Erratum: Optimized norm-conserving Vanderbilt pseudopotentials [Phys. Rev. B 88, 085177 (2013)]

D. R. Hamann

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

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

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 $x_2,...,x_{N-M}$ to zero using Eq.(15) for x_1 yields

$$x_i = -f_i \big/ \left(e_i - e_1 - f_1/x_1 \right). \qquad (16)$$

Since all of the e_i are positive with e_1 the smallest and f_1/x_1 is negative, the denominator in 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 $\left\{ 0, D_{\rm norm}^{1/2} \right\}$ to find $|x_1|$ satisfying Eq.(15) will yield the unique minimum of $E^{\rm r}$. The previously-described hypersphere search is unnecessary. While 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. Release 3.3.0, available at www.mat-simresearch.com, 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 log-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 the 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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