Convergence of the discrete dipole approximation. I. Theoretical analysis: erratum

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The following errors in the analysis of the weighted discretization in [1] resulted from the incorrect interpretation of this formulation of the discrete dipole approximation, originally proposed by Piller [2]. Moreover, this interpretation was not fully expressed in [1], which also cast ambiguity on the definition of the formulation. So we start with explicit statement of a correct interpretation, as corresponding to a numerical scheme,

$$E_i = E_i^{nc} + \sum_{j;i,j} G_{ij}^{(9)} V_j \chi_j E_j + (M_i \chi_i - L_i \chi_i) E_i, \quad (E1)$$

which is a direct cast of Eq. (13) in [2] into the notation of [1] and can be considered an extension of Eq. (10) in the latter.

The first error was in the multiplier of $G^i$ in the second integral in Eq. (92) in [1], which also contained a typographical error (“$r$” instead of “$\bar{r}$”). The correct expression is

$$M_i \chi_i E_i = \left( \int_{V_i} d^3r' (G(r_i, r') - \bar{G}(r_i, r')) \chi_p^i \right) E_i$$

$$+ \int_{V_i} d^3r' (\bar{G}(r_i, r') P_i - \bar{G}(r_i, r') \chi_p^i) E_i, \quad (92)$$

where the left-hand side is updated according to the notation of Eq. (E1) to explicitly indicate that it is an approximation to the rigorous $M_i(V_i, r_i)$ given by Eq. (4) in [1]. The corrected Eq. (92) is equivalent to Eq. (9) in [2].

The second error was in the third line of Eq. (96) in [1] in a multiplier of $L_i$, cf. Eq. (E1). Correcting both errors also results in vanishing of the last two lines of Eq. (96). The final corrected expression is

$$h_i^{sh} = (M(V_p, r_i) - L(\partial V_p, r_i) P_i^p)$$

$$- \left( \int_{V_i} d^3r' (\bar{G}(r_i, r') - \bar{G}(r_i, r')) P_i^p \right)$$

$$= \int_{V_i} d^3r' (\bar{G}(r_i, r') (P(r') - P_i^p)$$

$$+ \int_{V_i} d^3r' (\bar{G}(r_i, r') (P(r') - P_i^p).$$

Also, there was a typographic error in the expression in the beginning of a text line immediately before Eq. (96)—it should read $h_i^{sh}$.

Then, it follows that the phrase “and the third one is transformed to $L_i$, the same way as in expression (80)” after Eq. (96) should be removed, and Eq. (97) should read

$$\| h_i^{sh} \| \leq c_{88} d.$$

The whole paragraph after Eq. (97) should be removed, i.e., the original weighted discretization effectively reduces shape errors and requires no further improvements. That is the main conclusion of this erratum.

Finally, Eq. (98) should read

$$\| h_i^{sh} \| \leq \sum_{j \in dV} \left( \sum_{l=1}^{K_{max}} c_{84} n_l l^{-4} + c_{88} d \right) \leq c_{89} N d, \quad (98)$$

i.e., the term $c_{87}$ is removed, but the total order of errors is unchanged.
There was also a sign error in Eq. (6); the correct one is

\[ \mathbf{L}(\delta V_{m}, \mathbf{r}) = \frac{-2}{\Delta \omega_{q}} \int d \mathbf{r} \frac{2 \hat{\mathbf{r}}}{\Delta \omega_{q}}, \]  

(6)

All other parts of [1], including abstract and conclusions, remain unchanged and are not affected by this erratum.

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REFERENCES
