Erratum: Optimized norm-conserving Vanderbilt pseudopotentials [Phys. Rev. B 88, 085117 (2013)]

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Errors have been found in Eqs. (15) and (16). The correct constraint equation is

$$x_1 = s\left[D_{\rm norm} - \sum_{i=2}^{N-M} x_i^2\right]^{1/2}. \tag{15}$$

By inspection of the residual energy $E^{\rm r}$ given in Eq. (14), it is clear that the sign s of x_1 at the $E^{\rm r}$ minimum must be opposite to that of f_1. Setting the derivatives of $E^{\rm r}$ with respect to $x_2, \ldots, x_{N-M}$ to zero using Eq. (15) for x_1 yields

$$x_i = -f_i/(e_i - e_1 - f_1/x_1)\,. \tag{16}$$

Since all of the e_i's are positive with e_1 as the smallest and f_1/x_1 is negative, the denominator in the revised Eq. (16) is always positive. When Eq. (16) is now substituted back into Eq. (15), the magnitude of the right-hand side is seen to be a monotonically decreasing function of $|x_1|$ with maximum value $D_{\rm norm}^{1/2}$ at $x_1 = 0$. Thus a simple interval-halving search on $\{0, D_{\rm norm}^{1/2}\}$ to find $|x_1|$ satisfying Eq. (15) will yield the unique minimum of $E^{\rm r}$. The previously described hypersphere search is unnecessary. Whereas the correct form of Eq. (15) was used in the open-source ONCVPSP code, the erroneous version of Eq. (16) was coded and used as originally described. Reference [1] is corrected and employs this simple algorithm.

This error was inconsequential for the accuracy that pseudopotentials generated with this code achieved in representing all-electron atoms. Continuity, generalized norm conservation, and logarithmic derivatives were not compromised. The error resulted in a small sacrifice in convergence optimization since the exact minimum of $E^{\rm r}$ was not achieved. Extensive testing with the corrected code shows no significant changes in benchmark metrics against all-electron solid-state calculations and nearly undetectable differences in observed convergence. This is attributable to the very large dynamic range spanned by e_i, $\sim 10^6 - 10^8$, which effectively isolated the damage that could be done by the sign and coefficient errors in Eq. (16). Changes in the published figures in this paper would be imperceptible.

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[1] ONCVPSP, Release 3.3.0, available at www.mat-simresearch.com

