Erratum: Electrostatics in periodic boundary conditions and real-space corrections [Phys. Rev. B 77, 115139 (2008)]

Ismaila Dabo,* Boris Kozinsky, Nicholas E. Singh-Miller, and Nicola Marzari

(Received 14 October 2011; published 31 October 2011)

DOI: 10.1103/PhysRevB.84.159910 PACS number(s): 71.15.−m, 31.15.−p, 31.70.−f, 99.10.Cd

We correct two errors in Sec. II.D of Ref. 1, appearing in the derivation of Eq. (21) as an alternative expression for the point countercharge (PCC) correction (for which the original Makov-Payne derivation in Ref. 2 stands true) and in the associated plot in Fig. 5. The rest of the paper is not affected by these corrections, and all conclusions, including the comparative assessment of real-space countercharge corrections and the performance of the density-countercharge correction, remain valid.

First, in deriving Eq. (21), we considered the parabolic expansion of the corrective potential of a single PCC [Eq. (11)]:

$$v^{\text{corr}}_{\text{PCC,single}} = \frac{\alpha_0 q}{L} - \frac{2\pi q}{3L^3} r^2.$$

Substituting the expression of the potential $v^{\text{corr}}_{\text{PCC,single}}$ into Eq. (20) yields Eq. (21). Instead, the general derivation should take into account multiple countercharges [Eq. (13)]:

$$v^{\text{corr}}_{\text{PCC,multiple}} = \frac{\alpha_0 q}{L} - \frac{2\pi q}{3L^3} r^2 + \frac{4\pi}{3L^3} \mathbf{p} \cdot \mathbf{r} - \frac{2\pi Q}{3L^3}.$$

Inserting the expression for the potential $v^{\text{corr}}_{\text{PCC,multiple}}$ into Eq. (20), we obtain the general equation of the multiple-point energy correction,

$$\Delta E^{\text{corr}}_{\text{PCC,multiple}} = \frac{\alpha_0 q^2}{2L} + \frac{2\pi}{3L^3}(p^2 - qQ),$$

whose quadrupole term is identical to that derived by Makov and Payne, at variance with Eq. (21), which relies on the restrictive single-point expansion.

Second, in computing the corrective terms for the electrostatic interaction of two Gaussian charges in Fig. 5 of Ref. 1, we inadvertently set the origin of the coordinate system to be one of the Gaussian centers, yielding a quadrupole moment Q of 303 a.u. instead of 153 a.u., which caused a twofold overestimation of the quadrupole correction. Corrected results are presented in Fig. 1 here, highlighting the slow asymptotic convergence of the single-point correction relative to the multiple-point correction, notwithstanding the fortuitous accuracy of the former for small supercells. To confirm this conclusion, we consider the electrostatic energy of four Gaussian charges in Fig. 2 here, showing the improved performance of the multiple-point correction in comparison with its single-point counterpart.

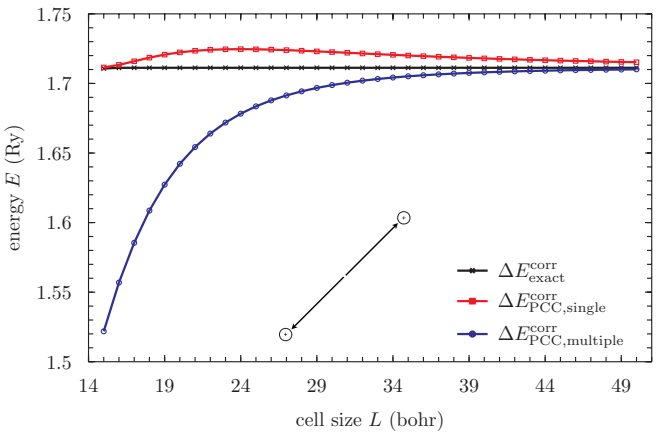

FIG. 1. (Color online) Electrostatic energy of two Gaussians of unit charge and unit spread calculated via exact real-space integration, reciprocal-space interaction with a single point countercharge (PCC), and reciprocal space intergration with a multiple PCC (the Makov-Payne correction). Gaussian charges are positioned at (–5,–5,–5) and (5,5,5), corresponding to a quadrupole moment Q of 153 a.u.

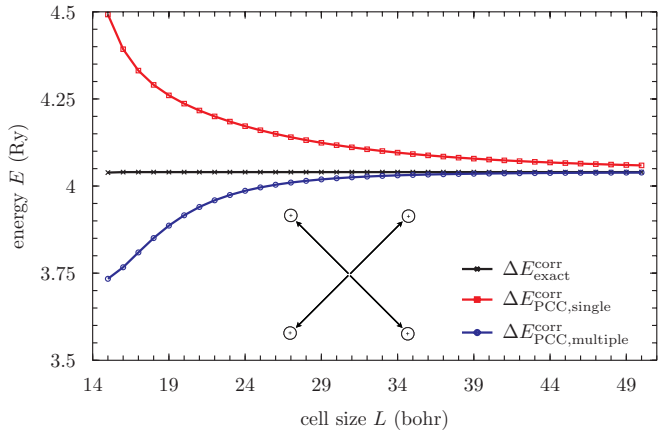

FIG. 2. (Color online) Electrostatic energy of four Gaussians of unit charge and unit spread. Gaussian charges are positioned at (–5,–5,5), (–5,5,–5), (5,–5,–5), and (5,5,5), forming a tetrahedron and corresponding to a quadrupole moment Q of 306 a.u.

We are grateful to Stefano de Gironcoli for elegantly rederiving the Makov-Payne correction from Eq. (13) and Oliviero Andreussi for pointing out errors in the figure. We thank Fabiano Corsetti for valuable discussions on alternative derivations of the Makov-Payne expansion.

---

*daboi@cermics.enpc.fr

[1]I. Dabo, B. Kozinsky, N. E. Singh-Miller, and N. Marzari, Phys. Rev. B **77**, 115139 (2008).

[2]G. Makov and M. C. Payne, Phys. Rev. B **51**, 4014 (1995).