Addition and Correction: "Perspectives of relativistic quantum chemistry: The negative energy cat smiles" [Phys. Chem. Chem. Phys. 14, 35 (2012)]

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Some of the equations are corrected to be general enough. However, none of the statements needs to be revised.

Although claimed for a many electron system, some of the (nonradiative and nonretarded) QED energy expressions (i.e., Eqs. (92), (95), and (107)) in Ref.[1] are found to hold only for the special case of two electrons. In particular, except for the diagrams considered before[1] (see Figs. (3a) to (3h)), the so-called three-electron-two-photon diagram[2] shown in Fig. (3i) should also be included for the second order energy $E^{(2)}$ of a many-electron system. Without going into details, the energy for Fig. (3d) should read

$$E^{(2)}_{L++} = \frac{1}{4}\frac{\bar{g}^{ab}_{ij}\bar{g}^{ij}_{ab}}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}, \quad (1)$$

$$E^{(2)}_{L--} = -\frac{1}{4}\frac{\bar{g}^{\tilde{i}\tilde{j}}_{ij}\bar{g}^{ij}_{\tilde{i}\tilde{j}}}{\varepsilon_i+\varepsilon_j-\varepsilon_{\tilde{i}}-\varepsilon_{\tilde{i}}}, \quad (2)$$

$$E^{(2)}_{Lov} = \frac{\bar{g}^{aj}_{ij}\bar{g}^{ij}_{aj}}{\varepsilon_i-\varepsilon_a} + \frac{1}{2}\frac{\bar{g}^{ka}_{ij}\bar{g}^{ij}_{ka}}{\varepsilon_i+\varepsilon_j-\varepsilon_k-\varepsilon_a}|_{i\neq j\neq k}, \quad (3)$$

while the energy for Fig. (3i) reads

$$E^{(2)}_{3i,1+} = \frac{(V_{HF})^a_i(V_{HF})^i_a}{\varepsilon_i-\varepsilon_a}, \quad (4)$$

$$E^{(2)}_{3iov} = -\frac{\bar{g}^{aj}_{ij}\bar{g}^{ij}_{aj}}{\varepsilon_i-\varepsilon_a} - \frac{1}{2}\frac{\bar{g}^{ka}_{ij}\bar{g}^{ij}_{ka}}{\varepsilon_i+\varepsilon_j-\varepsilon_k-\varepsilon_a}|_{i\neq j\neq k}, \quad (5)$$

$$E^{(2)}_{3i,1-} = \frac{(V_{HF})^{\tilde{i}}_i(V_{HF})^i_{\tilde{i}}}{\varepsilon_i-\varepsilon_{\tilde{i}}} - \frac{\bar{g}^{\tilde{i}j}_{ij}\bar{g}^{ij}_{\tilde{i}j}}{\varepsilon_i-\varepsilon_{\tilde{i}}}, \quad (6)$$

$$E^{(2)}_{3i,2-} = -\frac{1}{2}\frac{\bar{g}^{k\tilde{i}}_{ij}\bar{g}^{ij}_{k\tilde{i}}}{\varepsilon_i+\varepsilon_j-\varepsilon_k-\varepsilon_{\tilde{i}}}|_{i\neq j\neq k}. \quad (7)$$

Note that the term $E^{(2)}_{3iov}$ (5) will cancel the term $E^{(2)}_{Lov}$ in Eq. (3). Likewise, the energy for Fig. (3e) should be corrected as

$$E^{(2)}_X = \frac{i\gamma}{2}[4\langle\alpha|S^{(4)}|\alpha\rangle] \quad (8)$$

$$= -\frac{g^{pj}_{i\tilde{j}}g^{i\tilde{j}}_{pj}}{\varepsilon_i+\varepsilon_{\tilde{j}}-\varepsilon_j-\varepsilon_p} + \frac{g^{pi}_{i\tilde{j}}g^{\tilde{j}j}_{jp}}{\varepsilon_{\tilde{j}}-\varepsilon_p}, \quad (9)$$

where the summation over p includes all the occupied and virtual PES. Note that $E^{(2)}_X$ vanishes for the same occupied orbitals (i.e., $i = j$). The final two-body terms of $E^{(2)}_{QED}$ include Eqs. (1), (2), (7), and (9), while the one-body terms in Eqs. (4) and (6) and those in Eqs. (99), (100), (104) and (105) in Ref.[1] can be regrouped into

$$E^{(2)}_{QED,1+} = \frac{(V_{HF}-U)^a_i(V_{HF}-U)^i_a}{\varepsilon_i-\varepsilon_a} = E^{(2)}_{CS,1+}, \quad (10)$$

$$E^{(2)}_{QED,1-} = \frac{(V_{HF}-U)^{\tilde{i}}_i(V_{HF}-U)^i_{\tilde{i}}}{\varepsilon_i-\varepsilon_{\tilde{i}}} - \frac{\bar{g}^{\tilde{i}j}_{ij}\bar{g}^{ij}_{\tilde{i}j}}{\varepsilon_i-\varepsilon_{\tilde{i}}} \quad (11)$$

$$= E^{(2)}_{CS,1-} - \frac{\bar{g}^{\tilde{i}j}_{ij}\bar{g}^{ij}_{\tilde{i}j}}{\varepsilon_i-\varepsilon_{\tilde{i}}}. \quad (12)$$

Consequently, Eqs. (95) and (107) in Ref.[1] should be replaced with the present Eqs. (9) and (12), respectively. Although formerly the same, Eq. (92) in Ref.[1] (actually the first term of the present Eq. (3)) should be understood as the present Eq. (4) arising from Fig. (3i). Retaining only the terms in Eqs. (1) and (10) goes back to the standard no-pair approximation that has an intrinsic error of order $(Z\alpha)^3$ and is dependent on the mean-field potential generating the orbitals. Fortunately, such an error as well as the potential dependence can largely be removed by further accounting for the simple counter terms (100) and (105) in Ref.[1], leading to a 'potential-independent no-pair approximation'.

As a final remark, what has been discussed so far is exclusively the nonradiative correlation aspect of NES. In a forthcoming paper, we will show that the Fock space approach con-

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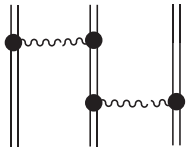
tains also some radiative effects (vacuum polarization and vertex correction) and is therefore different from the purely non-radiative QED approach. In short, the Fock space approach can be characterized as 'systematic but inconsistent'.



(i)

Fig. 3 The three-electron-two-photon Feynman diagram.

Acknowledgments

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Notes and references

1 W. Liu, Phys. Chem. Chem. Phys. **14**, 35-48 (2012).
2 J. Sapirstein and K. T. Cheng, Phys. Rev. A **64**, 022502-1-9 (2001).