Erratum: Hamiltonian for the inclusion of spin effects in long-range Rydberg molecules **[Phys. Rev. A *95*, 042515 (2017)]**

Matthew T. Eiles and Chris H. Greene

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There are several typographical errors in the “multipole moments” section along with some poor and confusing notational conventions. The changes below rectify these issues. In particular, several times the letter L was used rather than the letter k , or the letter k was used with multiple meanings. Making the appropriate replacements frees L to replace L' , which improves the legibility of this notation. We additionally removed two extraneous expressions [Eqs. (25) and (26) in the original article] involving reduced matrix elements, which are unrelated to the final result and thus introduced additional confusion due to their dependence on the convention of the Wigner-Eckart theorem.

These replacements are as follows:

Equation (22) should be replaced with

$$T_q^k = -r^k C_{kq}(\hat{r}), \quad C_{kq}(\hat{r}) = \sqrt{\frac{4\pi}{2k+1}} Y_{kq}(\hat{r}). \quad (22)$$

Equation (23) should be replaced by

$$\Psi_{LM_L}(\vec{R}, \vec{r}) = \frac{\sum_l Q_{LM_L}^{nl}(R) Y_{lM_L}(\hat{r}) r^{-1} f_{nl}(r)}{\sqrt{\mathcal{N}_{nLM}(R)}}, \quad (23)$$

where $\mathcal{N}_{nLM}(R) = \sum_l |Q_{LM_L}^{nl}(R)|^2$. Equation (24) should be replaced by

$$\begin{aligned} \langle T_q^k \rangle &= \langle \Psi_{LM} | T_q^k | \Psi_{LM} \rangle \\ &= \sum_{l,l'} \frac{Q_{LM}^{nl}(R) Q_{LM}^{n'l'}(R)}{\mathcal{N}_{nLM}(R)} \langle nLM | T_q^k | n'l'M \rangle. \end{aligned} \quad (24)$$

The text and equations between Eq. (24) and [including Eq. (28)] should be replaced with:

The matrix element separates into a radial integral $R_{nl}^{n'l'}(k) = \int dr f_{nl}(r) r^k f_{n'l'}(r)$ multiplying an angular integral which is evaluated with standard techniques to obtain the result,

$$\langle T_q^k \rangle = \sum_{l,l'} \frac{Q_{LM}^{nl}(R) Q_{LM}^{n'l'}(R)}{\mathcal{N}_{nLM}(R)} R_{nl}^{n'l'}(k) C_{l'M,kq}^{lM} (-1)^{k-l'} \sqrt{(2l'+1)} \begin{pmatrix} l & l' & k \\ 0 & 0 & 0 \end{pmatrix}. \quad (25)$$

The Clebsch-Gordan coefficient causes any term with $M' \neq 0$ to vanish, reflecting the cylindrical symmetry. The $k=1$ moments agree exactly with Ref. [18]. These multipole moments scale in size as n^{2k} and are displayed in Fig. 8 up to the octupole moments. Within the full spin model, the multipole moments are derived similarly but using the numerically calculated eigenstates $|s\rangle = \sum_{\kappa} a_{s\kappa} |\kappa\rangle$, where $|s\rangle$ is an electronic eigenstate, κ is a composite quantum number $\kappa = \{n(l s_1) j m_j m_2 m_i\}$, and $a_{s\kappa}$ is the eigenvector corresponding to the s th eigenstate. The multipole moments are then

$$\langle s | T_q^k | s \rangle = \sum_{\kappa, \kappa'} \left[a_{s\kappa}^* a_{s\kappa'} \delta_{m_2, m_2'} \delta_{m_i, m_i'} \delta_{m_j, m_j'} R_{nlj}^{n'l'j}(k) (-1)^{s_1+j'+l-l'} \sqrt{(2j+1)(2l+1)(2l'+1)} C_{j'm_j', kq}^{j m_j} \begin{pmatrix} l & l' & k \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l' & s_1 & j' \\ j & k & l \end{Bmatrix} \right].$$

These typographical errors or confusing conventions do not affect any other part of the paper or the calculations displayed in Figs. 8 and 9.