

Erratum: “Compressible generalized hybrid Monte Carlo” [J. Chem. Phys. 140, 174108 (2014)]

Youhan Fang, J. M. Sanz-Serna, and Robert D. Skeel

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Erratum: “Compressible generalized hybrid Monte Carlo” [J. Chem. Phys. **140**, 174108 (2014)]

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Section V of Ref. 1 contains mathematical errors and misprints, which do not affect the conclusions of the paper.

1. A false claim is made that satisfying *modified* detailed balance implies the probability propagator is self-adjoint. The flaw in the argument is the restriction to the set of functions $u(z)$ for which $u(R(z)) = u(z)$. Such a set is not closed under the operation of probability propagation.
2. Section V B, item (2) should read “set $x'' = p'$ and $p'' = -x$.”
3. Section V B, Equation (16) is an unmotivated and unnatural assumption.
4. Section V B, final paragraph should read “variance $1 - (1 - 2\gamma\tau)^{1/2}$.”

¹Y. Fang, J. M. Sanz-Serna, and R. D. Skeel, “Compressible generalized hybrid Monte Carlo,” *J. Chem. Phys.* **140**, 174108 (2014).

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