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Erratum: "A finite difference Davidson procedure to sidestep full *ab initio* hessian calculation: Application to characterization of stationary points and transition state searches" [J. Chem. Phys. 140, 164115 (2014)]

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Certain key contributions to the field were not presented in the Introduction section of our recent paper.[1] In addition to the variational method described in Ref. 14 and iterative diagonalization methods in Refs. 15–17, we wish to direct the attention of the reader to other significant efforts that have utilized similar principles for various applications. Reiher and Neugebauer developed a mode-tracking algorithm using the Davidson method for calculating only the modes relevant for vibrational analysis.[2] Similarly, a block-Davidson approach via finite differentiation of the gradient was implemented for calculating hessian-vector products for normal mode analysis.[3] Deglmann and Furche developed a method for stationary point characterization with density functional theory where full solution of all coupled-perturbed Kohn-Sham equations, the bottleneck in hessian calculation, could be avoided through iterative calculation of hessian-vector products to determine only the lowest eigenvalues.[4]

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[1]S. Mallikarjun Sharada, A. T. Bell, and M. Head-Gordon, "A finite difference Davidson procedure to sidestep full *ab initio* hessian calculation: Application to characterization of stationary points and transition state searches," J. Chem. Phys. **140**, 164115–164123 (2014).
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