Journal of Mathematical Chemistry Vol. 34, Nos. 1–2, July 2003 (© 2003)

Lower bounds to ground-state eigenvalues II

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Received 29 January 2003

An alternative to the Temple method for calculating a lower bound to the ground-state eigenvalue of an operator is presented. The method presented is an improvement and generalization upon a similar method [M.G. Marmorino, J. Math. Chem. 32 (2002) 19–29]. For the system tested the lower bound of the current method is significantly superior to the Temple method and the previous method. Furthermore, the current method (like its predecessor) is able to generate a lower bound when the Temple method fails.

KEY WORDS: lower bounds, Temple, ground state, eigenvalues

1. Introduction

A previous report [1] introduced a new method for generating a lower bound to the ground-state eigenvalue of a Hamiltonian. It was shown that the method was similar to the Temple bound but, in some cases, was able to provide a rigorous lower bound when the Temple method could not. Despite this success the previous method suffers from several restrictions:

1. Bounds the ground-state only.
2. Requires an exactly soluble base Hamiltonian (in part).
3. Requires the full Hamiltonian to be a positive perturbation from the base Hamiltonian.
4. Requires a separate calculation to bound an overlap integral.

In this paper we remove restrictions 2–4 so that a general ground-state lower bound results comparable to the Temple bound. This method and the Temple bound require information which is generally not available and so the bounds produced are usually not rigorous lower bounds. In the special case when restrictions 2, 3 are satisfied, then rigorous lower bounds can be obtained by both our method and the Temple method. Restriction 2 is severe for our method where a very large number of the base Hamiltonian's eigenfunctions and eigenvalues are used; on the other hand, the Temple method requires knowledge of only the first excited-state eigenvalue of the base problem.

0259-9791/03/0700-0059/0

2. Theory

We begin with an intermediate Hamiltonian H':

$$H' = P_{\mathbf{S}} H P_{\mathbf{S}} + P_{\boldsymbol{R}}(H + C) P_{\mathbf{R}}, \tag{1}$$

where C is a constant and H is the full Hamiltonian of interest. **S** is an N-dimensional variational subspace and **R** is the complement of **S**; $P_{\mathbf{S}}$ and $P_{\mathbf{R}}$ are projection operators onto **S** and **R**, respectively. We assume that the lowest n variational eigenpairs $(\lambda_1, f_1), \ldots, (\lambda_n, f_n)$ of the operator $H|_{\mathbf{S}}$ are also the lowest n eigenpairs of H': $(E'_1, \psi'_1), \ldots, (E'_n, \psi'_n)$, where $2 \leqslant n \leqslant N$.

The perturbation of H' to the full Hamiltonian H is $P' = H - H'$. Our lower bound formula is derived from the variational theorem:

$$E_1 = \langle \psi_1 | H' | \psi_1 \rangle + \langle \psi_1 | P' | \psi_1 \rangle \geqslant E'_1 + \langle \psi_1 | P' | \psi_1 \rangle, \tag{2}$$

where (E_1, ψ_1) is the ground-state eigenpair of the full Hamiltonian. It remains to bound the non-positive $\langle \psi_1 | P' | \psi_1 \rangle$ from below, which is the subject of the section 3. (The non-positive nature is evident from (2) since $E'_1 \geqslant E_1$.)

If we are not certain that the lowest n eigenstates of $H|_{\mathbf{S}}$ and H' are the same, then there will be a lack of rigor in our method. A similar situation occurs in the Temple ground-state lower bound which requires a lower bound, E_2^{lower}, to the first excited-state eigenvalue, E_2, as input:

$$E_1 \geqslant \langle \phi | H | \phi \rangle - \frac{\langle \phi | H^2 | \phi \rangle - \langle \phi | H | \phi \rangle^2}{E_2^{\text{lower}} - E'_1}, \tag{3}$$

where ϕ is often obtained from a variational calculation and thus equated with f_1. (A rigorous E_2^{lower} is usually E_2^0 from a base Hamiltonian H^0 which becomes the full Hamiltonian $H = H^0 + P$ under a positive perturbation P.) Furthermore, in the Temple bound, the variational estimate $\langle \phi | H | \phi \rangle$ (often equated with λ_1) must be less than E_2^{lower}. The Temple bound is sometimes used without a rigorous lower bound for E_2 [2]. In general we are unable to prove that the lowest n eigenstates of $H|_{\mathbf{S}}$ and H' are the same for our lower bound. Thus both methods are non-rigorous except in special cases, i.e., when restrictions 2 and 3 listed in the introduction are satisfied.

Because both bounds are usually non-rigorous it is important to consider which one is more trustworthy. We consider the case when $C = 0$ and, hopefully, $n = 2$. To ensure that λ_1 and λ_2 are the lowest eigenvalues of H', we must show that they are less than the lowest eigenvalue, χ, of $H'|_{\mathbf{R}}$:

$$\chi = \inf_{\substack{\varphi \in \mathbf{R} \\ \langle \varphi | \varphi \rangle = 1}} \langle \varphi | H | \varphi \rangle = \sum_{k=1}^{\infty} \langle \psi_k | \varphi \rangle^2 E_k, \tag{4}$$

where $H\psi_k = E_k \psi_k$. The overlap coefficients are limited by how much overlap there is between the eigenfunctions of H and **S**. Since **S** is an N-dimensional variational subspace, a large calculation usually ensures that $\langle \psi_k | \mathbf{S} \rangle$ are close to one for the first

several k, say $k = 1, \ldots, M \ll N$. This implies that $\langle \psi_k | \varphi \rangle$ would be close to zero for $k = 1, \ldots, M \ll N$. Thus an *approximate* lower bound to χ would be E_{M+1}. As the variational subspace increases in size, M increases. Since λ_1 and λ_2 are expected to be close to E_1 and E_2, they should be less than E_{M+1}, and thus be the lowest two eigenvalues of H'. This is all very approximate and when the variational subspace is small or not well-chosen the previous discussion does not apply.

The Temple bound, on the other hand, requires that λ_1 be less than E_2 (assume that $\langle \varphi | H | \varphi \rangle$ is the result of a variational calculation and thus equal to λ_1). This is a much tighter restriction on λ_1 than that given above (less than E_{M+1}). Furthermore, we must pick an *explicit* lower bound to E_2; even if λ_1 is less than the unknown E_2, an incorrect bound on E_2 renders the Temple bound invalid. No explicit bounds are made on E_2 for our method, and our assumption that λ_1 and λ_2 are less than E_{M+1} is often more reasonable than the Temple bound assumption that λ_1 is less than E_2.

In addition, the parameter C, if chosen positive, can be used to increase the chance that the lowest variational eigenvalues are less than the lowest eigenvalue of $H'|_{\mathbf{R}}$ by increasing all the eigenvalues in $\mathbf{R}$ by C. This would worsen the bound, although make it more reliable. If the lowest eigenvalue of $H'|_{\mathbf{R}}$ is known or somehow bounded, then C can be chosen negative to make the bound on E_1 better. This is done in an example in section 4. Our method thus offers more flexibility than the Temple method.

3. Derivation

3.1. General approach

Write ψ_1 as

$$\psi_1 = S_0 \delta + \sum_{k=1}^{N} S_k f_k, \tag{5}$$

where $\delta \in \mathbf{R}$ is normalized and S_0 and S_k are the (real) coefficients of the expansion of ψ_1. The N orthonormal functions f_k span the variational subspace $\mathbf{S}$. The function f_1 is the ground-state variational eigenfunction of $H|_{\mathbf{S}}$; the remaining f_k can be, but are not required to be, the excited-state variational eigenfunctions. We then write the expectation value of P':

$$\begin{aligned} 0 \geqslant \langle \psi_1 | P' | \psi_1 \rangle &= \left\langle S_0 \delta + \sum_{k=1}^{N} S_k f_k \middle| P' \middle| S_0 \delta + \sum_{k=1}^{N} S_k f_k \right\rangle \\ &= S_0^2 \langle \delta | P' | \delta \rangle + 2 S_0 \sum_{k=1}^{N} S_k \langle f_k | P' | \delta \rangle + \sum_{c=1}^{N} \sum_{k=1}^{N} S_c S_k \langle f_c | P' | f_k \rangle \\ &= S_0^2 \langle \delta | H - P_{\mathbf{S}} H P_{\mathbf{S}} - P_{\mathbf{R}} (H + C) P_{\mathbf{R}} | \delta \rangle \end{aligned}$$

$$+2S_0\sum_{k=1}^{N} S_k\langle f_k|H - P_{\mathbf{S}}HP_{\mathbf{S}} - P_{\mathbf{R}}(H+C)P_{\mathbf{R}}|\delta\rangle$$
$$+\sum_{c=1}^{N}\sum_{k=1}^{N} S_cS_k\langle f_c|H - P_{\mathbf{S}}HP_{\mathbf{S}} - P_{\mathbf{R}}(H+C)P_{\mathbf{R}}|f_k\rangle. \tag{6}$$

Because of the projection operators (6) simplifies dramatically to:

$$0 \geqslant \langle\psi_1|P'|\psi_1\rangle = -CS_0^2 + 2S_0\sum_{k=1}^{N} S_k\langle f_k|H - P_{\mathbf{S}}HP_{\mathbf{S}} - P_{\mathbf{R}}(H+C)P_{\mathbf{R}}|\delta\rangle. \tag{7}$$

The remaining $P_{\mathbf{S}}HP_{\mathbf{S}}$ and $P_{\mathbf{R}}(H+C)P_{\mathbf{R}}$ can both be removed, but it is useful to keep the former.

$$0 \geqslant \langle\psi_1|P'|\psi_1\rangle = -CS_0^2 + 2S_0\sum_{k=1}^{N} S_k\langle f_k|H - P_{\mathbf{S}}HP_{\mathbf{S}}|\delta\rangle. \tag{8}$$

We rewrite (8) as:

$$0 \geqslant \langle\psi_1|P'|\psi_1\rangle = -CS_0^2 + 2S_0S_1\langle f_k|H - P_{\mathbf{S}}HP_{\mathbf{S}}|\delta\rangle + 2S_0S_g\langle g|H - P_{\mathbf{S}}HP_{\mathbf{S}}|\delta\rangle, \tag{9}$$

where $g = \sum_{k=2}^{N} S_k f_k \in \mathbf{S}(N)$ and $S_g^2 = S_2^2 + S_3^2 + \cdots + S_N^2$ but is perpendicular to f_1. Taking absolute values of the majority of the right-hand side gives:

$$\begin{aligned} 0 &\leqslant -\langle\psi_1|P'|\psi_1\rangle \\ &\leqslant CS_0^2 + 2|S_0||S_1|\big|\langle f_1|H - P_{\mathbf{S}}HP_{\mathbf{S}}|\delta\rangle\big| + 2|S_0||S_g|\big|\langle g|H - P_{\mathbf{S}}HP_{\mathbf{S}}|\delta\rangle\big|. \end{aligned} \tag{10}$$

Then using the Cauchy–Schwarz inequality we have:

$$0 \leqslant -\langle\psi_1|P'|\psi_1\rangle \leqslant CS_0^2 + 2|S_0||S_1|F + 2|S_0||S_g|G, \tag{11}$$

where $F = \langle f_1|(H - P_{\mathbf{S}}HP_{\mathbf{S}})^2|f_1\rangle^{1/2}$, $G = \langle g|(H - P_{\mathbf{S}}HP_{\mathbf{S}})^2|g\rangle^{1/2}$. We replace $|S_1|$ with the upper bound of one and $|S_g|$ with the upper bound $(1 - S_1^2)^{1/2}$:

$$0 \leqslant -\langle\psi_1|P'|\psi_1\rangle \leqslant CS_0^2 + 2|S_0|F + 2|S_0|\big(1 - S_1^2\big)^{1/2}G. \tag{12}$$

We now introduce the Eckart inequality [3]:

$$\big\langle\psi_1\big|\psi_1'\big\rangle^2 = S_1^2 \geqslant \frac{E_2' - \langle\psi_1|H'|\psi_1\rangle}{E_2' - E_1'}. \tag{13}$$

Letting $H' = H - P'$ in (13) gives:

$$\begin{aligned} S_1^2 \geqslant \frac{E_2' - \langle\psi_1|H|\psi_1\rangle + \langle\psi_1|P'|\psi_1\rangle}{E_2' - E_1'} &= \frac{E_2' - E_1 + \langle\psi_1|P'|\psi_1\rangle}{E_2' - E_1'} \\ &\geqslant \frac{E_2' - E_1^{\text{upper}} + \langle\psi_1|P'|\psi_1\rangle}{E_2' - E_1'}. \end{aligned} \tag{14}$$

Since E'_1 is an upper bound to E_1, (14) can be written as:

$$1 - S_1^2 \leqslant \frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_2 - E'_1}. \tag{15}$$

Substituting (15) in (12) gives:

$$0 \leqslant -\langle\psi_1|P'|\psi_1\rangle \leqslant CS_0^2 + 2|S_0|F + 2|S_0|G\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_2 - E'_1}\right)^{1/2}. \tag{16}$$

3.2. When $C \geqslant 0$

To bound S_0^2 and $|S_0|$ in (16) we first prove an Eckart-like inequality. We have:

$$E'_1 - E'_n \geqslant E_1 - E'_n = \langle\psi_1|H - E'_n|\psi_1\rangle = \langle\psi_1|H' + P' - E'_n|\psi_1\rangle, \tag{17}$$

where n is as defined previously, i.e., that the lowest n eigenstates of H' and $H'|_{\mathbf{S}}$ coincide, where $2 \leqslant n \leqslant N$. Then expand ψ_1 in terms of the eigenfunctions ψ'_k of the intermediate Hamiltonian:

$$\begin{aligned} E'_1 - E'_n - \langle\psi_1|P'|\psi_1\rangle &\geqslant \sum_{k=1}^{\infty} S_k^2\big(E'_k - E'_n\big) \\ &\geqslant \sum_{k=1}^{n-1} S_k^2\big(E'_k - E'_n\big) \geqslant \big(E'_1 - E'_n\big)\sum_{k=1}^{n-1} S_k^2. \end{aligned} \tag{18}$$

This can be rearranged to give a lower bound to the square of the projection (overlap) of ψ_1 on the subspace $\mathbf{S}$, denoted by $S_{\mathbf{S}}^2$:

$$S_{\mathbf{S}}^2 \geqslant \sum_{k=1}^{n-1} S_k^2 \geqslant \frac{E'_n - E'_1 + \langle\psi_1|P'|\psi_1\rangle}{E'_n - E'_1} = 1 + \frac{\langle\psi_1|P'|\psi_1\rangle}{E'_n - E'_1}. \tag{19}$$

When $n = 2$, (19) reduces to the Eckart inequality. Referring to the decomposition of ψ_1 in (5) it is clear that $S_0^2 = 1 - S_{\mathbf{S}}^2$. Substitution of (19) in $S_0^2 = 1 - S_{\mathbf{S}}^2$ and then in (16) to bound $|S_0|$ gives:

$$0 \leqslant -\langle\psi_1|P'|\psi_1\rangle \leqslant CS_0^2 + 2\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_n - E'_1}\right)^{1/2}\left[F + G\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_2 - E'_1}\right)^{1/2}\right]. \tag{20}$$

We can use the square of the previous result to bound S_0^2 as well:

$$\begin{aligned} 0 \leqslant -\langle\psi_1|P'|\psi_1\rangle \leqslant{}& C\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_n - E'_1}\right) \\ &+ 2\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_n - E'_1}\right)^{1/2}\left[F + G\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_2 - E'_1}\right)^{1/2}\right]. \end{aligned} \tag{21}$$

Next divide by $(-\langle\psi_1|P'|\psi_1\rangle)^{1/2}$, rearrange and square:

$$0 \geqslant \langle\psi_1|P'|\psi_1\rangle \geqslant -\frac{4F^2}{E'_n - E'_1}\left(1 - \frac{C}{E'_n - E'_1} - \frac{2G}{(E'_n - E'_1)^{1/2}(E'_2 - E'_1)^{1/2}}\right)^{-2} \quad (22)$$

provided the quantity $(1 - C\cdots)$ is positive. Combining (22) with (2) gives us a lower bound to E_1:

$$E_1 \geqslant E'_1 - \frac{4F^2}{E'_n - E'_1}\left(1 - \frac{C}{E'_n - E'_1} - \frac{2G}{(E'_n - E'_1)^{1/2}(E'_2 - E'_1)^{1/2}}\right)^{-2}. \quad (23)$$

The quantity $F = \langle f_1|(H - P_{\mathbf{S}}HP_{\mathbf{S}})^2|f_1\rangle^{1/2}$ can straightforwardly be determined since $f_1 = \psi'_1$ is known. The quantity, $G = \langle g|(H - P_{\mathbf{S}}HP_{\mathbf{S}})^2|g\rangle^{1/2}$, however, is a bit trickier since g is an unknown function. Instead an upper bound to G is calculated by determining the maximum eigenvalue of $(H - P_{\mathbf{S}}HP_{\mathbf{S}})^2$ on the variational subspace $\mathbf{S}$. This requires another variational calculation.

In (23) the constant C may be taken as zero, or as some positive number to increase the chance that the lowest n variational eigenvalues are less than the lowest eigenvalue of $H'|_{\mathbf{R}}$ by increasing all the eigenvalues in $\mathbf{R}$ by C. The price to pay for this increased likelihood of getting a trustworthy bound is that a positive C worsens the lower bound. An upper limit on C is determined so that the $(1 - C\cdots)$ term in (23) is always positive.

3.3. *When $C < 0$*

The constant C can be made positive when there is uncertainty that the lowest n variational eigenvalues are less than the lowest eigenvalue of $H'|_{\mathbf{R}}$; however, when we are certain of this, then C can be made negative to improve the bound, being the difference between the $\lambda_n = E'_n$ and the lowest eigenvalue of $H'|_{\mathbf{R}}$. We encounter such a case in section 4 when we apply our method to an example. For such certainty it is usually necessary for restrictions 2 and 3 listed in the introduction to be satisfied. When $C < 0$ a different approach must be taken than in the latter part of section 3.2 because the S_0^2 term in (20) must be bounded from below instead of above as before:

$$0 \leqslant -\langle\psi_1|P'|\psi_1\rangle \leqslant CS_0^2 + 2\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_n - E'_1}\right)^{1/2}\left[F + G\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_2 - E'_1}\right)^{1/2}\right]. \quad (20)$$

A lower bound to S_0^2 can be found be found by first assuming a trivial lower bound of zero in (16):

$$0 \leqslant -\langle\psi_1|P'|\psi_1\rangle \leqslant 2|S_0|\left(F + G\left(\frac{-\langle\psi_1|P'|\psi_1\rangle}{E'_2 - E'_1}\right)^{1/2}\right) \quad (24)$$

which leads to the lower bound:

$$0 \leqslant \frac{(-\langle\psi_1|P'|\psi_1\rangle)^2}{4(F + G(-\langle\psi_1|P'|\psi_1\rangle/(E'_2 - E'_1))^{1/2})^2} \leqslant S_0^2. \quad (25)$$

Combining (25) and (20) and rearranging gives an inequality cubic in $x = (-\langle\psi_1|P'|\psi_1\rangle)^{1/2}$:

$$0 \leqslant x^3\left(\frac{C}{8} + \frac{\gamma^3}{\Delta_n^{1/2}} - \frac{\gamma^2}{2}\right) + x^2\left(\frac{3\gamma}{\Delta_n^{1/2}} - 1\right)F\gamma + x\left(\frac{3\gamma}{\Delta_n^{1/2}} - \frac{1}{2}\right)F^2 + \frac{F^3}{\Delta_n^{1/2}}, \quad (26)$$

where $\Delta_n = E'_n - E'_1$ and $\gamma = G/(E'_2 - E'_1)$. If (26) can provide an upper bound to x, then the bound x_{upper} is squared and negated to give a lower bound to $\langle\psi_1|P'|\psi_1\rangle$ and used in (2) for a lower bound to E_1:

$$E_1 \geqslant E'_1 + \langle\psi_1|P'|\psi_1\rangle \geqslant E'_1 - x^2_{\text{upper}}. \quad (2)$$

One way to determine if an upper bound to x exists is to plot the right-hand side of (26) versus positive x. If this curve intersects the x-axis sloping downward and does not rise up to intersect the x-axis again, then this final intersection x_{upper} is the maximum value of x, since by (26) x must be such that the curve is positive.

4. Example

We illustrate the method on the following one-dimensional Hamiltonian:

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{\text{box}} + px, \quad (27)$$

where V_{box} is the particle-in-a-box potential for a box from $x = 0$ to $x = \pi$ (zero inside and infinite outside) and p is a constant. For the N-dimensional variational subspace **S** we use the N lowest eigenfunctions of the particle-in-a-box Hamiltonian (restriction 2). Since the perturbation from the particle-in-a-box Hamiltonian to H is positive (restriction 3), the eigenvalues of the particle-in-a-box Hamiltonian $E_k(\text{box})$ are lower bounds to the eigenvalues of H. In particular, $E_{N+1}(\text{box})$ is a lower bound to the lowest eigenvalue of $H'|_{\mathbf{R}}$. For the choices of N tested, all the variational eigenvalues were lower than this so that $n = N$.

Furthermore, we are able to let C be negative which improves the lower bound slightly. We let $C = E'_N - E_{N+1}(\text{box})$, where $E'_N = \lambda_N$ and $E_{N+1}(\text{box})$ is a lower bound to the lowest eigenvalue of $H'|_{\mathbf{R}}$. This lowers all the eigenvalues in **R** by C while still keeping them above the N variational eigenvalues in **S**. Results for $p = 1/2$ and $p = 3/2$ are shown in tables 1 and 2, respectively. In both cases, our current lower bounds are higher than those from our previous method and the Temple formula.

5. Conclusion

We have presented a new lower bound formula for the ground-state eigenvalue of a Hamiltonian. In the general case, where the Temple method and ours may be applied non-rigorously, we propose that our method is more likely to give a reliable bound although the calculation is more intense due mainly to an additional matrix-eigenvalue

Table 1
Lower bounds to E_1 for the perturbed particle-in-a-box Hamiltonian ($p = 1/2$) are shown for the two bounds derived in this paper, the best bound of our previous method, and the Temple bound. Two hartree is used as a rigorous lower bound to E_2 for the Temple method. The variational upper bound E_1' is also shown. Hartree units are used for the energy.

Method	$N = 10$	$N = 50$
Upper bound	1.232950164	1.23295014815474
$C < 0$	1.232950071	1.23295014815298
$C = 0$	1.232950039	1.23295014815285
Previous	1.2329498	1.23295014812
Temple	1.2329484	1.23295014707

Table 2
Lower bounds to E_1 for the perturbed particle-in-a-box Hamiltonian ($p = 3/2$) are shown calculated from the two bounds derived in this paper and the best bound of our previous method. For this size perturbation the variational upper bound E_1' is greater than the only available lower bound to E_2, i.e., 2 hartree, so a Temple bound cannot be calculated. Hartree units are used for the energy.

Method	$N = 10$	$N = 50$
Upper bound	2.435902	2.435902312140
$C < 0$	2.435899	2.435902312106
$C = 0$	2.435898	2.435902312103
Previous	2.435895	2.435902311697
Temple	NA	NA

problem that must be solved. For rigorous applications, the increase in calculational difficulty from the Temple bound stems from two additional reasons: (1) more knowledge of the base Hamiltonian's eigenvalues and eigenfunctions; and (2) being forced to use a subspace of the base Hamiltonian eigenspace for a variational calculation using the full Hamiltonian.

To justify this increase in difficulty we note that in the first case tested ($p = 1/2$), our lower bound surpasses the Temple bound. Furthermore, in the second case ($p = 3/2$), our bound works when the Temple bound fails. The improvement over our previous method is two-fold: (1) the resulting bound is better in both cases tested; (2) the calculation is simpler (at least, in the $C \geqslant 0$ case).

Although we feel we have made a significant improvement in the numerical bound and the bounding method itself from the introduction of a similar method, we still lack an extension to excited states.

References

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