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Lower bounds to ground-state eigenvalues

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A new lower bound method is presented for ground-state eigenvalues which relies on the Eckart inequality. The method bears similarity to the variational method and the Temple lower bound formula. Restrictions are that an exactly soluble base Hamiltonian must be available with a positive-semidefinite perturbation to the Hamiltonian of interest. A sample calculation shows that our method is able to sometimes best the Temple bound and also perform rigorously when the Temple bound does not.

KEY WORDS: lower bounds, Temple, variational method

1. Introduction

Eigenvalue problems abound in mathematics, physics and chemistry, and a standard method to approximate the eigenvalues is the variational method. Although the variational method produces rigorous upper bounds, it does not give corresponding lower bounds – without which the quality of variational approximations cannot be rigorously judged. Thus the calculation of lower bounds is very important. Unfortunately, lower bound calculations have not enjoyed the success of upper bound calculations. Lower bound calculations typically suffer from theoretical as well as computational difficulties. Numerous methods exist to calculate lower bounds to eigenvalues, such as: intermediate problems [1–7], variance-like formulas [8–14], effective fields [15–19], local energy [20,21], inequalities between systems of the same or different numbers of particles [22–24] and Temple–Lehmann methods [25]. No current method of lower bound calculation has proved adequate for general use in quantum chemistry and thus variational upper bound calculations or approximate calculations are the methods of choice.

We present a simple and general strategy to calculate a lower bound to *any* eigenvalue of *any* Hamiltonian and then construct a very restricted but explicit method. The restrictions are that a lower bound to only the *ground-state* eigenvalue of a Hamiltonian is provided and the Hamiltonian must be greater than another *exactly soluble* Hamiltonian (which we call the base Hamiltonian).

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2. Strategy

We begin by taking the Gram determinant of the functions ϕ, $H\phi$ and ψ_n where ϕ is an arbitrary function in the domain of the Hamiltonian H and ψ_n is the nth eigenfunction of the Hamiltonian H with corresponding eigenvalue E_n. Assume that both ϕ and ψ_n are normalized and real. Letting S denote $\langle\phi|\psi_n\rangle = \langle\psi_n|\phi\rangle$, the result is:

$$\langle\phi|H^2|\phi\rangle(1 - S_n^2) - \langle\phi|H|\phi\rangle^2 + 2E_n S_n^2\langle\phi|H|\phi\rangle - E_n^2 S_n^2 \geqslant 0. \quad (1)$$

Using the quadratic formula to solve for E_n and rearranging gives:

$$\left[\langle\phi|H|\phi\rangle - E_n\right]^2 \leqslant \left(S_n^{-2} - 1\right)\left(\langle\phi|H^2|\phi\rangle - \langle\phi|H|\phi\rangle^2\right). \quad (2)$$

This result was derived by Weinhold [26]. If S_n^2 can be bounded from below then an upper bound and lower bound are available for E_n through (2). Since upper bounds are relatively simple to calculate by the variational theorem we concentrate on the lower bound. Weinstein [10] and others have derived bounds similar to (2) but missing the overlap term:

$$\left[\langle\phi|H|\phi\rangle - E_n\right]^2 \leqslant \left(\langle\phi|H^2|\phi\rangle - \langle\phi|H|\phi\rangle^2\right). \quad (3)$$

The interpretation of this is that *some* eigenvalue (or spectral point, in general) is bounded in the range indicated by (3) but there is no indication as to which quantum number n (3) refers. When we incorporate S_n in (2) we assume that we know (or at least can bound) the overlap of ϕ with a *specific* eigenfunction ψ_n; the result is an error bracket around a *specific* (the nth) eigenvalue. When $S_n = 1/2$, (2) gives the same numerical bound as (3) but allows a specific eigenvalue to be bounded.

3. The Temple lower bound

We now introduce the Eckart inequality:

$$S_1^2 \geqslant \frac{E_2 - \langle\phi|H|\phi\rangle}{E_2 - E_1} \quad (4)$$

which gives a non-trivial lower bound to S_1^2 only if $\langle\phi|H|\phi\rangle < E_2$, otherwise the bound is zero or negative. Only in the non-trivial case can the Eckart inequality be properly substituted in (2) to give the Temple lower bound:

$$E_1 \geqslant \frac{E_2\langle\phi|H|\phi\rangle - \langle\phi|H^2|\phi\rangle}{E_2 - \langle\phi|H|\phi\rangle}, \quad (5)$$

where the limitation $\langle\phi|H|\phi\rangle < E_2$ carries over from the Eckart inequality. Usually E_2 is not known; instead a lower bound E_2^{low} can be substituted for E_2 in the Eckart inequality (4), which translates to the same substitution in the Temple lower bound (5):

$$E_1 \geqslant \frac{E_2^{\text{low}}\langle\phi|H|\phi\rangle - \langle\phi|H^2|\phi\rangle}{E_2^{\text{low}} - \langle\phi|H|\phi\rangle} \quad (6)$$

with the modified limitation $\langle\phi|H|\phi\rangle < E_2^{\mathrm{low}}$. A rigorous bound to E_2 is sometimes available, but when it is not available the Temple lower bound cannot be applied or must be applied with "good faith" using an estimate or experimental value for E_2. Estimation of E_2 ruins the rigor of the Temple bound so that an estimate of E_1 results instead of a lower bound to E_1. An experimental value of E_2 forces the calculation to be semi-empirical instead of independent of experiment.

4. A new lower bound

Suppose that the Hamiltonian H is related to an exactly soluble Hamiltonian H' by the relation

$$H = H' + P'. \tag{7}$$

Suppose also that ϕ is the ground-state eigenfunction of H' with eigenvalue E_1'. Then the Eckart inequality supplies two different lower bounds to $S_1^2 = \langle\phi|\psi_1\rangle^2$. The first is (4) above and the second is:

$$S_1^2 \geqslant \frac{E_2' - \langle\psi_1|H'|\psi_1\rangle}{E_2' - E_1'} \tag{8}$$

obtained by interchanging ϕ with ψ_1 and all unprimed with primed quantities (E_2' is the first excited-state eigenvalue of H'). Insertion of (8) in (2) gives the lower bound:

$$E_1 \geqslant \langle\phi|H|\phi\rangle - \left[\frac{\langle\psi_1|H'|\psi_1\rangle - E_1'}{E_2' - \langle\psi_1|H'|\psi_1\rangle}\right]^{1/2}\left[\langle\phi|H^2|\phi\rangle - \langle\phi|H|\phi\rangle^2\right]^{1/2} \tag{9}$$

when $\langle\psi_1|H'|\psi_1\rangle < E_2'$. This is to be compared with the Temple lower bound (5) since they are derived in the same fashion. In (5) E_2 must be bounded from below, while in (9) $\langle\psi_1|H'|\psi_1\rangle$ must be bounded from above. Another difficulty involved in (5) and (9) is that the integral $\langle\phi|H^2|\phi\rangle$ is needed, in addition, to the simpler integral $\langle\phi|H|\phi\rangle$; only the latter is needed in variational (upper bound) calculations.

The bound given by (9) illustrates the idea involved, but unfortunately, the only practical upper bound to $\langle\psi_1|H'|\psi_1\rangle$ we have found makes use of the unknown S_1, so that (9) still has two unknowns: E_1 and S_1. Thus (9) is not practical.

Instead we first use the upper bound to $\langle\psi_1|H'|\psi_1\rangle$ which makes use of the unknown S_1 to get a *numerical* bound to S_1^2 using (8) and then substitute this numerical bound in the following version of (2):

$$E_1 \geqslant \langle\phi|H|\phi\rangle - \left[S_1^{-2} - 1\right]^{1/2}\left[\langle\phi|H^2|\phi\rangle - \langle\phi|H|\phi\rangle^2\right]^{1/2}. \tag{10}$$

Furthermore, since $H'\phi = E_1'\phi$ and $H = H' + P'$, (10) simplifies to:

$$E_1 \geqslant E_1' - \left[S_1^{-2} - 1\right]^{1/2}\left[\langle\phi|(P')^2|\phi\rangle - \langle\phi|P'|\phi\rangle^2\right]^{1/2}. \tag{11}$$

The Temple bound can also be simplified in this case:

$$E_1 \geqslant \frac{E_2^{\text{low}} E_1' - (E_1')^2 - 2E_1' \langle \phi | P' | \phi \rangle - \langle \phi | (P')^2 | \phi \rangle}{E_2^{\text{low}} - E_1'}. \tag{12}$$

5. Intermediate problem

We introduce three Hamiltonians:

1. Base Hamiltonian H^0:

$$H^0 \psi_n^0 = E_n^0 \psi_n^0.$$

2. Intermediate Hamiltonian H':

$$H' \psi_n' = E_n' \psi_n'.$$

3. Full Hamiltonian H:

$$H \psi_n = E_n \psi_n.$$

The eigenfunctions ψ_n^0 and eigenvalues E_n^0 of the base Hamiltonian H^0 are exactly known. The ground-state eigenvalue E_1 of the full Hamiltonian H is what we wish to bound from below. The full Hamiltonian is greater than the base Hamiltonian by a positive-semidefinite perturbation P so that $H = H^0 + P$. This means that the eigenvalues E_n^0 of the base Hamiltonian are already lower bounds (though probably poor) to the eigenvalues E_n of the full Hamiltonian. Thus it may very well be possible to calculate the Temple lower bound to E_1 (which requires a lower bound to E_2) so our new lower bound formula must be able to compete with the Temple lower bound.

Suppose that we perform a linear variational calculation with H in the subspace $\mathbf{S}(N)$ which is the N-dimensional subspace spanned by the N eigenfunctions $\psi_1^0, \ldots, \psi_N^0$ of H^0 that have the lowest eigenvalues. Define $f_1, \ldots, f_N$ as the N eigenfunctions (with eigenvalues $\lambda_1, \ldots, \lambda_N$) of this variational problem. Let $\mathbf{R} = \mathbf{S}(N)^\perp$ be the orthogonal complement of $\mathbf{S}(N)$ so that the span of $\mathbf{R}$ and $\mathbf{S}(N)$ is the complete Hilbert space. We define the intermediate Hamiltonian H' as:

$$H' = H^0 + P_{\mathbf{S}(N)} P P_{\mathbf{S}(N)}, \tag{13}$$

where $P_{\mathbf{S}(N)}$ are projection operators onto the subspace $\mathbf{S}(N)$. $\mathbf{S}(N)$ and $\mathbf{R}$ are reducing spaces for H' so that for any function $f \in \mathbf{S}(N)$, $H'f \in \mathbf{S}(N)$ and for any function $f \in \mathbf{R}$, $H'f \in \mathbf{R}$. The eigenfunctions and eigenvalues for H' are then those of $H'|_{\mathbf{S}(N)}$ and $H'|_{\mathbf{R}}$. The eigenfunctions and eigenvalues of $H'|_{\mathbf{S}(N)}$ are those of the variational problem of H in $\mathbf{S}(N)$. These are readily calculated. The eigenfunctions and eigenvalues of $H'|_{\mathbf{R}}$ are those of $H^0|_{\mathbf{R}}$ since $P_{\mathbf{S}(N)} P P_{\mathbf{S}(N)}|_{\mathbf{R}} = 0$. These are known by assumption. Thus the eigenfunctions and eigenvalues of H' are completely known. In a simple case the eigenvalues of H' are

$$E_1' = \lambda_1, \quad E_2' = \lambda_2, \quad \ldots, \quad E_N' = \lambda_N, \quad E_{N+1}' = E_{N+1}^0, \quad E_{N+2}' = E_{N+2}^0, \quad \ldots .$$

This is not the only case; there can be much mixing of the variational and unused base-Hamiltonian eigenstates. It can even be that the variational ground state is not the ground state of H'; however, for our lower bound formula to work λ_1 must be E_1'. In general, we use only E_2' of the other intermediate eigenvalues and do not care if it is a variational eigenvalue $(=\lambda_2)$ or unused base-Hamiltonian eigenvalue $(=E_{N+1}^0)$. In section 7 we specialize the lower bound formula to require the simple case shown above.

The perturbation of H' to the full Hamiltonian is $P' = P - P_{\mathbf{S}(N)} P P_{\mathbf{S}(N)}$ so that $H = H' + P' = H^0 + P$. With this choice of the intermediate Hamiltonian inequalities (11) and (12) simplify to:

$$E_1 \geqslant E_1' - \left[S_1^{-2} - 1\right]^{1/2} \left[\langle \psi_1' | P^2 | \psi_1' \rangle - \langle \psi_1' | \underline{P}^2 | \psi_1' \rangle\right]^{1/2} \tag{14}$$

and

$$E_1 \geqslant \frac{E_2^{\text{low}} E_1' - (E_1')^2 - \langle \psi_1' | P^2 | \psi_1' \rangle + \langle \psi_1' | \underline{P}^2 | \psi_1' \rangle}{E_2^{\text{low}} - E_1'}, \tag{15}$$

respectively, where $\phi = \psi_1' = f_1$, and $\underline{P} = P_{\mathbf{S}(N)} P P_{\mathbf{S}(N)}$ is the matrix representation of P on the subspace $\mathbf{S}(N)$.

6. Method 1

As noted towards the end of section 5, for our lower bound formula to work, the ground state of H' must be the ground state of the variational problem: $\psi_1' = f_1$ and $E_1' = \lambda_1$. We rewrite negative $\langle \psi_1 | H' | \psi_1 \rangle$:

$$-\langle \psi_1 | H' | \psi_1 \rangle = -\langle \psi_1 | H | \psi_1 \rangle + \langle \psi_1 | P' | \psi_1 \rangle = -E_1 + \langle \psi_1 | P' | \psi_1 \rangle. \tag{16}$$

Since $E_1' \geqslant E_1$ by the variational construction of H' we have the inequality:

$$-\langle \psi_1 | H' | \psi_1 \rangle \geqslant -E_1' + \langle \psi_1 | P' | \psi_1 \rangle. \tag{17}$$

Thus we now have to bound only $\langle \psi_1 | P' | \psi_1 \rangle$ from below. We know that $\langle \psi_1 | P' | \psi_1 \rangle$ is non-positive since:

$$E_1' \geqslant E_1 = \langle \psi_1 | H' | \psi_1 \rangle + \langle \psi_1 | P' | \psi_1 \rangle \geqslant E_1' + \langle \psi_1 | P' | \psi_1 \rangle. \tag{18}$$

We write ψ_1 as

$$\psi_1 = S_0 \delta + \sum_{k=1}^{N} S_k f_k, \tag{19}$$

where δ is some normalized function in the complement of the subspace $\mathbf{S}(N)$, and S_0 and S_k are merely the (real) coefficients of the expansion of ψ_1. We then write the expectation value of P' with considerable simplification since the integral $\langle f|P'|g\rangle = 0$ for any two functions $f, g \in \mathbf{S}(N)$ and $\langle h|P'|h\rangle = \langle h|P|h\rangle$ for any function $h \in \mathbf{S}(N)^{\perp}$:

$$\begin{aligned}
0 \geqslant \langle\psi_1|P'|\psi_1\rangle &= \left\langle S_0\delta + \sum_{j=1}^{N} S_j f_j \middle| P' \middle| S_0\delta + \sum_{k=1}^{N} S_k f_k \right\rangle \\
&= S_0^2\langle\delta|P'|\delta\rangle + \sum_{j=1}^{N} S_j S_0\langle f_j|P'|\delta\rangle \\
&\quad + \sum_{k=1}^{N} S_0 S_k\langle\delta|P'|f_k\rangle + \sum_{j=1}^{N}\sum_{k=1}^{N} S_j S_k\langle f_j|P'|f_k\rangle \\
&= S_0^2\langle\delta|P|\delta\rangle + \sum_{j=1}^{N} S_j S_0\langle f_j|P'|\delta\rangle + \sum_{k=1}^{N} S_0 S_k\langle\delta|P'|f_k\rangle. \qquad (20)
\end{aligned}$$

For positive-semidefinite P we have

$$0 \geqslant \langle\psi_1|P'|\psi_1\rangle \geqslant \sum_{j=1}^{N} S_j S_0\langle f_j|P'|\delta\rangle + \sum_{k=1}^{N} S_0 S_k\langle\delta|P'|f_k\rangle. \qquad (21)$$

Since $\langle\psi_1|P'|\psi_1\rangle$ is non-positive the magnitude of the right-hand side is larger than the magnitude of $\langle\psi_1|P'|\psi_1\rangle$:

$$\left|\langle\psi_1|P'|\psi_1\rangle\right| \leqslant 2|S_1||S_0|\left|\langle\delta|P'|f_1\rangle\right| + 2\sum_{k=2}^{N}|S_k||S_0|\left|\langle\delta|P'|f_k\rangle\right|. \qquad (22)$$

Then using the Cauchy–Schwarz inequality we have:

$$\left|\langle\psi_1|P'|\psi_1\rangle\right| \leqslant 2|S_1||S_0|\langle f_1|(P')^2|f_1\rangle^{1/2} + 2|S_0|\sum_{k=2}^{N}|S_k|\langle f_k|(P')^2|f_k\rangle^{1/2}. \qquad (23)$$

Inequality (23) does not contain the unknown function δ; it was removed by the Cauchy–Schwarz inequality (22)–(23) and the positive-semidefinite character of the perturbation P ((20)–(21)). Since we must remove the unknown δ, it was thus necessary for $P \geqslant 0$. Since we are expecting $|S_1|$ to be large (close to 1) while $|S_k|$ for $k \neq 1$ to be small (close to zero), it is not unreasonable to replace $|S_k|$ for $k \neq 1$ with the upper bound $(1 - S_1^2)^{1/2}$:

$$\left|\langle\psi_1|P'|\psi_1\rangle\right| \leqslant 2|S_1||S_0|\langle(P')^2\rangle_1^{1/2} + 2|S_0|\left(1 - S_1^2\right)^{1/2}\sum_{k=2}^{N}\langle(P')^2\rangle_k^{1/2}, \qquad (24)$$

where the integral $\langle\cdot\rangle_k$ refers to f_k. We similarly replace $|S_0|$ with the upper bound $(1-S_1^2)^{1/2}$:

$$\bigl|\langle\psi_1\big|P'\big|\psi_1\rangle\bigr| \leqslant 2|S_1|\bigl(1-S_1^2\bigr)^{1/2}\bigl\langle\bigl(P'\bigr)^2\bigr\rangle_1^{1/2} + 2\bigl(1-S_1^2\bigr)\sum_{k=2}^{N}\bigl\langle\bigl(P'\bigr)^2\bigr\rangle_k^{1/2}. \tag{25}$$

We now bound $\langle\psi_1|P'|\psi_1\rangle$ by the negative of the right-hand side of (25):

$$\bigl\langle\psi_1\big|P'\big|\psi_1\bigr\rangle \geqslant -2|S_1|\bigl(1-S_1^2\bigr)^{1/2}\bigl\langle\bigl(P'\bigr)^2\bigr\rangle_1^{1/2} - 2\bigl(1-S_1^2\bigr)\sum_{k=2}^{N}\bigl\langle\bigl(P'\bigr)^2\bigr\rangle_k^{1/2}. \tag{26}$$

Coupling (26) with (8) and (17) gives:

$$S_1^2 - 1 + \frac{2|S_1|(1-S_1^2)^{1/2}\langle(P')^2\rangle_1^{1/2} + 2(1-S_1^2)\sum_{k=2}^{N}\langle(P')^2\rangle_k^{1/2}}{E_2'-E_1'} \geqslant 0. \tag{27}$$

This inequality can sometimes be used to calculate a non-trivial lower bound to S_1^2 by plotting the left-hand side as a function of S_1^2 and noting the intersections with the S_1^2 axis. When such a bound is available, it can be substituted in (14) to give a lower bound to E_1.

7. Method 2

To improve upon the inequality used to bound S_1^2 in section 6 we require that the lowest M ($1 < M \leqslant N$) eigenfunctions ψ_n' of H' are the variational eigenfunctions f_n; this is unlike in section 6 where we required only $\psi_1' = f_1$ ($M = 1$). We start by proving an Eckart-like inequality:

$$E_1' - E_{M+1}' \geqslant E_1 - E_{M+1}' = \bigl\langle\psi_1\big|H - E_{M+1}'\big|\psi_1\bigr\rangle = \bigl\langle\psi_1\big|H' + P' - E_{M+1}'\big|\psi_1\bigr\rangle. \tag{28}$$

Then expand ψ_1 in terms of the eigenfunctions ψ_k' of the intermediate Hamiltonian:

$$\begin{aligned} E_1' - E_{M+1}' - \bigl\langle\psi_1\big|P'\big|\psi_1\bigr\rangle &\geqslant \sum_{k=1}^{\infty} S_k^2\bigl(E_k' - E_{M+1}'\bigr) \\ &\geqslant \sum_{k=1}^{M} S_k^2\bigl(E_k' - E_{M+1}'\bigr) \geqslant \bigl(E_1' - E_{M+1}'\bigr)\sum_{k=1}^{M} S_k^2. \end{aligned} \tag{29}$$

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

$$S_{\mathbf{S}(N)}^2 \geqslant \sum_{k=1}^{M} S_k^2 \geqslant \frac{E_{N+1}^0 - E_1' + \langle\psi_1|P'|\psi_1\rangle}{E_{N+1}^0 - E_1'} = 1 + \frac{\langle\psi_1|P'|\psi_1\rangle}{E_{N+1}^0 - E_1'}, \tag{30}$$

where we have replaced E'_{M+1} with E^0_{N+1}. Referring to the decomposition of ψ_1 in (19) it is clear that $S_0^2 = 1 - S^2_{\mathbf{S}(N)}$, which will be equal to or superior to the bound $S_0^2 \leqslant 1 - S_1^2$ used in section 6. Thus a new bound for S_0^2 is developed using (30):

$$S_0^2 = 1 - S^2_{\mathbf{S}(N)} \leqslant -\frac{\langle\psi_1|P'|\psi_1\rangle}{E^0_{N+1} - E'_1} = \frac{|\langle\psi_1|P'|\psi_1\rangle|}{E^0_{N+1} - E'_1}. \tag{31}$$

We now use (24) as a bound for $|\langle\psi_1|P'|\psi_1\rangle|$, insert it in (31) and solve for $|S_0|$. The result is:

$$|S_0| \leqslant \frac{2|S_1|\langle(P')^2\rangle_1^{1/2} + 2(1 - S_1^2)^{1/2}\sum_{k=2}^{N}\langle(P')^2\rangle_k^{1/2}}{E^0_{N+1} - E'_1}. \tag{32}$$

This bound for $|S_0|$ cannot be *numerically* calculated without knowledge of S_1 but instead it is used *symbolically* in (24). Inequality (24) is combined with (8) and (17) to give:

$$S_1^2 \geqslant 1 - \frac{2|S_1||S_0|\langle(P')^2\rangle_1^{1/2} + 2|S_0|(1 - S_1^2)^{1/2}\sum_{k=2}^{N}\langle(P')^2\rangle_k^{1/2}}{E'_2 - E'_1}. \tag{33}$$

When (32) is used to bound $|S_0|$ in (33) the result is a single inequality with the single unknown S_1^2:

$$S_1^2 - 1 + \frac{4S_1^2\langle(P')^2\rangle_1 + 8|S_1|(1 - S_1^2)^{1/2}\langle(P')^2\rangle_1^{1/2}\sum_{k=2}^{N}\langle(P')^2\rangle_k^{1/2}}{(E'_2 - E'_1)(E^0_{N+1} - E'_1)} + \frac{4(1 - S_1^2)[\sum_{k=2}^{N}\langle(P')^2\rangle_k^{1/2}]^2}{(E'_2 - E'_1)(E^0_{N+1} - E'_1)} \geqslant 0. \tag{34}$$

When (34) provides a non-trivial lower bound to S_1^2, found by plotting the left-hand side as a function of S_1^2 and noting the intersections with the S_1^2 axis, the bound can be substituted in (14) to calculate a lower bound to E_1.

8. Example

We illustrate the two methods on the following one-dimensional Hamiltonian:

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{\text{box}} + px, \tag{35}$$

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. In accordance with section 3 we define the following:

$$H^0 = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{\text{box}}, \qquad P = px,$$
$$H' = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_{\text{box}} + pP_{\mathsf{S}(N)}xP_{\mathsf{S}(N)}, \qquad P' = px - pP_{\mathsf{S}(N)}xP_{\mathsf{S}(N)}. \tag{36}$$

In regards to (27) of method 1 and (34) of method 2, the expectations values $\langle f_k|(P')^2|f_k\rangle$ are equal to $\langle f_k|P^2|f_k\rangle - \langle f_k|\underline{P}^2|f_k\rangle$. In table 1 lower bounds to E_1 for $p = 1/2$ are shown using methods 1 and 2 of this paper and the Temple bound. Method 2 is not inferior to method 1 as is expected since the bound on $|S_0|$ in the derivation is better in method 2. The Temple bound is superior to the methods in this paper for small sized calculations ($N = 1$) and remains superior to method 1. Method 2, however, begins to best the Temple bound rather quickly.

When the perturbation is increased to $p = 3/2$ (table 2), method 1 fails to give a nontrivial bound to S_1^2, making it impossible to calculate a lower bound to E_1. The

Table 1
Lower bounds to E_1 for the slightly perturbed particle-in-a-box Hamiltonian ($p = 1/2$) are shown calculated from both methods in this paper and the Temple method. Also shown are the variational upper bound and lower bounds to S_1^2. Results are shown for three different sized calculations. $E_2^{\text{low}} = E_2^0 = 2$ for the Temple method. All energies have units hartree.

$p = 1/2$	$N = 1$	$N = 10$	$N = 50$
method 1: $S_1^2 \geqslant$	0.612	0.999988	0.999999993
method 2: $S_1^2 \geqslant$	0.612	0.999999930	0.999999999998
$E_1 \leqslant E_1' =$	1.285	1.232950164	1.232950148154
method 1: $E_1 \geqslant$	1.059	1.232946279	1.232950146152
method 2: $E_1 \geqslant$	1.059	1.232949861	1.232950148128
Temple: $E_1 \geqslant$	1.172	1.232948435	1.232950147407

Table 2
Lower bounds to E_1 for the moderately perturbed particle-in-a-box Hamiltonian ($p = 3/2$) are shown calculated from method 2 of this paper. Also shown are the variational upper bound and lower bounds to S_1^2. Results are shown for three different sized calculations. $\langle\psi_1'|H|\psi_1'\rangle > E_2^{\text{low}} = E_2^0 = 2$ so the Temple method cannot be applied. Method 1 fails to yield nontrivial bounds to S_1^2 and thus cannot be used to bound E_1. All energies have units hartree.

$p = 3/2$	$N = 1$	$N = 10$	$N = 50$
$S_1^2 \geqslant$	NA	0.999998	0.999999999981
$E_1 \leqslant E_1' =$	2.856	2.435902	2.435902312140
method 2: $E_1 \geqslant$	NA	2.435895	2.435902311697

Temple bound also fails because the lower bound on E_2 from the base Hamiltonian is too poor: we always have $\langle\psi_1'|H|\psi_1'\rangle > E_2^{\rm low} = E_2^0 = 2$. Only method 2 is able to provide a lower bound to E_1 although it too fails when $N = 1$ (for in this case it is equivalent to method 1).

9. Summary

A new method for calculating a lower bound to the ground-state eigenvalue of a Hamiltonian has been introduced. It relies on the construction of an exactly soluble intermediate Hamiltonian which is related to the matrix representation of the full operator on a special finite-dimensional subspace. A lower bound to the overlap of the lowest state of the intermediate Hamiltonian and full Hamiltonian is calculated and then used to generate a lower bound to the lowest eigenvalue of the full Hamiltonian. An explicit example is shown and the lower bound complements very well the upper bound to the ground-state eigenvalue of a one-dimensional Hamiltonian operator. Although we are quite satisfied with the performance of method 2 in this example we must remember that it is very restricted and its superior performance over the Temple bound may not be universal. Further progress must be made before a variation of these methods are suitable for a wide range of Hamiltonians; however, the current success is very encouraging.

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