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Alternatives to Bazley's special choice for eigenvalue lower bounds

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Bazley's special choice operator is a lesser operator to a positive perturbation of a self-adjoint semi-bounded operator that possesses an exactly soluble base eigenvalue problem. It allows the construction of an exactly soluble intermediate problem that gives eigenvalues not less than the base problem and not greater than the perturbed problem so that lower bounds to the eigenvalues of the perturbed operator are produced. This paper considers alternate derivations of Bazley's special choice which lead to two alternate methods to determine eigenvalue lower bounds. One is simpler, but gives poorer bounds; the other is more difficult, but sometimes yields superior bounds. Lower bounds to the particle in a box model with a linear perturbation and lower bounds to the helium atom are calculated using the two methods introduced and are compared to those given with Bazley's special choice.

KEY WORDS: Bazley's special choice, lower bounds, intermediate problems

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1. Introduction

Although the variational theorem allows for a straightforward and practical method to determine upper bounds to the eigenvalues of the quantum mechanical Hamiltonian operator, a practical method for corresponding lower bounds has proved elusive. A variety of methods are available for one-dimensional systems, but application to the many-body (each with three dimensions) electronic chemical systems has been restricted to a handful of methods, none of which have proved successful in general. The simplest methods, related to the Temple formula, have been successfully applied to the helium [1] and lithium atoms [2, 3], but the difficulty of calculating expectation values of the square Hamiltonian and some theoretical issues for many-electron atoms has prevented application to larger systems. The effective field method is easily applied to very large systems, but the resulting lower bounds are poor [4–6]. The method of intermediate problems proved useful for the helium atom [7], but was inadequate for

the lithium atom [8, 9] until supplemented with the effective field method [10]. The local energy method has been applied to the helium atom, and although it avoids difficult integrals, it has its own problems [11]. Attempts to determine energy lower bounds for molecules have been less successful [12].

Consider a [base] self-adjoint operator A^o whose [base] eigenvalue equation $A^o\psi_n^o = \lambda_n^o\psi_n^o$ is exactly soluble. In many situations one wishes to solve a related eigenvalue equation $A\psi_n = \lambda_n\psi_n$ where $A = A^o + V$ so that V is a perturbation. If V is positive then a variety of related methods to determine lower bounds to λ_n are available which utilize the base problem. One method is Bazley's special choice [7] in which the perturbation V is replaced by the lesser operator L_B:

$$L_B \equiv P_B[V^{-1}]^{-1}P_B \leq V, \tag{1}$$

where P_B is a projection operator onto the N-dimensional subspace, S_B, spanned by the eigenfunctions $\psi_1^o, \ldots, \psi_N^o$ of A^o and $[V^{-1}]$ is the matrix representation of V^{-1} on S_B. The form of L_B given in (1) is practical; however, Bazley defines L_B as VQ where Q is the (non-orthogonal) projection operator onto the subspace $V^{-1}S_B$ which is a form more suitable for discussing the favorable properties of L_B. Except for Q, all projection operators in this work are orthogonal. Both S_B and $S_B^\perp$ (the complement subspace of S_B) are reducing subspaces for L_B: L_B takes the form of $[V^{-1}]^{-1}$ on S_B, while on $S_B^\perp$ the operator L_B is zero. S_B and $S_B^\perp$ are also reducing subspaces for A^o so that the eigenvalues of the operator $A^o + L_B$ are $\lambda_{N+1}^o, \lambda_{N+2}^o, \ldots$ and the N eigenvalues of $[A^o + L_B]$. (Note that the former set of eigenvalues are unchanged from the base problem so that they are called *persistent* eigenvalues.) Thus only an $N \times N$ matrix eigenvalue problem needs to be solved to determine lower bounds to each λ_n, and this is the advantage of using L_B over V.

Bazley's proof of (1) by defining a new inner product is well-known [7]. His proof illustrates that the operator L_B is not only less than V, but has two important properties: (1) it is non-negative; (2) as N increases, L_B does not decrease. The former property means that the resulting lower bounds are not worse than λ_n^o (which themselves serve as lower bounds due to the positive nature of V). The latter property guarantees that the lower bounds are not worsened as more effort is expended (from working with larger matrices). Nevertheless, the fundamental property of (1), that $L_B \leq V$ is easy to prove in a variety of ways – some of which yield new lesser operators to V. In this paper, some alternate derivations of (1) are explored which lead us to new lesser operators.

At this point we emphasize that although the application of (1) by Bazley was very restricted, i.e., coupled to an exactly soluble base problem through the projection operator P_B, the result is valid for a general projection operator P onto a general subspace S.

2. Existing alternate derivations

After the introduction of (1), Bazley and Fox [13] discovered that the same lower bounds to λ_n resulted from the use A^o with the lesser operator L_{BF} to V where $L_{BF} \equiv V^{1/2} P_{BF} V^{1/2}$ and P_{BF} is the projection operator onto the subspace generated by $V^{-1/2} S_B$. The equivalence of the lower bounds lead to the realization that the operators L_{BF} and L_B were the same. Consider the general inequality below for a projection operator P and positive operator X.

$$X^{1/2}(1 - P)X^{1/2} \geq 0. \tag{2}$$

L_{BF} results from (2) when $P = P_{BF}$ and $X = V$.

Bazley's special choice can also be derived from the general comparison operator $Y \equiv W - (I - R)X(I - R)$ where $W \leq A$, $X \geq 0$, and R is a finite rank operator (such as, but not limited to, a projection operator) [14]. Note that $Y \leq W \leq A$ so that Y is a lesser operator to A as desired and the eigenvalues of Y serve as lower bounds to the eigenvalues of A. This comparison operator Y simplifies to $Y = W - X + XR$ [14]. Letting $W = A$ and $X = V$ one arrives at

$$A \geq Y = A^o + VR, \tag{3}$$

which gives (1) when $R = Q$ so that $VQ = P_B[V^{-1}]^{-1} P_B$.

Miller [15] derived (1) from a general theorem originating from the work of Ref. [16] which he used to also derive a number of other results pertaining to lower bound calculations. The theorem states that given a self-adjoint operator X with matrix representation $[X]$, both of which have N eigenvalues below a number α which is not in the spectrum of X, then

$$(X - \alpha)^{-1} \geq P_X[X - \alpha]^{-1} P_X, \tag{4}$$

where P_X is a projection operator onto the subspace used to generate the matrix $[X]$. Bazley's special choice bound (1) is regained with positive $X = V^{-1}$ so that $\alpha = 0$ for any subspace used to form the matrix $[X]$. Miller remarks that with $X > 0$ and $\alpha = 0$, (4) is equivalent to the Schwarz inequality. We consider the Schwarz inequality below for a general function f and projection operator P:

$$|\langle f|Pf\rangle|^2 = \left|\left\langle fV^{1/2}|V^{-1/2}Pf\right\rangle\right|^2 \leq \langle f|V|f\rangle \left\langle f|PV^{-1}P|f\right\rangle \tag{5}$$

for $V > 0$ which rearranges to give a lower bound to $\langle f|V|f\rangle$ from which an operator less than V can be determined and (1) is regained.

If (1) is altered with a positive coefficient c so that cB replaces B then the poorer result $V \geq cB$ for $0 < c < 1$ is obvious. Nevertheless, Wilson [17] has shown in a different setting, that use of cB with $c > 1$ can be used to give rigorous lower bounds to the eigenvalues λ_n (not a lower bound to the operator V) that substantially improves those obtained with $c = 1$ in the special choice method.

3. Another derivation

A simple proof of (1) is the following. Consider a general finite-dimensional subspace S and its complement $S^{\perp}$ with projection operators P onto the former and $P^{\perp}$ onto the latter. We non-rigorously define $\chi^{-1} = PX^{-1}P + P^{\perp}\infty P^{\perp}$ where operator $X > 0$. If a function ϕ has any component in $S^{\perp}$ then $\langle\phi|\chi^{-1}|\phi\rangle = \infty > \langle\phi|X^{-1}|\phi\rangle$ while if $\phi \in S$, then $\langle\phi|\chi^{-1}|\phi\rangle = \langle\phi|X^{-1}|\phi\rangle$. It follows that $0 < X^{-1} \leq \chi^{-1} \leq \infty$ and by inversion that $\infty > X \geq \chi \geq 0$ where $\chi = P[X^{-1}]^{-1}P$. Bazley's inequality (1) is thus proved for positive operators $X = V$.

If we instead let $X = V + c$, with real number $c > 0$ and $V > 0$, then one can define the lesser operator L_c such that

$$L_c \equiv P\left([(V+c)^{-1}]^{-1} - c\right)P - P^{\perp}cP^{\perp} \leq V \tag{6}$$

and (1) is a special case of (6) for which $c = 0$. When the subspaces and projection operators are defined as in the introduction, the component $P^{\perp}cP^{\perp}$ of L_c *lowers* the already existing lower bounds $\lambda^o_{N+1}, \lambda^o_{N+2}, \ldots$ to the eigenvalues $\lambda_{N+1}, \lambda_{N+2}, \ldots$ of A each by c. The other component of L_c, however, *raises* the lower bounds given by the $N \times N$ matrix eigenvalue problem. The cost for this improvement is the more difficult construction of the matrix operator $[(V+c)^{-1}]$ due to more difficult integrations. Bazley and Fox described this method (proved again by defining a new inner product) [18]. Miller derived a more general lower bound approach which gives this method as a special (inferior) case [19].

Consider next that $X = V + f + c$, with real number $c > 0$ such that $X > 0$ although operator f may not be positive. Then one can derive the lesser operator L_f

$$L_f \equiv P\left([(V+f+c)^{-1}]^{-1}\right)P - (f+c) \leq V. \tag{7}$$

If the positive projection onto S of (7) is completely ignored the worse lesser operator $-(f+c)$ is formed. This simpler bound is more quickly determined from the positive nature of $X = V + f + c > 0$ and is the essence of the effective field method [4]. Practical use of (7) has not yet been achieved.

4. Bazley's special choice without inversion

A proof without infinities results from the positive nature of $X^{-1} > 0$ so that

$$(X - C)^* X^{-1}(X - C) \geq 0, \tag{8}$$

where C is a general linear operator. This expression is similar to that used in defining general comparison operators of [14] mentioned in section 2. Letting $X = V$, the inequality expands to give

$$L' \equiv C + C^* - C^* V^{-1} C \leq V. \tag{9}$$

Table 1
Lower bounds to the first six eigenvalues of the one-dimensional linearly perturbed particle in a box model calculated with L'' and L_B (in parentheses) in place of the perturbation $V = x$. Upper bounds were obtained from a variational calculation using the first 20 eigenfunctions of the unperturbed system. Bounds in italics are the best for a given eigenvalue using L''. Units are hartree.

N	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1	1.72706					
	(1.78878)					
2	1.79887	3.37258				
	(1.82377)	(3.47043)				
3	1.85687	3.57408	5.73535			
	(1.86186)	(3.59124)	(5.88345)			
4	1.86776	3.60907	6.06968	9.13608		
	(1.86888)	(3.61358)	(6.08405)	(9.32488)		
5	1.86971	3.61847	6.09519	9.55980	13.5675	
	(1.87021)	(3.61929)	(6.10038)	(9.57278)	(13.7893)	
6	*1.87054*	*3.61950*	*6.10550*	*9.57998*	*14.0545*	*19.0162*
	(1.87074)	(3.62007)	(6.10635)	(9.58581)	(14.0668)	(19.2658)
Upper bound	1.87113	3.62101	6.10822	9.59403	14.0862	19.5817

Letting $C = L_B = P[V^{-1}]^{-1}P$ gives Bazley's special choice (1). This derivation immediately generalizes Bazley's special choice by allowing a variety of other operators lesser than V by the choice of C; however, we believe the choice $C = L_B$ to be optimal, for only in this case is L' guaranteed to be non-negative. Careful choices of C keep one from calculating the inverse matrix $[V^{-1}]^{-1}$, which is difficult for large matrices, but one then discards the optimal nature of the bound. A good compromise is $C = P[V]P$ since as S increases one might expect $P[V]P$ and $P[V^{-1}]^{-1}P$ to become more similar, e.g., when S is the entire Hilbert space, then $P = I$ so that $P[V]P = V$ and $P[V^{-1}]^{-1}P = V$. This choice of C gives

$$L'' \equiv 2\,P[V]P - P[V][V^{-1}][V]\,P \leq V, \tag{10}$$

which can, but is not guaranteed to, give lower bounds very close to those obtained with L_B. The quality of the lower bounds given by L'' is judged by how close they are to those obtained with L_B, as our choice of C is now non-optimal.

As a first example we consider the operator $A = A^o + V$ with $A^o = -1/2\ d^2/dx^2$ on a domain of $x \in [0, \pi]$ and $V = x$ using the N-dimensional subspace S_B spanned by the eigenfunctions $\psi_n^o = (2/\pi)^{1/2} \sin(nx)$ of A^o for $n = 1$ to N. The lower bounds using L'' and L_B (in parentheses) are reported in table 1; the latter bounds are superior as expected, but not by much. The best lower bound given for a particular eigenvalue using L'' is reported in italics. For this example, lower bounds from L'' increase with N, which is very desirable.

For a second example we consider the S states of the non-relativistic helium atom Hamiltonian operator $A = A^o + V$ where V is the electron–electron

Table 2
Lower bounds to the first six eigenvalues of the helium atom calculated with L'' and L_B (in parentheses) in place of the perturbation $V = 1/r_{12}$. Bounds in italics are the best for a given eigenvalue using L''. Bounds underlined are persistent eigenvalues of the base problem. Units are hartree.

N	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1	−3.20898					
	(−3.08571)					
2	*−3.20479*	−2.23114				
	(−3.06787)	(−2.15533)				
3	−3.21223	*−2.22227*	−2.10101			
	(−3.06373)	(−2.16554)	(−2.12500)			
4	−3.21925	−2.22462	*−2.09278*	−2.08000		
	(−3.06210)	(−2.16539)	(−2.08000)	(−2.06649)		
5	−3.22498	−2.22782	−2.09293	*−2.05556*	*−2.04914*	
	(−3.06128)	(−2.16526)	(−2.06652)	(−2.05556)	(−2.04082)	
6	−3.22959	−2.23084	−2.09366	−2.09366	−2.04937	−2.04082
	(−3.06082)	(−2.16517)	(−2.06652)	(−2.04937)	(−2.04082)	(−2.03569)
Upper bound [7]	−2.9037	−2.1460	−2.0613	−2.0336	−2.0212	−2.0146

repulsion potential $(1/r_{12})$ and A^o is the difference (for which exact eigenvalues and eigenfunctions are available). The N-dimensional subspace S_B is spanned by the symmetrical combinations $(1/2)^{1/2}[\phi_1(\mathbf{r}_1)\phi_n(\mathbf{r}_2) + \phi_n(\mathbf{r}_1)\phi_1(\mathbf{r}_2)]$ of hydrogenic functions ϕ_n for $n = 1$ to N. Lower bounds using L'' and L_B (in parentheses) are reported in table 2; the latter bounds are superior. Persistent eigenvalues from the base problem are underlined and the best lower bound using L'' is reported in italics. For this example the lower bounds given by L'' do not increase with N – instead they tend to decrease.

Further improvement of this method could be achieved by letting $C = cP[V]P$ where c is an adjustable parameter; but one must then run a series of lower bound calculations to optimize the bounds with respect to c. This would, however, allow the bounds to approach those obtained with (1).

5. Exponential special choice

Attempts to create a lesser operator to V using the exponential function and (8) with $X = e^V$ and $X = e^V - 1$ were not successful. Nontrivial lower bounds did sometimes result, but for the systems studied bounds were poor and/or did not improve with increasing effort. A more successful route using the exponential function is discussed below, although there is very little resemblance to Bazley's special choice method.

Given a finite-dimensional space S, let R be the subspace defined by $e^{-V}S \cap S^{\perp}$ and let T be the complement space of $R \oplus S$. Then the representation of the

operator e^{-V} takes the following form:

$$e^{-V} = \begin{bmatrix} P_S\mathrm{e}^{-V}P_S & P_S\mathrm{e}^{-V}P_R & P_S\mathrm{e}^{-V}P_T \\ P_R\mathrm{e}^{-V}P_S & P_R\mathrm{e}^{-V}P_R & P_R\mathrm{e}^{-V}P_T \\ P_T\mathrm{e}^{-V}P_S & P_T\mathrm{e}^{-V}P_R & P_T\mathrm{e}^{-V}P_T \end{bmatrix} = \begin{bmatrix} \alpha & \beta & \gamma \\ \beta^* & \delta & \varepsilon \\ \gamma^* & \varepsilon^* & \chi \end{bmatrix}, \tag{11}$$

where $\gamma = 0$ by construction since for any $s \in S$ and $t \in T$ we have $\langle s|e^{-V}|t\rangle = \langle \mathrm{e}^{-V}s|t\rangle = 0$ since $\mathrm{e}^{-V}s \in R \oplus S$ which is orthogonal to T. Construction of a lesser operator to V proceeds as follows where $\mathrm{e}^{-V} \leq I$ as we restrict $V \geq 0$.

$$\mathrm{e}^{-V} = \begin{bmatrix} \alpha & \beta & 0 \\ \beta^* & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & \delta & \varepsilon \\ 0 & \varepsilon^* & \chi \end{bmatrix} \leq \begin{bmatrix} \alpha & \beta & 0 \\ \beta^* & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \alpha & \beta & 0 \\ \beta^* & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{12}$$

The logarithm is operator monotone [20] so that the inequality in (12) is retained when one takes the logarithm of both sides. Then negate (12) to obtain (13)

$$L_E = \begin{bmatrix} -\ln\begin{bmatrix} \alpha & \beta \\ \beta^* & 1 \end{bmatrix} & 0 \\ 0 \quad 0 & 0 \end{bmatrix} \leq V. \tag{13}$$

Matrix α is straightforward to construct. Given an orthonormal basis set $s_1, s_2, \ldots, s_N$ for an N-dimensional space S the matrix elements of α are merely $\alpha_{ij} = \langle s_i|e^{-V}|s_j\rangle$ for $i, j = 1, 2, \ldots, N$. Matrix β requires more work. The domain of β is the subspace $R \equiv \mathrm{e}^{-V}S \cap S^{\perp}$. Combining the orthonormal set $s_1, s_2, \ldots, s_N$ with the non-orthogonal and unnormalized set $\mathrm{e}^{-V}s_1, \mathrm{e}^{-V}s_2, \ldots, \mathrm{e}^{-V}s_N$, the Gram–Schmidt orgthonormalization process returns the unchanged set $s_1, s_2, \ldots, s_N$ which spans S but also a set of M additional orthonormal functions $g_1, \ldots, g_M$ which span R where $M \leq N$. The β matrix elements are then $\beta_{ij} = \langle s_i|e^{-V}|g_j\rangle$ for $i = 1, 2, \ldots, N$ and $j = 1, 2, \ldots, M$.

Sample calculations with $S = S_B$ for the linearly perturbed particle in a box (table 3) and the helium atom (table 4) show that given the same information from the base problem, bounds superior to Bazley's special choice can be obtained, but are not guaranteed. Unfortunately, even with the same information this method requires a matrix twice the size used with Bazley's special choice. Furthermore, the examples studied suggest that competitive bounds for λ_n are obtained only when $n+1$ base problem eigenfunctions are used, instead of just n base problem eigenfunctions for Bazley's special choice.

If e^{-V} in (11) is replaced with the more general e^{-cV} where c is a constant then (13) is modified to

$$L_E = \frac{1}{c}\begin{bmatrix} -\ln\begin{bmatrix} \alpha' & \beta' \\ \beta'^* & 1 \end{bmatrix} & 0 \\ 0 \quad 0 & 0 \end{bmatrix} \leq V \tag{14}$$

Table 3
Lower bounds to the first six eigenvalues of the one-dimensional linearly perturbed particle in a box model calculated with L_E and L_B (in parentheses) in place of the perturbation $V = x$. Upper bounds were obtained from a variational calculation using the first 20 eigenfunctions of the unperturbed system. Bounds in italics for a given eigenvalue using L_E are those which are superior to calculation with L_B. Units are hartree.

N	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1	0.47466					
	(1.78878)					
2	1.79213	1.99967				
	(1.82377)	(3.47043)				
3	*1.87007*	*3.61003*	4.49181			
	(1.86186)	(3.59124)	(5.88345)			
4	*1.87101*	*3.62014*	*6.10265*	7.98206		
	(1.86888)	(3.61358)	(6.08405)	(9.32488)		
5	*1.87108*	*3.62087*	*6.10716*	*9.58936*	12.4783	
	(1.87021)	(3.61929)	(6.10038)	(9.57278)	(13.7893)	
6	*1.87111*	*3.62093*	*6.10800*	*9.59283*	*14.0817*	17.9763
	(1.87074)	(3.62007)	(6.10635)	(9.58581)	(14.0668)	(19.2658)
Upper bound	1.87113	3.62101	6.10822	9.59403	14.0862	19.5817

Table 4
Lower bounds to the first six eigenvalues of the helium atom calculated with L_E and L_B (in parentheses) in place of the perturbation $V = 1/r_{12}$. Bounds in italics for a given eigenvalue using L_E are those which are superior to calculation with L_B. Bounds underlined are persistent eigenvalues of the base problem. Units are hartree.

N	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1	*−3.05661*					
	(−3.08571)					
2	*−3.01655*	−2.32965				
	(−3.06787)	(−2.22222)				
3	*−3.00908*	−2.25811	−2.15435			
	(−3.06373)	(−2.16554)	(−2.12500)			
4	*−3.00623*	−2.22992	−2.13113	−2.08781		
	(−3.06210)	(−2.16539)	(−2.08000)	(−2.06649)		
5	*−3.00481*	−2.21685	−2.12081	−2.07317	−2.05740	
	(−3.06128)	(−2.16526)	(−2.06652)	(−2.05556)	(−2.04082)	
6	*−3.00400*	−2.20988	−2.11498	−2.06658	−2.04710	−2.04123
	(−3.06082)	(−2.16517)	(−2.06652)	(−2.04937)	(−2.04082)	(−2.03569)
Upper bound [7]	−2.9037	−2.1460	−2.0613	−2.0336	−2.0212	−2.0146

(where α' and β' are matrix elements of e^{-cV}) in a manner similar to (6) although there are notable differences. In (6) $c > 0$ was *added* to V. Addition produces no change in the current method and so we multiply by the factor c; coincidentally, multiplication by c produces no change in method of section 3. In the present case c deviates from one in either direction and is not guaranteed to give better bounds; whereas in (6) the parameter c was increased from zero and did not give inferior bounds. Furthermore, there is no effect of c on the persistent eigenvalues of the base problem in the present method, while for (6) those eigenvalues were lowered. Calculations with (14) on both the perturbed particle in a box and the helium atom showed some improvement for optimal values of c, but not enough to detail here. It is worth noting, however, that the optimal c varied for both different-sized calculations *and* for different eigenvalues.

6. Conclusion

We have presented two new methods to obtain lower bounds to eigenvalues of a self-adjoint operator related by a positive perturbation of a base self-adjoint operator with an exactly-soluble eigenvalue equation. The first is a simple modification of Bazley's special choice which constructs a lesser operator to the positive perturbation V of the form $2P[V]P - P[V][V^{-1}][V]P$ where P is a projection operator onto the subspace used to construct the matrix representations $[V]$ of V and $[V^{-1}]$ of V^{-1}. This uses no information that is not used in Bazley's special choice or a variational (upper bound) calculation and avoids inverting $[V^{-1}]$ which is necessary for Bazley's special choice and thus we recommend this new approach to be tried before using Bazley's special choice. Unfortunately, the bounds of the former are inferior to those of the latter, and thus if performance is not sufficient then Bazley's special choice should be tried. For lower bounds superior to those obtained with Bazley's special choice, our second method (exponential special choice) may be helpful. It performed very well for the perturbed particle in a box giving superior lower bounds to the $N-1$ lowest eigenvalues for an N-dimensional matrix eigenvalue problem. For the helium atom, only the lowest eigenvalue was bounded better. Although we have numerical evidence for the "goodness" of the two methods we have presented, Bazley's special choice is still more desirable *in general* because it guarantees that with increasing effort there is no reduction in the quality of the lower bounds.

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