization of large components can be addressed in a quite general way.

As is well known, there exist several methods for obtaining semirelativistic, up-to-order $(v/c)^2$ approximations to the Dirac equation. One of them, the elimination of small components, is the one used in [2]. Another possibility is to use Hamiltonians obtained from the Dirac Hamiltonian, in which the odd terms (those connecting large and small components) are removed by applying unitary transformations, e.g., the Foldy-Wouthuysen transformation. This is the approach used by Cohen and Leung in a recent paper [3]. All of these approaches are equivalent up to order $(v/c)^2$, but not all of them are suitable for generalization to calculate higher-order corrections. Given this equivalence, it is interesting to investigate possible discrepancies between results obtained through different approaches.

The normalization of large components can be introduced through an operator N defined [4] by introducing the normalized two-component spinor $|\tilde{i}\rangle=N|i^L\rangle$, where $N=[1+(\sigma\cdot\mathbf{p})K^2(\sigma\cdot\mathbf{p})]^{1/2}=1+p^2/8m^2c^2+O(\alpha^4)$. Then, a corrected closure relation for large components can be recovered:

$$\sum_n |i^L\rangle\langle i^L|=\sum_n N^{-1}|\tilde{i}\rangle\langle\tilde{i}|N^{-1}=N^{-2}=1-p^2/4m^2c^2+O(\alpha^4), \tag{1}$$

where the sum runs over both occupied and vacant large components $|i^L\rangle$. Hence the sum over the vacant states used in [2] can be replaced by

$$\sum_n |n^L\rangle\langle n^L|=1-p^2/4m^2c^2-|\chi^L\rangle\langle\chi^L|+O(\alpha^4), \tag{2}$$

χ denoting the only occupied orbital. Finally, the expectation values of the various operators have to be calculated using the non-normalized wave function,

$$|\chi^L\rangle=N^{-1}|\tilde{\chi}\rangle=(1-p^2/8m^2c^2)|\tilde{\chi}\rangle. \tag{3}$$

Inserting these replacements into our formulas for the one-electron case makes our results coincide with Cohen and Leung's [1], and the correction for the sum rules becomes

$$\Delta S_1=-\frac{5}{3mc^2}\left\langle\chi\left|\frac{p^2}{2m}\right|\chi\right\rangle. \tag{4}$$

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[1] S. M. Cohen and P. T. Leung, Phys. Rev. A **59**, 4847 (1999).
[2] R. H. Romero and G. A. Aucar, Phys. Rev. A **57**, 2212 (1998).
[3] S. M. Cohen and P. T. Leung, Phys. Rev. A **57**, 4994 (1998).
[4] R. E. Moss, *Advanced Molecular Quantum Mechanics* (Chapman and Hall, London, 1972), p. 136.

