

Abstract Submitted
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Partial derivatives of eigenvalues without finite differences¹ J.F. BABB, ITAMP, Harvard-Smithsonian — Partial derivatives of eigenvalues and eigenvectors with respect to parameters appear widely in descriptions of collisional and spectroscopic phenomena. Usually finite difference methods are employed for evaluations but they are sometimes inefficient or unstable. There are, however, several algorithms that can yield partial derivatives by iterative solution of matrix equations. The methods do not appear to be widely used in atomic and molecular physics. The algorithms will be described in this paper and results of tests on model problems and on the hydrogen molecular ion will be presented.

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James Babb
Harvard-Smithsonian CfA

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