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On the Temple lower bound for eigenvalues

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Abstract. In the first part of this paper we examine the relation between the Temple, Weinstein and Stevenson bounds for an arbitrary eigenvalue of a Hamiltonian H . We show that, in a sense which we define, the Temple and Stevenson bounds are numerically equivalent, while the Weinstein bound is inferior to either.

In the second part, the Temple bound is reformulated and it is shown that the usual restriction on its validity may be relaxed; the relaxation leads to rather more convenient calculations in the presence of excited states, but not to improved lower bounds. A numerical example demonstrating the extension is given.

1. Introduction

There exists a large number of methods for computing lower bounds on the eigenvalues of an hermitian operator H . These methods differ in their ease of computation; in their efficiency for a given class of trial functions; and in the input knowledge they assume. This knowledge may be either of the structure of H (such as a split of the form $H_0 + V$ for soluble H_0) or of the approximate position of adjacent eigenvalues.

We consider here only the 'classical' lower bounds, which introduce the operator H^2 and assume some knowledge of the level spacing. The best known of these are the formulae of Temple, Stevenson, and Weinstein. These are usually quoted only for the ground state, but apply equally well to excited states; we can write them in the conventional form as follows. For a given (normalized) trial function Ψ we define

$$\begin{aligned}\eta &= (\Psi, H\Psi) \\ \delta^2 &= (H\Psi, H\Psi).\end{aligned}\tag{1}$$

Then lower bounds to the p th ordered eigenvalue of H are given by:
Weinstein (1934)

$$E_p \geq E_w = \eta - (\delta^2 - \eta^2)^{1/2}\tag{2a}$$

provided

$$\eta \leq \frac{1}{2}(E_p + E_{p+1}).\tag{2b}$$

Temple (1928a, 1928b)

$$E_p \geq E_T(\alpha) = \eta - \frac{\delta^2 - \eta^2}{\alpha - \eta}\tag{3a}$$

provided that

$$\eta < \alpha \leq E_{p+1} \quad (3b)$$

Stevenson (1938)

$$E_p \geq E_S(\beta) = \beta - (\beta^2 - 2\beta\eta + \delta^2)^{1/2} \quad (4a)$$

provided that

$$\beta \leq \frac{1}{2}(E_p + E_{p+1}). \quad (4b)$$

These formulae differ both in their accuracy for a given trial function, and in their ease of optimization when this contains a number of linear parameters. Their accuracy has been compared by a number of authors. In § 2 we add to these comparisons, and we hope clarify the situation in which one or other will yield the better results. In § 3 we compare the computational convenience of the methods, and in particular rederive the Temple bound in a convenient form which allows us to ease the restriction (3b). A calculation on helium which demonstrates this is discussed.

2. Relation between the Temple, Weinstein and Stevenson bounds

The bounds (3), (4), (5) have been compared by a number of authors, with varying conclusions. These variations stem from the presence of the parameters α , β in E_T , E_S ; both E_T and E_S are monotonic increasing functions of these parameters, which are therefore taken in practice to be as large as possible. It is easy to make different assumptions concerning the 'possible size' which affect the detailed comparisons. We remark further on this below.

2.1. E_W and E_S

The Weinstein bound can be viewed as a special case of the Stevenson bound for the choice $\beta = \eta$

$$E_W = E_S(\eta).$$

Hence we have as remarked by Walmsley (1967)

$$E_S(\beta) \geq E_W \quad \text{if } \beta \geq \eta. \quad (5a)$$

2.2. E_W and E_T

It is straightforward to derive the identity

$$E_T(\alpha) - E_W = \frac{(\delta^2 - \eta^2)^{1/2}}{\alpha - \eta} \{(\alpha - \eta) - (\eta - E_W)\}.$$

The denominator in this expansion is positive, as is the factor $(\delta^2 - \eta^2)^{1/2}$. We therefore conclude that

$$E_T > E_W$$

provided that

$$\alpha - \eta > \eta - E_W. \tag{5b}$$

Comment: Both the inequalities (5a), (5b) may be violated in particular calculations; however, the calculations will then inevitably be very inaccurate. We recall that η should approximate E_p while in a practical calculation we will choose β as close to $(E_p + E_{p+1})/2$ as possible. In terms of the *level spacing* $\Delta = E_{p+1} - E_p$ we may therefore write the second inequality in (5a) approximately in the form

$$\eta - E_p \leq \frac{1}{2}\Delta. \tag{5c}$$

Moreover, in a practical calculation α will be chosen as close as possible to E_{p+1} . Hence if η is close to E_p , the second inequality in (5b) becomes approximately

$$\Delta \geq \eta - E_W. \tag{5d}$$

Thus E_W is worse than either E_S or E_T provided only that the calculation has an accuracy comparable with or better than the spacing between energy levels. This is a rather modest accuracy to aim at in most circumstances. Worse, inequality (5c) is a condition for the *validity* of the Weinstein bound; hence, to a good approximation, we may say that E_W is *never* preferable whenever it is valid.

2.3. E_S and E_T

There has been some confusion over the relation between E_S and E_T in the past. Kato (1949) has shown that, if the only available information is given by η , δ and E_1 , then $E_T(E_1)$ is the *best possible uniform bound* in the sense that, for all systems and some Ψ_T , the Temple bound may be exact (see also Schmid and Schwager 1968). Walmsley (1967) on the other hand has derived the straightforward algebraic identity.

$$E_S(E_p + \alpha) \geq E_T(\alpha)$$

provided

$$\eta \leq \alpha \leq E_{p+1} \tag{6}$$

and concludes that the Stevenson bound is uniformly *better* than the Temple. This conclusion rests on the assumption that the comparative choice of parameters $\beta = E_p + \alpha$ is valid; however, the numerical implementation of such a comparison involves knowing E_p , and Schmid and Schwager (1968) have tartly remarked that this knowledge leads to the best of all lower bounds: $E_L = E_p$. In practice, the choice of α requires prior knowledge of a lower bound on E_{p+1} ; the choice of β requires in addition a lower bound on E_p . We can perform one consistent comparison by either taking E_T as this input lower bound, or by a self consistent procedure in which we set $\beta = E_S + \alpha$. In either case it is straightforward to derive the following identity (Schmid *et al* 1963):

$$E_S(E_T + \alpha) = E_S(E_S + \alpha) = E_T(\alpha). \tag{7}$$

This equation indicates a close relation between E_S and E_T . We now ask which would be preferable, for any legitimate choice of α , β , if we are to attempt a calculation of high accuracy. For such a calculation, or sequence of calculations, we have $E_S, E_T, \eta \simeq E_p$.

We write $E_S = \eta - \Delta_S$, $E_T = \eta - \Delta_T$ and compute the ratio Δ_S/Δ_T . We first rewrite E_S in the form

$$\begin{aligned} E_S &= \beta - (\beta^2 - 2\beta\eta + \delta^2)^{1/2} \\ &= \beta - (\beta - \eta) \left(1 + \frac{\delta^2 - \eta^2}{(\beta - \eta)^2} \right)^{1/2} \\ &= \eta - \frac{\delta^2 - \eta^2}{2(\beta - \eta)} + \frac{(\delta^2 - \eta^2)^2}{8(\beta - \eta)^3} + O(\delta^2 - \eta^2)^3. \end{aligned} \quad (8)$$

Whence we find immediately

$$\frac{\Delta_S}{\Delta_T} = \frac{(\alpha - \eta)}{2(\beta - \eta)} \left(1 - \frac{\delta^2 - \eta^2}{4(\beta - \eta)^2} + O(\delta^2 - \eta^2)^2 \right) \simeq \frac{\alpha - \eta}{2(\beta - \eta)}. \quad (9)$$

Now the ratio (9) is *finite*, and to first order independent of the accuracy of the trial function Ψ_T (which enters only via η). Thus, for any α, β a sequence of calculations with increasing number of terms in Ψ_T (for example) will yield identical convergence rates from E_S and E_T . Moreover, any choice of α, β close to their 'optimal' values will make the ratio (9) close to unity. This is not so for the Weinstein bound; the corresponding ratio Δ_W/Δ_T becomes *infinite* in this limit, and hence E_W converges *more slowly* than either E_T or E_S .

2.4. Input and output bounds

Despite these results, there will be many situations in which the Temple bound is poor, and in which the Stevenson and Weinstein bounds appear better; the calculations of Walmsley (1967) form such a case. This gain is then essentially *illusory*. Both E_S and E_W require for their validity information which we can interpret as an *input lower bound* on the eigenvalue E_p . For E_W this is given by (2b), which may be written

$$E_p \geq 2\eta - E_{p+1} = E_{W1} \quad (\text{Weinstein input bound}). \quad (2b')$$

While any given choice of the parameter β yields a similar input bound for E_S

$$E_p \geq 2\beta - E_{p+1} = E_{S1} \quad (\text{Stevenson input bound}). \quad (4b')$$

If the *output* bounds E_W, E_S lie below the *input* bounds E_{W1}, E_{S1} , it cannot be said that we have gained much. The discussion above then shows that *this will always be so* whenever E_W, E_S are better than E_T .

We illustrate this remark with numerical results from a calculation in the three-nucleon system ${}^3\text{H}$ with the Hamada-Johnston potential (Hamada and Johnston 1962). The upper and Temple lower bounds E_u and E_T for this work have been published (Delves and Hennell 1971); the latter are very bad. Table 1 gives these bounds, and also the input and output Stevenson and Weinstein bounds, for several wavefunctions. For this calculation E_{p+1} represents the two-body deuteron energy, and is known; the upper bound appeared to be converging to -6.5 MeV. The input E_{S1} determines β , and has been set at -10 MeV, well below this. We see from table 1 that indeed we get less out of E_W and E_S than we put into them, although they are attractively higher than E_T .

Table 1. Bounds for the energy $E(^3\text{H})$ with the Hamada–Johnston potential

N	Ψ	Ritz	Temple	Weinstein		Stevenson	
		E_u	E_T	Input E_{wi}	Output E_w	Input E_{si}	Output E_s
6	Ψ_u	-4.73	-294.0	-7.2	-31.7	-10.0	-33.1
	Ψ_L	-3.66	-187.6	-5.1	-20.0	-10.0	-22.6
13	Ψ_u	-5.60	-429.4	-9.0	-43.5	-10.0	-44.0
	Ψ_L	-3.78	-129.4	-5.3	-17.8	-10.0	-20.3
23	Ψ_u	-5.72	-359.5	-9.2	-41.0	-10.0	-41.3
	Ψ_L	-3.80	-67.0	-5.4	-13.8	-10.0	-16.4
66	Ψ_u	-6.40	-206.2	-10.6	-35.3	-10.0	-35.0
	Ψ_L	-3.93	-41.2	-5.6	-11.9	-10.0	-14.4

These results come from the calculation of (Delves and Hennell 1971). N is the number of linear parameters in the trial function; Ψ_u and Ψ_L represent trial functions whose linear parameters have been optimized for the upper (E_u) and Temple lower (E_T) bounds respectively. E_{wi} , E_{si} are the input bounds (2b'), (4b') for the Weinstein and Stevenson lower bounds E_w , E_s .

3. Extension of the Temple bound

We now rederive the Temple bound in a computationally convenient form. The Schrödinger equation for an eigenvalue E is

$$(H - E)\Psi = 0.$$

We write this in the form

$$(L - \gamma)\Psi = 0 \quad L = H - \alpha \quad \gamma = E - \alpha$$

whence premultiplying by the operator L we find

$$(L - \epsilon L^2)\Psi = 0 \quad \epsilon = 1/\gamma. \tag{10}$$

This equation is formally similar to the original Schrödinger equation, since the operator L^2 is positive definite (we exclude the case that α is an eigenvalue of H). A linear trial function $\Psi_T = \sum_{i=1}^N a_i^{(N)} h_i$ with N terms leads to the finite matrix equation for $\epsilon^{(N)}$, $\mathbf{a}^{(N)}$:

$$(L_{(N)} - \epsilon^{(N)} L_{(N)}^2) \mathbf{a}^{(N)} = 0. \tag{11}$$

Moreover, the Hylleraas–Undheim theorem holds for the pair (10), (11); that is, if we order the eigenvalues ϵ_i and approximations $\epsilon_i^{(N)}$

$$\begin{aligned} \epsilon_1 &\leq \epsilon_2 \leq \epsilon_3 \dots \\ \epsilon_1^{(N)} &\leq \epsilon_2^{(N)} \leq \dots \end{aligned} \tag{12}$$

Then

$$\epsilon_i^{(N)} \geq \epsilon_i \quad i = 0, 1, 2, \dots, N. \tag{13}$$

Now the ordering (12) induces a mapping between the ϵ_i and the (ordered) E_i . Let us suppose that $\epsilon_i = 1/(E_{j_i} - \alpha)$; then (13) reads

$$\epsilon_i^{(N)} \geq \frac{1}{E_{j_i} - \alpha}. \tag{13a}$$

Now if $E_{j_i} < \alpha$, the right hand side is negative. If $\epsilon_i^{(N)}$ is positive, (13a) is then not very useful. If $\epsilon_i^{(N)}$ is *negative*, we invert the inequality to read

$$E_{j_i} \geq \alpha + \frac{1}{\epsilon_i^{(N)}} \quad E_j < \alpha \quad \epsilon_i^{(N)} < 0. \tag{14}$$

Equation (14) has the form of the Temple bound. To see this, let us choose (as is usual)

$$E_1 < \alpha < E_2.$$

Then there exists only one negative $\epsilon_i = \epsilon_1$; and $E_{j_i} = E_1$. Moreover, the solution of (11) yields the Rayleigh quotient

$$\begin{aligned} \epsilon_1^{(N)} &= \frac{\mathbf{a}^T L^{(N)} \mathbf{a}^{(N)}}{\mathbf{a}^T L^{(N)2} \mathbf{a}^{(N)}} \\ &= \frac{\eta - \alpha}{\delta^2 - 2\alpha\eta + \alpha^2} \end{aligned}$$

whence (14) may be put in the form (3).

However, we may use (14) to ease the restriction (3b) on the parameter α . Let us suppose that $E_p < \alpha < E_{p+1}$; there are then p negative eigenvalues ϵ_i . Moreover, the correspondence between the first p ϵ_i and E_{j_i} is as follows:

$$(\epsilon_1, E_p) \quad (\epsilon_2, E_{p-1}) \quad (\epsilon_3, E_{p-2}) \dots (\epsilon_p, E_1).$$

Let us suppose that there are $q \leq p$ negative eigenvalues $\epsilon_i^{(N)}, i = 1 \dots q$. Then these q eigenvalues yield via (14) lower bounds on $E_p, E_{p-1} \dots E_{p-q+1}$. For a ‘sufficiently good’ trial function we shall have $q = p$; we then have in particular a lower bound on the ground state E_1 using the Temple formula with a value of $\alpha > E_2$. If $q < p$, the lower bounds which we obtain can however be expected to be rather poor; the numerical results below show clearly that they then tend to be *approximations to* $E_q \dots E_1$, although of course valid lower bounds to $E_p \dots E_{p-q+1}$. We may use this extension to find improved lower bounds on any eigenvalue: we compute the eigenvalues $\epsilon_i^{(N)}$ for increasing α , checking meanwhile that the appropriate number of negative $\epsilon_i^{(N)}$ exists. We illustrate the extension with a calculation on the 1^1S and 2^1S states of the helium atom, using the basis $\exp\{-S(lr_1 + mr_2 + nr_{12})\}$. The calculation was performed using a general purpose program which has been described elsewhere (Delves and Kalotás 1968). The first three eigenvalues of this system are in atomic units

$$E(1^1S) = -2.9037243 \quad E(2^1S) = -2.1459681 \quad E(3^1S) = -2.0612558.$$

Calculations were performed using 40 and 60 term functions, with $\alpha = -2.06128 \approx E(3^1S)$. The results are shown in figure 1 as a function of the scale parameter S . For small values of the scale ($S \lesssim 2.0$) only one negative eigenvalue $\epsilon_1^{(N)}$ was found. This then yields via (14) a lower bound on $E(2^1S)$; however, it is evident from figure 1 that it is in fact a rather good approximation to $E(1^1S)$ and an extremely poor lower bound to $E(2^1S)$.

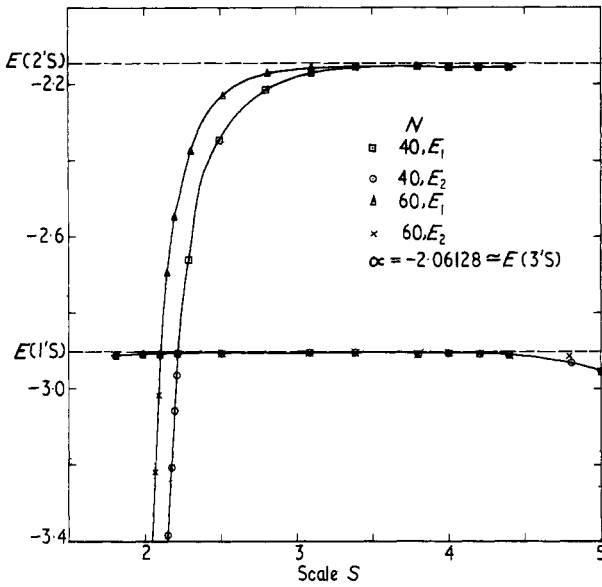


Figure 1. Temple lower bounds for the singlet states of the helium atom using a basis $\exp\{-S(lr_1 + mr_2 + nr_{12})\}$ with $N = 40$ and 60 terms. The reference energy α used is $\alpha = -2.06128 \approx E(3^1S)$; ϵ_1, ϵ_2 are the algebraically smallest and second smallest eigenvalues of equation (11). These lead to lower bounds on $E(2^1S)$ and $E(1^1S)$ respectively. Note that the definition in terms of their ordering induces a break in the curves of ϵ_1, ϵ_2 as a function of the scale S , and that for small S ϵ_1 yields a good approximation to $E(1^1S)$ rather than to $E(2^1S)$.

This result is to be expected, on continuity grounds. For larger scale factors, we found two negative $\epsilon_i^{(N)}$ for both $N = 40$ and $N = 60$, and hence obtained lower bounds on both $E(1^1S)$ and $E(2^1S)$. The best lower bounds found in this way are shown in table 2, together with the values obtained for the ‘conventional’ Temple bound using $\alpha = -2.146 \approx E(2^1S)$.

Table 2. Temple lower bounds for the helium atom

State	1 ¹ S	2 ¹ S
<i>E</i> exact	-2.9037243	-2.1459681
$N = 40, \alpha = -2.06128$	-2.90411	-2.15328
$N = 60, \alpha = -2.06128$	-2.90373	-2.14605
$N = 40, \alpha = -2.146$	-2.90388	—
$N = 60, \alpha = -2.146$	-2.90372	—

The last figure in each result may be in error by one unit due to round-off errors.

4. Discussion

The conventional results above show clearly that there is a nett loss in accuracy for the ground state from the use of the generalization given for the Temple bound. In this sense the gain has been negative. However, we have the advantage that it is no longer

necessary to know the number or location of the excited states of the system used. For any choice of the parameter α (such that there is only a finite number of levels below α), a calculation with increasing N will 'eventually' yield the full number of bound states and hence a lower bound on these low-lying levels. The form (14) is also useful in that it leads, via (11), to a straightforward optimization of the linear parameters in the trial function. A similar formalism exists for the Stevenson bound, by replacing (10) by the equation

$$(L^2 - \gamma^2)\Psi = 0 \quad L = H - \beta \quad \gamma = E - \beta.$$

In practice, the Stevenson and Temple bounds are therefore essentially equivalent in both convenience and in results; the Temple bound then has the advantage that its side conditions do not involve the eigenvalue to be computed. The Weinstein bound on the other hand does not appear to lead to such straightforward optimization procedures, and despite suggestions to the contrary (Goodison 1967) would seem to have little to recommend it as a procedure for bounding excited states.

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