Journal of Mathematical Chemistry Vol. 38, No. 4, November 2005 (© 2005)
DOI: 10.1007/s10910-004-6893-8

Improvement of Weyl's inequality

M.G. Marmorino
Department of Chemistry, Indiana University South Bend, South Bend, IN, 46634, USA
E-mail: mmarmori@iusb.edu

Received 26 October 2004; revised 4 November 2004

Consider the construction of an operator from the sum of two component operators. Weyl's inequality gives a lower bound to an eigenvalue of the constructed operator using a single eigenvalue from each of the component operators. Using such minimal information gives a poor bound, however, and when the eigenvectors that correspond to the said eigenvalues of the component operators are known, Weyl's inequality can be significantly improved by considering the overlap of the two eigenvectors. This improvement can sometimes be further improved when several eigenvectors of each component operator are known so that the overlap of sub-eigenspaces are considered instead. The improvement is best when there is minimal overlap and Weyl's inequality returns when the overlap is complete. An example with the hydrogen molecular ion is presented which illustrates the superiority over Weyl's inequality when eigenvector or sub-eigenspace information is utilized.

KEY WORDS: Weyl, lower bound, inequality, energy

AMS (MSC) subject classification: 34L15, 35P15, 68Q17, 15A42

1. Introduction

Solution of the Schrödinger equation is a major goal of chemists, but as most problems of interest do not yield an equation that can be solved analytically, chemists are forced to numerically approximate the eigenvalues and eigenfunctions. The former, being real numbers instead of functions, are easier to approximate but require upper and lower bounds to accurately localize the true eigenvalue. Calculation of upper bounds has enjoyed phenomenol success whereas lower bounds are typically not sought due to theoretical and calculational difficulties in the many approaches. To date, the most complicated chemical system for which accurate lower bounds have been calculated is the lithium atom [1,2].

The simplest approach to the calculation of lower bounds is by Weyl's inequality [3] which gives a lower bound to an eigenvalue of a sum of component operators using eigenvalue information of the component operators. Weyl's inequality has theoretical significance (such as the fact that molecular energies

are bounded below by sums of atomic energies [4]) but has little impact in the realm of precise calculations. In this paper we improve Weyl's inequality by considering, in part, the eigenspaces of the component operators as well. In the first and simplest case (Section 3) we consider a single eigenvector from each component operator. In the second and more general case (Section 4) we consider sub-eigenspaces of dimension two or larger.

2. Weyl's inequality

Define $\lambda_n^{(C)}$ to be the nth eigenvalue of the operator C ordered from lowest (most negative) to highest (most positive). Let S_n be an n-dimensional subspace of a Hilbert space H and L_n be a subspace of dimension less than or equal to n.

The max-min formulation [5] of eigenvalues is usually written as

$$\lambda_{a+b-1}^{(C)} = \max_{S_{a+b-2}\subseteq H} \min_{f\in S_{a+b-2}^{\perp}} \langle Cf, f\rangle , \tag{1}$$

where f is restricted to the appropriate symmetry dictated by operator C and also to a norm of 1. Any subspace L_n of S_n will yield a complementary subspace $L_n^{\perp}$ larger than and including $S_n^{\perp}$. Minimizing $\langle Cf, f\rangle$ over this larger subspace may give smaller minimums, but since we then choose the maximum of these minimums, there is no change when including these subspaces of S_n in the max-min formulation of eigenvalues. Thus we can write:

$$\lambda_{a+b-1}^{(C)} = \max_{L_{a+b-2}\subseteq H} \min_{f\in L_{a+b-2}^{\perp}} \langle Cf, f\rangle . \tag{2}$$

We now assume that operator C is the sum of operators A and B. We define a particular subspace to be the span of the lowest $a-1$ eigenfunctions α_1, $\alpha_2, \ldots, \alpha_{a-1}$ of A and lowest $b-1$ eigenfunctions $\beta_1, \beta_2, \ldots, \beta_{b-1}$ of B. This subspace has a maximum dimension of $a+b-2$ if $\langle \alpha_i, \beta_j\rangle = 0$ for $i < a$ and $j < b$. It has a minimum dimension of the greater of $a-1$ or $b-1$ if the span of one set of eigenfunctions is included in the span of the other. Thus it qualifies as one of L_{a+b-2} but perhaps not of S_{a+b-2}, and we call it L_{AB}. Instead of maximizing the minimums over subspaces in (2) we consider only the subspace L_{AB}:

$$\lambda_{a+b-1}^{(C)} \geqslant \min_{f\in L_{AB}^{\perp}} \langle (A+B)f, f\rangle . \tag{3}$$

Weyl's inequality results in the next few steps

$$\lambda_{a+b-1}^{(C)} \geqslant \min_{f\in L_{AB}^{\perp}} \{\langle Af, f\rangle + \langle Bf, f\rangle\} \geqslant \min_{f\in L_{AB}^{\perp}} \langle Af, f\rangle + \min_{f\in L_{AB}^{\perp}} \langle Bf, f\rangle \geqslant \lambda_a^{(A)} + \lambda_b^{(B)}. \tag{4}$$

The last inequality results from the fact that f is perpendicular to the lowest $a-1$ eigenfunctions of A and the lowest $b-1$ eigenfunctions of B.

3. Improvement

Although the eigenfunctions of operators A and B appear symbolically in the derivation of Weyl's inequality, explicit knowledge of them is not required. However, if the eigenvectors are known then they can be used to improve the lower bound. This results from taking advantage of the fact that the ath and bth eigenfunctions of A and B, respectively, may overlap. We assume a discrete set of eigenfunctions for all operators but the analysis holds when parts of the spectra of A, B and/or C are continuous. We start with (3) subtracting $\lambda_{a+1}^{(A)}$ and $\lambda_{b+1}^{(B)}$ from both sides:

$$\begin{aligned}\lambda_{a+b-1}^{(C)} - \lambda_{a+1}^{(A)} - \lambda_{b+1}^{(B)} &\geqslant \min_{f\in L_{AB}^{\perp}} \left[\left\langle (A-\lambda_{a+1}^{(A)})f, f\right\rangle + \left\langle (B-\lambda_{a+1}^{(B)})f, f\right\rangle\right] \\ &= \min_{f\in L_{AB}^{\perp}} \left[\sum_{i=1}^{\infty} |\langle f \mid \alpha_i\rangle|^2 (\lambda_i^{(A)} - \lambda_{a+1}^{(A)}) \right. \\ &\qquad \left. + \sum_{j=1}^{\infty} \left|\langle f \mid \beta_j\rangle\right|^2 (\lambda_j^{(B)} - \lambda_{b+1}^{(B)})\right] \qquad (5)\end{aligned}$$

Given the particular subspace L_{AB}, all $f \in S_{AB}^{\perp}$ are orthogonal to α_i for $i < a$ and β_j for $j < b$ since L_{AB} is the span of these eigenfunctions. Thus the sums in (5) need not start with the index one:

$$\begin{aligned}\lambda_{a+b-1}^{(C)} - \lambda_{a+1}^{(A)} - \lambda_{b+1}^{(B)} \geqslant \min_{f\in L_{AB}^{\perp}} &\left[\sum_{i=a}^{\infty} |\langle f \mid \alpha_i\rangle|^2 (\lambda_i^{(A)} - \lambda_{a+1}^{(A)}) \right. \\ &\left. + \sum_{j=b}^{\infty} \left|\langle f \mid \beta_j\rangle\right|^2 (\lambda_j^{(B)} - \lambda_{b+1}^{(B)})\right]. \qquad (6)\end{aligned}$$

Furthermore, since only the $i = a$ and $j = b$ terms in the summations are negative we are able to write

$$\lambda_{a+b-1}^{(C)} - \lambda_{a+1}^{(A)} - \lambda_{b+1}^{(B)} \geqslant \min_{f\in L_{AB}^{\perp}} \left[|\langle f \mid \alpha_a\rangle|^2 (\lambda_a^{(A)} - \lambda_{a+1}^{(A)}) + |\langle f \mid \beta_b\rangle|^2 (\lambda_b^{(B)} - \lambda_{b+1}^{(B)})\right]. \qquad (7)$$

The resulting bound to $\lambda_{a+b-1}^{(C)}$ is more conveniently written as

$$\lambda_{a+b-1}^{(C)} \geqslant \lambda_{a+1}^{(A)} + \lambda_{b+1}^{(B)} + \min_{f\in L_{AB}^{\perp}} \{(r_a^2 + s_b^2)\Delta A + s_b^2(\Delta B - \Delta A)\}, \qquad (8)$$

where $\Delta A = \lambda_a^{(A)} - \lambda_{a+1}^{(A)}$, $\Delta B = \lambda_b^{(B)} - \lambda_{b+1}^{(B)}$, $r_a = |\langle f|\alpha_a\rangle|$, $s_b = |\langle f|\beta_b\rangle|$ and without loss of generality $\Delta B \leqslant \Delta A < 0$.

Ignoring restrictions on r_a and s_b, Weyl's inequality results when their squares are taken as one. When the restrictions are taken into consideration, however, Weyl's inequality improves. Noting that ΔA and $(\Delta B - \Delta A)$ are both negative, it is apparent that any such improvement is limited to $\lambda_{a+1}^{(A)} + \lambda_{b+1}^{(B)}$ at best. The restrictions are obtained using the Gram determinant of the functions f, α_a and β_b which gives:

$$r_a^2 + s_b^2 \leqslant 1 - s^2 + 2sr_a s_b, \tag{9}$$

where $s = |\langle \alpha_a, \beta_b \rangle|$. Using the relationship $(r_a - s_b)^2 \geqslant 0$ in (9) gives

$$r_a^2 + s_b^2 \leqslant 1 - s^2 + s(r_a^2 + s_b^2), \tag{10}$$

to yield the following bound

$$r_a^2 + s_b^2 \leqslant \frac{1 - s^2}{1 - s} = 1 + s. \tag{11}$$

Inserting (11) in (8) gives

$$\lambda_{a+b-1}^{(C)} \geqslant \lambda_{a+1}^{(A)} + \lambda_{b+1}^{(B)} + \min_{f \in L_{AB}^{\perp}} [(1+s)\Delta A + s_b^2(\Delta B - \Delta A)]. \tag{12}$$

If we now ignore the restriction on s_b by letting it equal one we obtain

$$\lambda_{a+b-1}^{(C)} \geqslant \lambda_b^{(B)} + \lambda_{a+1}^{(A)} + s(\lambda_a^{(A)} - \lambda_{a+1}^{(A)}), \tag{13}$$

since s is independent of f. Weyl's inequality is obtained only in the case when $s = 1$, i.e., $|\langle \alpha_a, \beta_b \rangle| = 1$, otherwise (13) is superior. The best result is obtained when $s = 0$.

4. Generalization

The result above can be generalized by considering a sub-eigenspace of dimension two or more of each component operator instead of just a single eigenvector. To this end, one subtracts $\lambda_{m+a+1}^{(A)}$ and $\lambda_{m+b+1}^{(B)}$, where integer $m > 0$, from both sides of (3) and continues the derivation as before. The significance of m is that it is the number of *additional* eigenvectors each of A and B considered. In place of (7) one obtains the following:

$$\lambda_{a+b-1}^{(C)} \geqslant \lambda_{m+a+1}^{(A)} + \lambda_{m+b+1}^{(B)} + \min_{f \in L_{AB}^{\perp}} \left[\sum_{i=a}^{m+a} |\langle f \mid \alpha_i \rangle|^2 \left(\lambda_i^{(A)} - \lambda_{m+a+1}^{(A)}\right) + \sum_{j=b}^{m+b} \left|\langle f \mid \beta_j \rangle\right|^2 \left(\lambda_j^{(B)} - \lambda_{m+b+1}^{(B)}\right) \right] \tag{14}$$

As the term to be minimized is negative, the best possible bound that could be obtained is $\lambda^{(A)}_{m+a+1}+\lambda^{(B)}_{m+b+1}$, which by virtue of "$m$" is more promising than the limit $\lambda^{(A)}_{a+1}+\lambda^{(B)}_{b+1}$ presented in Section 3. We simplify, which simultaneously worsens, (14) by taking the largest magnitude eigenvalue differences outside the summations:

$$\lambda^{(C)}_{a+b-1} \geqslant \lambda^{(A)}_{m+a+1}+\lambda^{(B)}_{m+b+1}+\min_{f\in L^{\perp}_{AB}}\left[(\lambda^{(A)}_{a}-\lambda^{(A)}_{m+a+1})\sum_{i=a}^{m+a}|\langle f \mid \alpha_i\rangle|^2 +(\lambda^{(B)}_{b}-\lambda^{(B)}_{m+b+1})\sum_{j=b}^{m+b}\left|\langle f \mid \beta_j\rangle\right|^2\right]. \quad (15)$$

It is this simplification that will make our more general bound not necessarily an improvement over the less general bound using a single eigenvector from each component operator. We define f_A to be the *normalized* projection of a normalized function f on the subspace spanned by the eigenfunctions α_a, $\alpha_{a+1},\ldots,\alpha_{m+a}$. We define f_B analogously, and then note that the summations in (15) can be written as $|\langle f|f_A\rangle|^2$ and $|\langle f|f_B\rangle|^2$,

$$\lambda^{(C)}_{a+b-1} \geqslant \lambda^{(A)}_{m+a+1}+\lambda^{(B)}_{m+b+1}+\min_{f\in L^{\perp}_{AB}}\left[\Delta A\,|\langle f \mid f_A\rangle|^2+\Delta B\,|\langle f \mid f_B\rangle|^2\right] \quad (16)$$

where we now let $\Delta A=\lambda^{(A)}_{a}-\lambda^{(A)}_{a+m+1}$ and $\Delta B=\lambda^{(B)}_{b}-\lambda^{(B)}_{b+m+1}$. Similar to before we require, without loss of generality, that $\Delta B\leqslant\Delta A<0$ and rearrange (16) to

$$\lambda^{(C)}_{a+b-1} \geqslant \lambda^{(A)}_{m+a+1}+\lambda^{(B)}_{m+b+1}+\min_{f\in L^{\perp}_{AB}}\left[\Delta A\left(|\langle f \mid f_A\rangle|^2+|\langle f \mid f_B\rangle|^2\right) +(\Delta B-\Delta A)\,|\langle f \mid f_B\rangle|^2\right]. \quad (17)$$

We then set up a Gram determinant with the functions f, f_A and f_B to obtain the inequality

$$|\langle f \mid f_A\rangle|^2+|\langle f \mid f_B\rangle|^2\leqslant 1+|\langle f_A \mid f_B\rangle|\,. \quad (18)$$

Since f is variable, so are f_A and f_B. Instead of the maximum value of $|\langle f_A|f_B\rangle|$, we seek the possibly larger, but not smaller, quantity $|\langle g_A|g_B\rangle|$ where g_A is any normalized function in the subspace spanned by the eigenfunctions α_a, $\alpha_{a+1},\ldots,\alpha_{m+a}$ – and analogously for g_B. Thus g_A and g_B are completely independent of each other while f_A and f_B are related through f. The maximum of $|\langle g_A|g_B\rangle|$ equals the magnitude of both the positive and negative extrema of $\langle g_A|g_B\rangle$ since $|\langle g_A|g_B\rangle|=|-\langle g_A|g_B\rangle|=|\langle -g_A|g_B\rangle|$ assuming real functions. We expand $\langle g_A|g_B\rangle$

$$\langle g_A \mid g_B\rangle=\left\langle\sum_{i=a}^{m+a}c_i\alpha_i\;\middle|\;\sum_{j=b}^{m+b}d_j\beta_j\right\rangle=\sum_{i=a}^{m+a}c_i\sum_{j=b}^{m+b}d_jx_{ij}, \quad (19)$$

where $x_{ij} = \langle \alpha_i \mid \beta_j \rangle$ and c_i and d_j are expansion coefficients and bound $\langle g_A | g_B \rangle$ in two stages: first eliminate c_i, then eliminate d_j. For the first stage we use the Lagrange method of undetermined multipliers with the partial constraint $\sum_{i=a}^{m+a} c_i^2 = 1$ so that the following is extremized

$$\sum_{i=a}^{m+a} c_i \sum_{j=b}^{m+b} d_j x_{ij} - \lambda \sum_{i=a}^{m+a} c_i^2, \tag{20}$$

which gives the optimal expansion coefficients of g_A as

$$c_i^* = \frac{1}{2\lambda} \sum_{j=b}^{m+b} d_j x_{ij}, \tag{21}$$

for all $i = a, a+1, \ldots, a+m$ where the "*" indicates these expansion coefficients are those that extremize $\langle g_A | g_B \rangle$. Next square and then sum both sides of (21) over i to get unity since g_A is normalized and solve for λ.

$$\lambda = \frac{\pm 1}{2} \sqrt{\sum_{i=a}^{m+a} \left[\left(\sum_{j=b}^{m+b} d_j x_{ij} \right)^2 \right]}. \tag{22}$$

Rearrange (21) to get

$$\sum_{j=b}^{m+b} d_j x_{ij} = 2\lambda c_i^*, \tag{23}$$

to substitute directly in (19) followed by substitution of (22):

$$\begin{aligned} \left| \langle g_A \mid g_B \rangle_{\text{extreme}} \right| &= \left| \sum_{i=a}^{m+a} c_i^* \sum_{j=b}^{m+b} d_j x_{ij} \right| = 2\,|\lambda| \sum_{i=a}^{m+a} (c_i^*)^2 \\ &= 2\,|\lambda| = \sqrt{\sum_{i=a}^{m+a} \left[\left(\sum_{j=b}^{m+b} d_j x_{ij} \right)^2 \right]}. \end{aligned} \tag{24}$$

Now that the expansion coefficients c_i of g_A have been optimized and eliminated we concentrate on the expansion coefficients d_j of g_B. We recognize that the final right-hand side of (24) is the length, or norm, of the vector Xd^*

$$\left| \langle g_A \mid g_B \rangle_{\text{extreme}} \right| = \left\| Xd^* \right\| = \left(Xd^* \bullet Xd^* \right)^{1/2} = \left(d^* \bullet X^T X d^* \right)^{1/2}, \tag{25}$$

where X is the $(m+1) \times (m+1)$ matrix with elements $x_{ij} = \langle \alpha_i \mid \beta_j \rangle$, X^{T} is its transpose (for a real matrix), and d^* is the vector $(d_b^*, d_{b+1}^*, \ldots, d_{b+m}^*)$ corresponding to the function g_B. All that remains is to note that $(d^* \bullet X^T X d^*)^{1/2}$ is the square-root, s^*, of the largest magnitude eigenvalue of $X^{\mathrm{T}}X$ so that the finding the extreme value of $\langle g_A | g_B \rangle$ reduces to a matrix-eigenvalue problem. We are now able to bound (18)

$$|\langle f \mid f_A \rangle|^2 + |\langle f \mid f_B \rangle|^2 \leqslant 1 + |\langle f_A \mid f_B \rangle| \leqslant 1 + |\langle g_A \mid g_B \rangle| \leqslant 1 + s^*, \qquad (26)$$

which is inserted in (17) where we also bound $|\langle f | f_B \rangle|$ with one. Upon simplification we arise at the final generalized bound to $\lambda_{a+b-1}^{(C)}$

$$\lambda_{a+b-1}^{(C)} \geqslant \lambda_{m+a+1}^{(A)} + \lambda_b^{(B)} + s^*(\lambda_a^{(A)} - \lambda_{m+a+1}^{(A)}), \qquad (27)$$

which reduces to (13) when $m = 0$ so that the more specific bound is included in the more general. Inequality (27) can be written in a different form which allows a better comparison with the simpler improvement of Weyl's inequality (13)

$$\lambda_{a+b-1}^{(C)} \geqslant \lambda_{a+1}^{(A)} + \lambda_b^{(B)} + s^*(\lambda_a^{(A)} - \lambda_{a+1}^{(A)}) + \delta \qquad (28)$$

where $\delta = (1 - s^*)(\lambda_{m+a+1}^{(A)} - \lambda_{a+1}^{(A)}) \geqslant 0$. Ignoring δ, (28) and (13) are identical if the overlap of the two eigenvectors, s, is the same as the overlap of two sub-eigenspaces, s^*. Considering the positive δ would then cause (28) to be a certain improvement of (13). Unfortunately the overlap of two sub-eigenspaces never decreases, and typically increases, as the sub-eigenspaces get larger. Thus s^*, which is the overlap of two many-dimensional sub-eigenspaces, will typically exceed s, the overlap of two one-dimensional sub-eigenspaces, and the improvement of (28) over (13) is not certain.

5. Example

To illustrate the improvement of Weyl's method using (13) and (27) and the fact that (27) is not necessarily an improvement of (13) we consider an example. The simplest diatomic molecule is the hydrogen molecular cation H_2^+ for which the Hamiltonian operator C is

$$C = T + V_+ + V_-, \qquad (29)$$

where T is the kinetic energy operator for the single electron and V_+ and V_- are the potential energy operators for the attraction of the electron to the first and second nuclei (i.e., protons), respectively, which are displaced from the origin along the positive and negative x-axis, respectively. The Hamiltonian C can also be written as the sum of the operators A and B:

$$A = \frac{1}{2}(T + 2V_+) \qquad B = \frac{1}{2}(T + 2V_-), \qquad (30)$$

each of which is half the Hamiltonian for a He^+ cation, but at a different location. Because V_+ and V_- are the same except for the center of the potential, the symmetry of the eigenfunctions of C is such that $r_a = s_b$ as long as $a = b$. The eigenvalues (in hartree energy units) of A and B are both $\lambda_1 = -1$, $\lambda_2 = \cdots = \lambda_5 = -1/4$, $\lambda_6 = \cdots = \lambda_{14} = -1/9, \ldots, \lambda_\infty = -1$. We seek a lower bound to $\lambda_1^{(C)}$. Bounds (13) and (27) reduce in this case to

$$\lambda_1^{(C)} \geqslant \frac{-5}{4} - \frac{3}{4}s \tag{31}$$

and

$$\lambda_1^{(C)} \geqslant \frac{-10}{9} - \frac{8}{9}s^* \tag{32}$$

respectively, while Weyl's bound is constant at -2.00. The eigenvectors for use in (13,31) are a $1s$ He^+ orbital placed at each nucleus. The sub-eigenspaces for use in (27,32) are the span of $1s$, $2s$, $2p_x$, $2p_y$ and $2p_z$ He^+ orbitals at each nucleus so that $m = 4$.

Figure 1 plots the lower bounds using the eigenvector improvement (13,31) and the sub-eigenspace improvement (27,32) along with accurate values of the energy [6] as the internuclear distance varies. Weyl's inequality is constant at -2.00 hartree and provides a very poor lower bound. At small internuclear

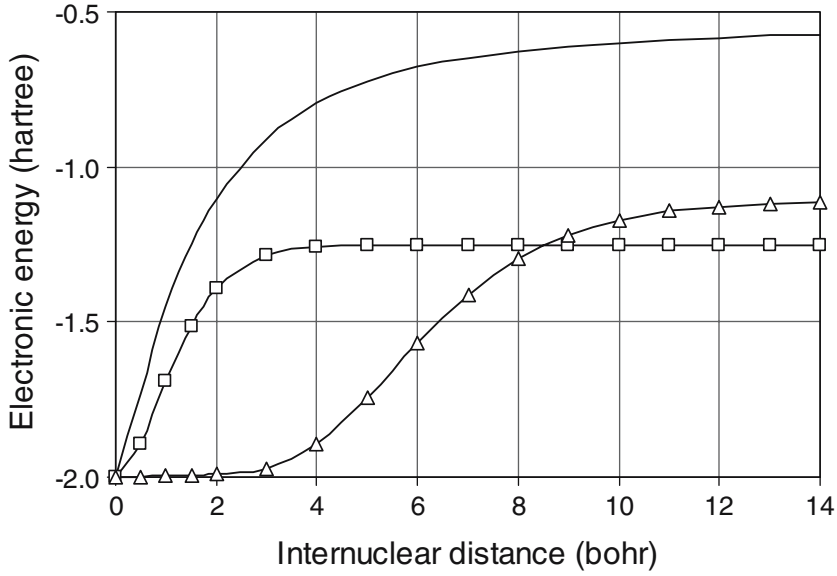

Figure 1. The true electronic energy of H_2^+ is plotted without data point markers [6]. Below it are lower bounds using (13, 31) with square data point markers and lower bounds using (27, 32) with triangular data point markers. Weyl's inequality gives a constant lower bound of -2.00 hartree.

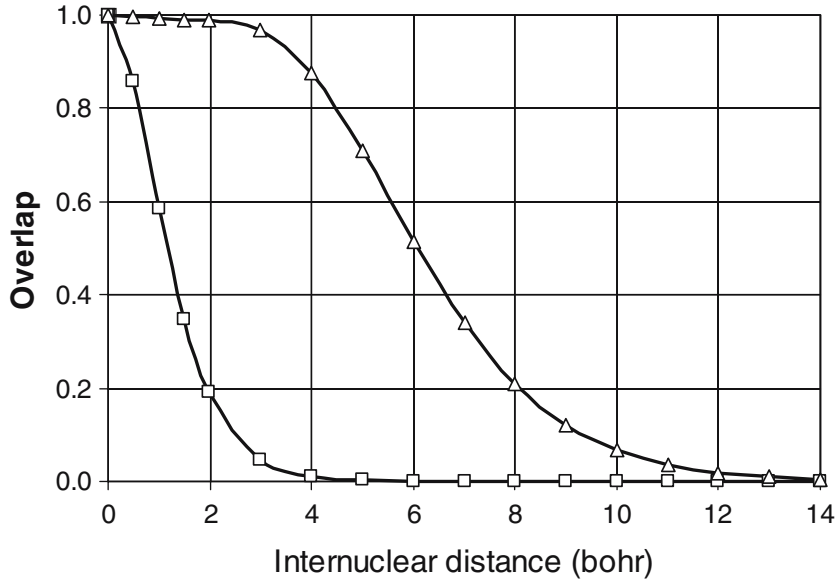

Figure 2. The overlaps s and s^* are plotted as a function of the internuclear distance. Square data point markers denote s (for the eigenvector case) while triangular data point markers denote s^* (for the sub-eigenspace case). Low values of s and s^* allow the associated lower bounds to reach their potential.

distances the sub-eigenspace improvement is poorer than the eigenvector improvement. Although the former has the more potential (-1.11 hartree vs. -1.25 hartree) the large value of s* causes poor performance. Only after the internuclear distance has increased beyond about eight bohr does s* become low enough (see figure 2) for the potential of the sub-eigenspace improvement to be realized. Using larger sub-eigenspaces in (27) would improve the lower bounds, though only at even larger internuclear distances as s* typically increases as the dimension of the sub-eigenspace increases. Furthermore the improvement would be small as there exists an ultimate limit of -1.00 hartree for the improvements presented here based on $\lambda_1 + \lambda_\infty$ in (27) when $m = \infty$ due to the bunching of the He^+ eigenvalues near -1.00 hartree.

6. Summary

Weyl's inequality provides a simple lower bound to the eigenvalue of a sum of two operators using the eigenvalues of the two component operators. This has been improved by considering the overlap of sub-eigenspaces of the individual operators and the improvement is better when the overlap is minimal. The general bound, which considers many-dimensional sub-eigenspaces, while never

inferior to Weyl's inequality, is sometimes inferior to the simpler bound which considers one-dimensional sub-eigenspaces (i.e., eigenvectors) due to a drastic simplification in the derivation of the more general bound.

References

[1] F.W. King, J. Chem. Phys. 102 (1995) 8053.
[2] A. Luchow and H. Kleindienst, Int. J. Quant. Chem. 51 (1994) 211.
[3] H. Weyl, Math. Ann. 71 (1912) 441.
[4] W.E. Thirring, *Quantum Mechanics of Atoms and Molecules: A course in Mathematical Physics*, Vol. 3 (Springer Verlag, 1978) theorem 4.6.14.
[5] A. Weinstein and W. Stenger, *Methods of Intermediate Problems for Eigenvalues: Theory and Ramifications* (Academic Press, 1972).
[6] H. Wind, J. Chem. Phys. 42 (1964) 2371.