

# Lower bounds to eigenvalues by the method of arbitrary choice without truncation

Matthew G. Marmorino

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John C. Schug, Chair      of the Department of Chemistry

Christopher A. Beattie      of the Department of Mathematics

Randy Heflin      of the Department of Physics

Herve Marand      of the Department of Chemistry

Jimmy Viers      of the Department of Chemistry

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(ABSTRACT)

After a detailed discussion of the variation theorem for upper bound calculation of eigenvalues, many standard procedures for determining lower bounds to eigenvalues are presented with chemical applications in mind. A new lower bound method, arbitrary choice without truncation is presented and tested on the helium atom. This method is attractive because it does not require knowledge of the eigenvalues or eigenvectors of the base problem. In application, however, it is shown that the method is disappointing for two reasons: 1) the method does not guarantee improved bounds as calculational effort is increased; and 2) the method requires some *a priori* information which, in general, may not be available. A possible direction for future work is pointed out in the end.

An extension of a lower bound method by Calogero and Marchioro has been developed and is presented in appendix G along with comments on the effective field method in appendix H for Virginia Tech access only.

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