Erratum: Multipole effects in atom-surface interactions: A theoretical study with an application to He–α-quartz [Phys. Rev. A 81, 052507 (2010)]

Grzegorz Łach, Maarten DeKieviet, and Ulrich D. Jentschura

(Received 24 May 2023; published 9 January 2024)

DOI: 10.1103/PhysRevA.109.019902

As recently outlined in Ref. [1], the general functional form of the multipole corrections defined in our original paper is valid in the asymptotic short-range and long-range limits, but the prefactors of the multipole correction terms receive modifications when one takes the details of the angular momentum decomposition into account. Specifically, the modifications are as follows. With the notation employed in Ref. [1] for the multipole polarizability $\alpha_\ell(\omega)$, of multipole order 2^ℓ, and the corresponding energy shifts $\mathcal{E}_\ell$, the expressions given in Eqs. (8)–(11) of our paper should have read

$$\mathcal{E}_{\ell=2} = -\frac{1}{12}\sum_{\vec{k}\lambda}\sum_{ij}\alpha_2(\omega)\left|\{\nabla^j E^i_{\vec{k}\lambda}(\vec{r})\}\right|_{\ell=2}|^2, \tag{1}$$

$$\mathcal{E}_{\ell=3} = -\frac{1}{180}\sum_{\vec{k}\lambda}\sum_{ijk}\alpha_3(\omega)\left|\{\nabla^j\nabla^k E^i_{\vec{k}\lambda}(\vec{r})\}\right|_{\ell=3}|^2, \tag{2}$$

$$\mathcal{E}_{\ell=4} = -\frac{1}{5040}\sum_{\vec{k}\lambda}\sum_{ijk}\alpha_4(\omega)\left|\{\nabla^j\nabla^k\nabla^l E^i_{\vec{k}\lambda}(\vec{r})\}\right|_{\ell=4}|^2, \tag{3}$$

$$\mathcal{E}_{L} = -\frac{2^{L-1}}{(2L)!}\sum_{\vec{k}\lambda}\sum_{j_1 j_2\ldots j_L}\sum_{i}\alpha_L(\omega)\left|\{\nabla^{j_1}\nabla^{j_2}\ldots\nabla^{j_L} E^i_{\vec{k}\lambda}(\vec{r})\}\right|_{\ell=L}|^2. \tag{4}$$

The specification of the ($\ell = L$) component assumes that a specific angular momentum can be isolated in Cartesian coordinates, a problem, which is discussed in Ref. [1] in detail.

The results in Eqs. (32)–(34) of our paper receive the following modifications:

$$\mathcal{E}_2(z) = -\frac{\hbar}{16\pi^2\epsilon_0 z^5}\int_0^\infty d\omega\,\alpha_2(i\omega)\,\exp\left(-\frac{2\omega z}{c}\right)\left[\frac{3}{4}+\frac{3}{2}\frac{\omega z}{c}+\frac{4}{3}\left(\frac{\omega z}{c}\right)^2+\frac{2}{3}\left(\frac{\omega z}{c}\right)^3+\frac{1}{6}\left(\frac{\omega z}{c}\right)^4\right], \tag{5}$$

$$\mathcal{E}_2(z) \overset{z\to 0}{=} -\frac{3\hbar}{64\pi^2\,\epsilon_0\,z^5}\int_0^\infty d\omega\,\alpha_2(i\omega), \tag{6}$$

$$\mathcal{E}_2(z) \overset{z\to \infty}{=} -\frac{35 c\hbar\,\alpha_2(0)}{384\pi^2\,\epsilon_0\,z^6}. \tag{7}$$

The results given in Eqs. (35)–(37) of our paper receive the following modifications:

$$\mathcal{E}_3(z) = -\frac{\hbar}{16\pi^2\epsilon_0 z^7}\int_0^\infty d\omega\,\alpha_3(i\omega)e^{-2\omega z/c}\left[\frac{2}{3}+\frac{4}{3}\frac{\omega z}{c}+\frac{92}{75}\left(\frac{\omega z}{c}\right)^2+\frac{152}{225}\left(\frac{\omega z}{c}\right)^3+\frac{6}{25}\left(\frac{\omega z}{c}\right)^3+\frac{4}{75}\left(\frac{\omega z}{c}\right)^4+\frac{4}{675}\left(\frac{\omega z}{c}\right)^6\right], \tag{8}$$

$$\mathcal{E}_3(z) \overset{z\to 0}{=} -\frac{\hbar}{24\pi^2\,\epsilon_0\,z^7}\int_0^\infty d\omega\,\alpha_3(i\omega), \tag{9}$$

$$\mathcal{E}_3(z) \overset{z\to \infty}{=} -\frac{77 c\hbar\,\alpha_3(0)}{800\pi^2\,\epsilon_0\,z^8}. \tag{10}$$

As explained in Ref. [1], the results given in Eqs. (38)–(40) of our paper receive the following modifications:

$$\mathcal{E}_4(z) = -\frac{\hbar}{16\pi^2\epsilon_0 z^9}\int_0^\infty d\omega\,\alpha_4(i\omega)e^{-2\omega z/c}\left[\frac{5}{8}+\frac{5}{4}\frac{\omega z}{c}+\frac{115}{98}\left(\frac{\omega z}{c}\right)^2+\frac{100}{147}\left(\frac{\omega z}{c}\right)^3 + \frac{79}{294}\left(\frac{\omega z}{c}\right)^4+\frac{11}{147}\left(\frac{\omega z}{c}\right)^5+\frac{32}{2205}\left(\frac{\omega z}{c}\right)^6+\frac{4}{2205}\left(\frac{\omega z}{c}\right)^7+\frac{1}{8820}\left(\frac{\omega z}{c}\right)^8\right], \tag{11}$$

$$\mathcal{E}_4(z) \overset{z\to 0}{=} -\frac{5\hbar}{128\pi^2\,\epsilon_0\,z^9}\int_0^\infty d\omega\,\alpha_4(i\omega), \tag{12}$$

$$\mathcal{E}_4(z) \overset{z\to\infty}{=} -\frac{1287c\hbar\,\alpha_4(0)}{12544\pi^2\,\epsilon_0\,z^{10}}. \tag{13}$$

The result reported in Eq. (49) of our paper (for the short-range regime, perfect conductor) receives an additional factor $(L+1)/(2L)$ and reads

$$\mathcal{E}_L(z) = -\frac{\hbar}{(4\pi)^2\epsilon_0 z^{2L+1}}\left\{\frac{L+1}{2L}\right\}\int_0^\infty d\omega\alpha_L(i\omega), \tag{14}$$

where the additional factor is given in curly brackets [1]. Furthermore, the result reported on the right-hand side of Eq. (61b) of our paper, for the idealized case of a perfect conductor, receives a global prefactor 3/4. The results reported in Eqs. (66) receives modified prefactors in the polynomial in ξ in the integrand,

$$\mathcal{E}_2(z) = -\frac{\hbar}{16\pi^2\,\epsilon_0\,c^5}\int_0^\infty d\omega\,\omega^5\,\alpha_2(i\omega)\int_1^\infty d\xi\,e^{-2\xi\omega z/c}\left(\frac{\xi^2}{2}-\frac{1}{3}\right)\mathrm{H}(\xi,\epsilon(i\omega)). \tag{15}$$

Finally, the results reported in Eqs. (67)–(69) of our paper receive the following modifications:

$$\mathcal{E}_2(z) \overset{z\to 0}{=} -\frac{3}{4}\,\frac{\hbar}{(4\pi)^2\epsilon_0 z^5}\int_0^\infty d\omega\,\alpha_2(i\,\omega)\,\frac{\epsilon(i\omega)-1}{\epsilon(i\omega)+1}, \tag{16}$$

$$\mathcal{E}_3(z) = -\frac{\hbar}{16\pi^2\,\epsilon_0\,c^7}\int_0^\infty d\omega\,\omega^7\,\alpha_3(i\omega)\int_1^\infty d\xi\,e^{-2\xi\omega z/c}\left(\frac{8\xi^4}{135}-\frac{16\,\xi^2}{225}+\frac{4}{225}\right)\mathrm{H}(\xi,\epsilon(i\omega)), \tag{17}$$

$$\mathcal{E}_4(z) = -\frac{\hbar}{16\pi^2\,\epsilon_0\,c^9}\int_0^\infty d\omega\,\omega^9\,\alpha_4(i\omega)\int_1^\infty d\xi\,e^{-2\xi\omega z/c}\left(\frac{\xi^6}{252}-\frac{\xi^4}{147}+\frac{\xi^2}{294}-\frac{1}{2205}\right)\mathrm{H}(\xi,\epsilon(i\omega)). \tag{18}$$

For reference, we would like to point out that all considerations regarding the order-of-magnitude of the multipole corrections, and their parametric scaling as reported in detail in Sec. IV A of our paper [especially, the scaling relations in Eqs. (45)–(48) of our paper] remain valid and are not affected by the modifications reported here and in Ref. [1].

In our original paper analytic representations have been obtained for the dielectric function of α quartz, based on fitting data from Ref. [2]. In the fitting function given in Eq. (70) in our original paper, a factor ω_k^2 was missing in the numerator; the correct fitting function reads

$$\rho(\omega) \equiv \frac{\epsilon(\omega)-1}{\epsilon(\omega)+2} \simeq \sum_{k=1}^{n}\frac{\alpha_k\,\omega_k^2}{\omega_k^2 - i\,\gamma_k\,\omega-\omega^2}. \tag{19}$$

The entries in Tables I and II of our paper remain valid. An update on a suitable fit for α quartz is given in Ref. [1].

The modified results for the quadrupole and octupole effects imply that coefficients C_5 and C_7 given in Table III of our paper receive multiplicative correction factors of 3/4 and 2/3, respectively. One may consult Ref. [1] for a discussion of the magnitude of the multipole effects and an update on α-quartz interactions for hydrogen and positronium, and applications to physisorption.

The authors acknowledge helpful conversations with Professor Carsten A. Ullrich. This research was supported by NSF Grant No. PHY–2110294.

[1] U. D. Jentschura, preceding paper, Revisiting the divergent multipole expansion of atom-surface interactions: Hydrogen and positronium, α-quartz, and physisorption, Phys. Rev. A **109**, 012802 (2024).

[2] H. R. Phillipp, Silicon dioxide (SiO_2), type α (cystalline), in *Handbook of Optical Constants of Solids*, edited by E. D. Palik (Academic Press, Boston, 1985), pp. 719–747.