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# Asymptotic behavior of the $t$ expansion

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The asymptotic behavior of a system's ground-state energy from the $t$ expansion of Horn and Weinstein has been suggested to have the form $E_1(t) = E_1 + \sum \exp(-a_n t + b_n)$. In the limit of very large $t$, this becomes $E_1(t) = E_1 + \exp(-a_1 t + b_1)$. A simple analysis shows that the parameters are $a_1 = E_2 - E_1$ and $b_1 = \ln[(E_2 - E_1)|c_2|^2/|c_1|^2]$. Functions are introduced which allow determination of $a_1, b_1$ and lower bounds to $E_1$.

**KEY WORDS:** lower bounds, $t$ expansion, asymptotic behavior

## 1. Introduction

Horn and Weinstein introduced the $t$ expansion [1], which generates the ground-state eigenfunction, $\phi_1$, of a Hamiltonian, $H$, from an initial guess, $\psi$, as follows:

$$\begin{aligned} \phi_1 &= \lim_{t\to\infty} \psi(t), \\ \psi(t) &= \frac{\mathrm{e}^{-tH/2}\psi}{\langle \mathrm{e}^{-tH/2}\psi | \mathrm{e}^{-tH/2}\psi\rangle^{1/2}} \end{aligned} \tag{1}$$

provided there is nonzero overlap between $\psi$ and $\phi_1$. This is easily seen if $\psi$ is expanded in terms of the unknown eigenfunctions, $\phi_n$, of $H$:

$$\psi(t) = \frac{\mathrm{e}^{-tH/2}\sum c_n\phi_n}{\langle \psi|\mathrm{e}^{-tH}|\psi\rangle^{1/2}} = \frac{\sum c_n \mathrm{e}^{-tE_n/2}\phi_n}{\langle \psi|\mathrm{e}^{-tH}|\psi\rangle^{1/2}} \underset{t\to\infty}{\to} \phi_1. \tag{2}$$

As $t$ increases, the low-energy states have more weight compared to the high-energy states until finally the ground state overwhelms all others as $t$ approaches infinity. Expand the trial function $\psi$ as a linear combination of the (we assume) complete set of unknown eigenfunctions, $\phi_n$, of $H$ (with corresponding eigenvalues $E_n$). The energy can then be written as

$$E_1(t) = \frac{\langle \psi(t)|H|\psi(t)\rangle}{\langle \psi(t)|\psi(t)\rangle} = \frac{\langle \mathrm{e}^{-tH/2}\psi|H|\mathrm{e}^{-tH/2}\psi\rangle}{\langle \mathrm{e}^{-tH/2}\psi|\mathrm{e}^{-tH/2}\psi\rangle} = \frac{\sum |c_n|^2 E_n \mathrm{e}^{-tE_n}}{\sum |c_n|^2 \mathrm{e}^{-tE_n}}. \tag{3}$$

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Although there have been no generalizations of the $t$ expansion to produce excited-state eigenfunctions, the $t$ expansion has been generalized to produce sums and differences of energy levels [2,3]. Since the operator $\mathrm{e}^{-tH}$ is not known for most systems, a direct calculation of $\psi(t)$ is not possible (except for $t = 0$), and therefore, $E_1(t)$ is not directly calculable.

## 2. Asymptotic form of $E_1(t)$

A number of researchers have continued the work of Horn and Weinstein [2–5]. In particular, Cioslowski [4] suggested that $E_1(t)$ could be written in the following form:

$$E_1(t) = E_1 + \sum_{n=1}^{\infty} \exp(-a_n t + b_n), \tag{4}$$

where $a_n > 0$ for all $n$. Without loss of generality, we assume that $a_m < a_n$ if $m < n$. We suggest that $E_1(t)$ asymptotically approaches $E_1$ as

$$E_1(t) = E_1 + \exp(-a_1 t + b_1). \tag{5}$$

Such treatment of an exponential series is well known in relating the ionization energy of atoms and molecules to the exponential decay of electron density; however, such an approach has been argued as non-rigorous by some [6,7]. Nevertheless, such treatment is fundamental to the $t$-expansion. The asymptotic form and constants $a_1$ and $b_1$ can be simply determined by expanding $E_1(t)$ as a ratio of power series according to (3):

$$E_1(t) = \frac{\sum |c_n|^2 E_n \exp(-E_n t)}{\sum |c_n|^2 \exp(-E_n t)}. \tag{6}$$

The limit of $E_1(t)$ is simply $E_1$, which can be derived by considering only the first terms in the power series of (6). Instead of the limit, we are interested in the asymptotic form. At large $t$, we consider only the first and second terms of the power series:

$$\begin{aligned}
E_1(t) &\approx \frac{|c_1|^2 E_1 \mathrm{e}^{-E_1 t} + |c_2|^2 E_2 \mathrm{e}^{-E_2 t}}{|c_1|^2 \mathrm{e}^{-E_1 t} + |c_2|^2 \mathrm{e}^{-E_2 t}} \\
&= \frac{|c_1|^2 E_1 \mathrm{e}^{-E_1 t} + |c_2|^2 E_1 \mathrm{e}^{-E_2 t}}{|c_1|^2 \mathrm{e}^{-E_1 t} + |c_2|^2 \mathrm{e}^{-E_2 t}} + \frac{|c_2|^2 E_2 \mathrm{e}^{-E_2 t} - |c_2|^2 E_1 \mathrm{e}^{-E_2 t}}{|c_1|^2 \mathrm{e}^{-E_1 t} + |c_2|^2 \mathrm{e}^{-E_2 t}} \\
&= E_1 + \frac{|c_2|^2 (E_2 - E_1) \mathrm{e}^{-E_2 t}}{|c_1|^2 \mathrm{e}^{-E_1 t} + |c_2|^2 \mathrm{e}^{-E_2 t}} \\
&\approx E_1 + \frac{|c_2|^2}{|c_1|^2} (E_2 - E_1) \mathrm{e}^{-(E_2 - E_1)t}.
\end{aligned} \tag{7}$$

Equating the final result with (5) shows that $a_1 = E_2 - E_1$ and $b_1 = \ln[(E_2 - E_1)|c_2|^2/|c_1|^2]$. A similar analysis can be done keeping the first $n$ terms of the power series and gives the general but incorrect results: $a_n = E_n - E_1$ and $b_n = \ln[(E_n - E_1)|c_n|^2/|c_1|^2]$. That these are incorrect is seen by their substitution in (4) for $t = 0$. Thus, our derivation of $a_n$ and $b_n$ for large $n$ is surely incorrect, although we believe the limit of $E_1$ and the asymptotic form with $a_1$ and $b_1$ is correct. For $a_1$ at least, the asymptotic slope $a_1 = E_2 - E_1$ can be rigorously proven if it is first assumed that a linear asymptotic form results:

$$\ln\left[E_1(t) - E_1\right] = -a_1 t + b_1. \tag{8}$$

The following two bounds on (8) are linear with identical slopes, $-(E_2 - E_1)$:

$$\begin{aligned}
\ln(E_1(t) - E_1) &= \ln\left(\frac{\sum |c_n|^2 (E_n - E_1) \mathrm{e}^{-E_n t}}{\sum |c_n|^2 \mathrm{e}^{-E_n t}}\right) \\
&\leqslant \ln\left(\frac{\sum |c_n|^2 (E_n - E_1) \mathrm{e}^{-E_2 t}}{|c_1|^2 \mathrm{e}^{-E_1 t}}\right) \\
&= \ln\left(\sum |c_n|^2 |c_1|^{-2} (E_n - E_1)\right) - (E_2 - E_1)t,
\end{aligned} \tag{9}$$

$$\begin{aligned}
\ln\left(E_1(t) - E_1\right) &\geqslant \ln\left(\frac{|c_2|^2 (E_2 - E_1) \mathrm{e}^{-E_2 t}}{\mathrm{e}^{-E_1 t} \sum |c_1|^2}\right) \\
&= \ln\left(|c_2|^2 (E_2 - E_1)\right) - (E_2 - E_1)t.
\end{aligned} \tag{10}$$

If the asymptotic form is linear, it must have this same slope to remain within the two bounds for infinitely large $t$. Thus, we have more justification for proposing $a_1 = E_2 - E_1$. Further justification for our proposed value of $b_1$ is just that it lies between the $t = 0$ intercepts of (9) and (10).

## 3. Discussion

Defining $f(t, \varepsilon) = \ln[E_1(t) - \varepsilon]$, it is straightforward to show that (i) if $\varepsilon$ is an upper bound to $E_1$ then $f(t, \varepsilon)$ goes to negative infinity and then for some $t$ (when $E_1(t) = \varepsilon$) becomes indeterminate; and (ii) if $\varepsilon$ is a lower bound to $E_1$ then $f(t, \varepsilon)$ asymptotically approaches the finite negative number $\ln[E_1 - \varepsilon]$. Thus, if $E_1(t)$ can be calculated to sufficient accuracy at large $t$, where $\ln[E_1(t) - E_1]$ is nearly linear, then upper bounds (in addition to $E_1(t)$) and, more importantly, lower bounds can be determined by varying $\varepsilon$ and observing the large $t$ behavior of $f(t, \varepsilon)$: negative curvature indicates an upper bound while positive curvature indicates a lower bound.

Direct measurement of the slope of the best (i.e., most linear) $f(t, \varepsilon)$ at large $t$ directly gives an estimate of the difference $E_2 - E_1$, and indirectly of $E_2$ using an accurate estimate of $E_1$ (e.g., from simply $E_1(t)$ or $\varepsilon$). Extension of the linear asymptotic form to $t = 0$ gives an estimate of the ratio $|c_2|^2/|c_1|^2$ through $b_1$. Although the difference $E_2 - E_1$ can be obtained from $f(t, \varepsilon)$, it is more readily apparent using

$$g(t,\varepsilon) = -\frac{\mathrm{d}f(t,\varepsilon)}{\mathrm{d}t} \stackrel{t\to\infty}{\longrightarrow} a_1 = E_2 - E_1. \tag{11}$$

This function $g(t, \varepsilon)$ is very similar to the function $D_0(t)$ introduced by Weinstein and Horn and generalized by Markoš and Olejník. Their limits are the same when $\varepsilon = E_1$, however, their function forms are different:

$$D_0(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\left(\ln\left(-\frac{\mathrm{d}}{\mathrm{d}t}E_1(t)\right)\right) = \frac{\langle H^3\rangle\langle H^0\rangle^2 - 3\langle H^0\rangle\langle H^1\rangle\langle H^2\rangle + 2\langle H^1\rangle^3}{\langle H^1\rangle[\langle H^2\rangle\langle H^1\rangle - \langle H^1\rangle^2]}, \tag{12}$$

$$g(t,\varepsilon) = -\frac{\mathrm{d}}{\mathrm{d}t}\bigl(\ln\bigl[E_1(t) - \varepsilon\bigr]\bigr) = \frac{\langle H^2\rangle\langle H^0\rangle - \langle H^1\rangle^2}{\langle H^0\rangle\langle H^1\rangle - \varepsilon\langle H^0\rangle^2}. \tag{13}$$

Our function $g(t, \varepsilon)$ is formally simpler, although it requires knowledge of $E_1$ to give the correct limit. However, by changing $\varepsilon$ one can determine $E_1$ at the same time one is determining $E_2 - E_1$. If and only if $\varepsilon = E_1$, then $g(t, \varepsilon)$ will be asymptotically constant at some nonzero number. By the same reasoning used for $f(t, \varepsilon)$, (i) if $\varepsilon$ is an upper bound to $E_1$ then $g(t, \varepsilon)$ goes to positive infinity and then for some $t$ (when $E_1(t) = \varepsilon$) becomes indeterminate; and (ii) if $\varepsilon$ is a lower bound to $E_1$ then $g(t, \varepsilon)$ asymptotically approaches zero. Methods to approximate $E_1(t)$ have been thoroughly discussed by Stubbins [5] and can also be applied to $f(t, \varepsilon)$ and $g(t, \varepsilon)$. Although $g(t, \varepsilon)$ gives $E_2 - E_1$ and $E_1$ directly, $f(t, \varepsilon)$ may still be useful to estimate the ratio $|c_2|^2/|c_1|^2$ at the $t = 0$ intercept using $b_1$.

We can also compare these two formulae for the energy difference with that from the Lanczos method which is a variational calculation with a two-dimensional basis set ($\psi$ and $H\psi$):

$$\begin{aligned} E_2 - E_1 \approx \Bigl(&\langle H^0\rangle^2\langle H^3\rangle^2 + 4\langle H^0\rangle\langle H^2\rangle^3 + 4\langle H^3\rangle\langle H^1\rangle^3 \\ &- 3\langle H^1\rangle^2\langle H^2\rangle^2 - 6\langle H^0\rangle\langle H^1\rangle\langle H^2\rangle\langle H^3\rangle\Bigr)^{1/2} \Big/ \Bigl(2\bigl(\langle H^0\rangle\langle H^2\rangle - \langle H^1\rangle^2\bigr)\Bigr). \end{aligned} \tag{14}$$

Comparison of (12)–(14) shows that $D_0(t)$ and the variationally-calculated energy difference both require the expectation value of $H^3$ while $g(t, \varepsilon)$ does not. In the event that expectation values of powers of $H$ are difficult to calculate, then $g(t, \varepsilon)$ can provide an estimate of the energy difference for $t = 0$ and some guess at $E_1$ by only calculating $\langle H\rangle$ and $\langle H^2\rangle$. However, the $t$ expansion is best suited for cases where such expectation values are calculable because they are used to establish large $t$ behavior of (12) and (13).

Simple tests with Hamiltonians where $\exp(-tH)$ is known, for example, the particle-in-a-box Hamiltonian, easily support our determination of $a_1$ and $b_1$ and illustrate the ability to bound $E_1$ from above and below. Figure 1 shows $f(t, \varepsilon)$ and its asymptotic form $-a_1 t + b_1$ for the trial function $\psi = (1/10)^{1/2}\phi_1 + (4/10)^{1/2}\phi_2 + (5/10)^{1/2}\phi_3$ for a particle in a box of length $\pi$ bohr and the linear function $-a_1 t + b_1$. The approximate energy $\varepsilon$ ranges from the exact $E_1$ to variations by $\pm 1\%$, $\pm 5\%$, and $\pm 10\%$ giving upper and lower bounds. Figure 2 shows the same, but with $g(t, \varepsilon)$ and its

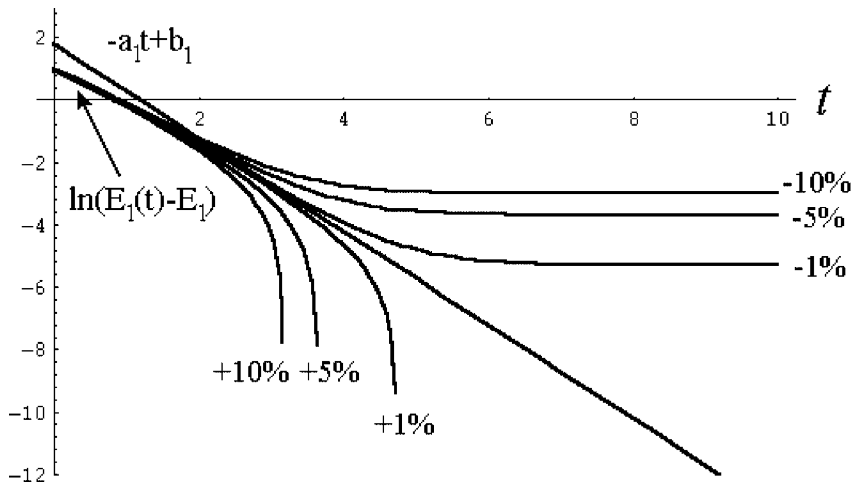


Figure 1. $f(t, \varepsilon)$ for the trial function $\psi = (1/10)^{1/2}\phi_1 + (4/10)^{1/2}\phi_2 + (5/10)^{1/2}\phi_3$ for a particle in a box of length $\pi$ bohr. The approximate energy $\varepsilon$ ranges from the exact $E_1$ to variations by $\pm 1\%$, $\pm 5\%$, and $\pm 10\%$.

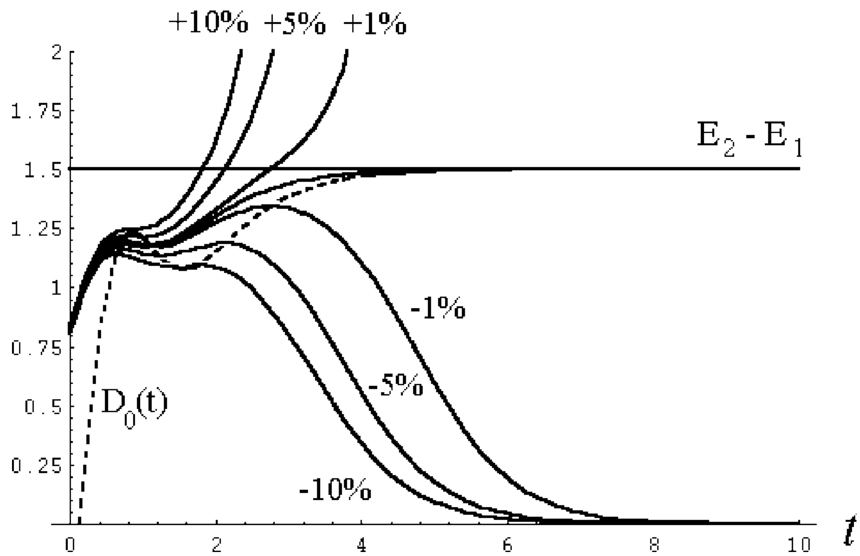


Figure 2. $g(t, \varepsilon)$ for the trial function $\psi = (1/10)^{1/2}\phi_1 + (4/10)^{1/2}\phi_2 + (5/10)^{1/2}\phi_3$ for a particle in a box of length $\pi$ bohr. The approximate energy $\varepsilon$ ranges from the exact $E_1$ to variations by $\pm 1\%$, $\pm 5\%$, and $\pm 10\%$.

asymptotic form $a_1$ in place of $f(t, \varepsilon)$ and $-a_1 t + b_1$. Also shown in figure 2 is $D_0(t)$ for comparison. In both figures, the asymptotic form is reached very quickly. Note that both $D_0(t)$ and $g(t, \varepsilon)$ do not approach $E_2 - E_1$ monotonically. This is in stark contrast to the monotonic approach of $E_1(t)$ to $E_1$ and the overlap $\langle \psi(t)|\phi_1\rangle / \langle \psi(t)|\psi(t)\rangle^{1/2}$ to unity.

The precision of the upper bounds does not allow an improvement upon the upper bounds obtained directly from $E_1(t)$; however, the presence of the lower bounds is exciting since even reasonable lower bounds are sometimes very difficult to determine. In addition, the precision is fair even at low $t$. Of course, to get lower bounds, one must be able to approximate $E_1(t)$ accurately – again see Stubbin's work [5]. Many methods to approximate $E_1(t)$ make use of expectation values of $H^n$; thus, $\langle H^2\rangle$ and $\langle H\rangle$ will probably be available and can be used to bound an eigenvalue with the variance:

$$\langle H\rangle - \sqrt{\left\langle H^2\right\rangle - \langle H\rangle^2} \leqslant E_n \leqslant \langle H\rangle + \sqrt{\left\langle H^2\right\rangle - \langle H\rangle^2}. \tag{15}$$

At first the bound (15) may seem more advantageous than ours since we need not worry whether the asymptotic form (linear or constant) has been sufficiently reached. Unfortunately, (15) can only be rigorously applied to $E_1$ if it is known that there is only one eigenvalue in this bounded range – otherwise the lower bound may apply to any one of possibly many eigenvalues in this range. Our asymptotic bounds, however, avoid this ambiguity and always give lower bounds to $E_1$ (assuming there is nonzero overlap of $\psi$ with $\phi_1$).

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