Remarks on a Recent Method for Lower Bounds to Energy Levels

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A procedure of Gay for lower bounds to energy eigenvalues is improved and extended to apply to excited states and more complex systems.

INTRODUCTION

RECENTLY Gay[1] introduced a modification of the method of intermediate problems[2–5] with which he obtained good numerical results in applications to ground-state calculations for helium-like atoms.[1,6] In this note we remark on this method and extend its applicability to excited states and more complex systems.

DISCUSSION

For convenience we shall use the notation and setting of the problem given by Gay.[1]

A self-adjoint Hamiltonian H is assumed to be decomposable as

$$H=H^0+V,$$

in which V is positive definite and H^0 is a resolvable self-adjoint Hamiltonian, i.e., H^0 has known eigenvalues E_ν^0 indexed in increasing order and corresponding eigenfunctions Ψ_ν^0. The eigenvalues E_ν^0, which give crude lower bounds to the eigenvalues E_ν of H, are improved by the eigenvalues E_ν^n of the problems,

$$H^n\Psi-E\Psi=0,$$

for intermediate Hamiltonians[4,5] H^n. The latter have the form

$$H^n=H^0+VO^n,$$

with O^n given by

$$O^n=\sum_{i,j=1}^{n}|\mathbf{p}_i\rangle\mathbf{\Lambda}^n{}_{ij}\langle\mathbf{p}_i|V,$$

where the $\mathbf{p}_i$ are linearly independent vectors in the domain of V and the matrix $\mathbf{\Lambda}^n$ is the inverse of the nth-order matrix having the elements $\langle\mathbf{p}_i|V|\mathbf{p}_j\rangle$. The improved lower bounds E_ν^n satisfy

$$E_\nu^0\leq E_\nu^n\leq E_\nu,\quad \nu=1,2,\cdots.$$

The eigenvalues E_ν^n which do not lie in the spectrum of H^0 are given[4,5] by the roots of the determinantal equation

$$|\langle\mathbf{p}_i|V|\mathbf{p}_j\rangle+\langle V\mathbf{p}_i|(H^0-E)^{-1}|V\mathbf{p}_j\rangle|=0. \tag{1}$$

A principal difficulty in finding these roots is that the resolvent operator $(H^0-E)^{-1}$ is rarely known in closed form.

Gay observed that if the vectors $\mathbf{p}_i$ were to have the form

$$\mathbf{p}_i=\mathbf{p}_i(E)=V^{-1}(H-E)f_i, \tag{2}$$

where the f_i are suitable linearly independent elements, then the equation would no longer contain the resolvent operator and the elements might be computed more easily. A problem arises since the theory of intermediate Hamiltonians is based on the use of *fixed* vectors $\mathbf{p}_i$, while those given in terms of the f_i by Eq. (2) depend on E. Thus, the meaning of the roots of (1) with vectors $\mathbf{p}_i$ of the form (2) must be interpreted, as Gay remarked.

To aid in this interpretation, Gay introduces a parameter ϵ in place of E (ultimately ϵ is put equal to E), i.e., vectors $\mathbf{p}_i(\epsilon)$ are defined by

$$\mathbf{p}_i(\epsilon)=V^{-1}(H-\epsilon)f_i, \tag{3}$$

and intermediate Hamiltonians $H^n(\epsilon)$, given by

$$H^n(\epsilon)=H^0+VO^n(\epsilon),$$

are constructed as before employing the $\mathbf{p}_i(\epsilon)$ of (3).

For each fixed real value of ϵ nothing is changed from the usual intermediate Hamiltonian theory; however if ϵ is put equal to E, then a solution Ψ^n, E^n (E^n real) of the *nonlinear* eigenvalue problem

$$H^n(E)\Psi-E\Psi=0 \tag{4}$$

is also a solution of the *linear* intermediate eigenvalue problem

$$H^n(\epsilon)\Psi-E\Psi=0$$

for ϵ having the *fixed* value E^n. Thus E^n may be interpreted as a lower bound for some eigenvalue of H; but for which one?

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[1] J. G. Gay, Phys. Rev. **135**, A1220 (1964).
[2] A. Weinstein, Mem. Sci. Math. (Paris) **88**, (1937).
[3] N. Aronszajn, in *Proceedings of the Oklahoma Symposium on Spectral Theory and Differential Problems, Stillwater, Oklahoma, 1950*, (Department of Mathematics, Oklahoma A & M, Stillwater, Oklahoma, 1955), p. 179.
[4] N. Bazley and D. W. Fox, J. Res. Natl. Bur. Std. **65B**, 105 (1961).
[5] N. Bazley and D. W. Fox, Phys. Rev. **124**, 483 (1961).
[6] P.-O. Löwdin, Phys. Rev. **139**, A357 (1965).

A second problem to be resolved for this method is how to proceed if the operator V does not have an inverse known in closed form.

We will give some answers to these questions in subsequent remarks, but to explain these clearly we must follow the theoretical development a little further.

The nonlinear equation (4) may be cast in the form

$$(H^0-E)[\Psi-\sum_1^n C_i(E)f_i]=0\,, \tag{5}$$

where the quantities $C_i(E)$ satisfy

$$\sum_{i=1}^n \langle (H^0-E)f_j|\, V^{-1}|\,(H^0-E)f_i\rangle C_i+\langle f_j|H^0-E|\Psi\rangle=0\,,\qquad j=1,2,\cdots. \tag{6}$$

If Ψ^n, E^n (E^n real) satisfy Eq. (5) with E^n not in the spectrum of H^0, then Ψ^n is given by

$$\Psi^n=\sum_{i=1}^n C_i(E^n)f_i\,, \tag{7}$$

and the system of equations resulting from (6),

$$\sum_{i=1}^n [\langle (H^0-E^n)f_j|\, V^{-1}|\,(H^0-E^n)f_i\rangle +\langle f_j|H^0-E^n|f_i\rangle]C_i=0\,,\quad j=1,2,\cdots,n\,, \tag{8}$$

must be satisfied by the $C_i(E^n)$. Conversely, if these equations have r linearly independent solutions for a real value E^n not in the spectrum of H^0, then the r resulting vectors of the form (7) are solutions of (5), (6) for the value E^n.

If Ψ^n, E^n satisfy (5) with E^n equal to an eigenvalue $E_\mu{}^0$ of H^0, then Ψ^n has the form

$$\Psi^n=\sum_{i=1}^n C_i(E_\mu{}^0)f_i+C_0\Psi^0\,, \tag{9}$$

where Ψ^0 is an eigenvector of H^0 corresponding to $E_\mu{}^0$, and the quantities $C_i(E_\mu{}^0)$ must satisfy the equations (8) which result from putting Ψ^n given by (9) into Eqs. (6). Clearly, every eigenfunction Ψ^0 of H^0 corresponding to $E_\mu{}^0$ satisfies (5) and (6) with E equal to $E_\mu{}^0$. Further, if the system (8) with E equal to $E_\mu{}^0$ has r linearly independent solutions, these yield r additional solutions of (5), (6) of the form (9) *unless* the span of the f_i contains eigenvectors Ψ^0 corresponding to $E_\mu{}^0$. In the latter case the number of solutions Ψ^n independent of the Ψ^0 is r minus the number of linearly independent eigenvectors Ψ^0 contained in the span of the f_i. We note that if the span of f_i does contain an eigenvector Ψ^0, then the vectors $\mathbf{p}_i$ given by Eq. (2) are not linearly independent.

REMARKS

We observe that if an eigenfunction Ψ_ν of H belongs to the span of the vectors $\mathbf{f}_i$, then Ψ_ν, E_ν satisfy (4). This follows from the fact that $O^n\mathbf{p}=\mathbf{p}$ for any vector $\mathbf{p}$ in the span of the vectors $\mathbf{p}_i$. Thus, $O^n\mathbf{p}=O^nV^{-1}(H^0-E_\nu)\Psi_\nu=V^{-1}(H^0-E_\nu)\Psi_\nu$; or, equivalently, since $(H^0-E_\nu)\Psi_\nu=-V\Psi_\nu$, we have $O^n\Psi_\nu=\Psi_\nu$ so that

$$H^n(E_\nu)\Psi_\nu=H^0\Psi_\nu+VO^n\Psi_\nu=H^0\Psi_\nu+V\Psi_\nu=E_\nu\Psi_\nu\,.$$

In general there is no certainty that E_ν will be the νth-ordered eigenvalue of the operator $H^n(E_\nu)$.

We now consider procedures for locating E^n, arising from a solution of (5) and (6), in the spectrum of the operator $H^n(E^n)$; (E^n is regarded as fixed).

This problem was considered by Gay,[1] who observed (we modify his statement slightly) that when $E^n<E_{\alpha+1}{}^0$, the fact that $H^0\leq H^n(E^n)$ implies that E^n is no larger than the αth eigenvalue of $H^n(E^n)$; thus $E^n<E_{\alpha+1}{}^0$ gives $E^n\leq E_\alpha$. This result is of practical use only in those problems for which the eigenvalues of H^0 lie close to those of H.

A more effective means for locating E^n is to use the operators $H^{l,n}(E^n)=H^{l,0}+VO^n(E^n)$, in which $H^{l,0}$ is the lth-order truncation[4,5] of H^0. The eigenvalues $E^{l,n}$ of the operator $H^{l,n}(E^n)$ are easily determined[4,5] and satisfy

$$E_\alpha{}^0\leq E_\alpha{}^{l,n}\leq E_\alpha\,,\quad \alpha=1,2,\cdots,l+1\,.$$

If E^n satisfies $E^n<E_{\alpha+1}{}^{l,n}$, then E^n can be no larger than the αth eigenvalue of $H^n(E^n)$, and it is a lower bound for E_α. Further, if sufficiently good upper bounds $\hat{E}_\nu$ are available and the inequalities

$$\hat{E}_{\alpha-1}<E_\alpha{}^{l,n}\leq E^n<E_{\alpha+1}{}^{l,n}$$

are satisfied, then E^n is the αth eigenvalue of $H^n(E^n)$ and is nondegenerate.

Now we turn to the problem of what to do if the inverse of V is not available in closed form. In this case a second projection[7] can be employed. This is done by replacing H by the smaller operator $H^0-\gamma+(VQ^m+\gamma)$, where γ is an arbitrary positive constant and Q^m is the projection with respect to the positive bilinear form generated by V on the linear span of a family of vectors $\mathbf{q}_1,\mathbf{q}_2,\cdots,\mathbf{q}_m$ in the domain of V. Then using $VQ^m+\gamma$, which always has an easily found inverse, in place of V and $H^0-\gamma$ in place of H^0, the technique developed by Gay can be applied.

[7] N. Bazley and D. W. Fox, J. Math. Phys. 3, 469 (1962).