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The t-Expansion – a Short Review*

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ABSTRACT

The t-expansion is a nonperturbative calculational tool recently developed for Hamiltonian systems. A short review of the method is given. It is followed by a summary of applications to two dimensional spin systems and to four dimensional non-abelian lattice gauge theories.

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1. Introduction

In this talk I would like to review some recent work [1,2,3,4] done on the t-expansion at SLAC and Tel-Aviv University.

Consider a quantum mechanical Hamiltonian H. Suppose now that you have some initial guess $|\psi_0\rangle$ for the ground state wavefunction. $|\psi_0\rangle$ can be expanded in a complete set of the eigenstates of H:

$$|\psi_0\rangle = \sum_n c_n |n\rangle ,$$

where

$$H|n\rangle = \epsilon_n |n\rangle \quad and \quad \sum_n |c_n|^2 = 1$$

It is easy to write down a wavefunction which is a better approximation to the ground state. Let us apply the operator $e^{-tH/2}$ to $|\psi_0\rangle$ and normalize the result:

$$|\psi_t\rangle = \frac{1}{\langle\psi_0| e^{-tH} |\psi_0\rangle^{1/2}} e^{-tH/2} |\psi_0\rangle , \tag{1.1}$$

$|\psi_t\rangle$ can again be expanded in the eigenstates of H:

$$|\psi_t\rangle \quad \alpha \quad \sum_n c_n e^{-\epsilon_n t/2} |n\rangle . \tag{1.2}$$

For any finite value of t, the contribution of the excited eigenstates $|n\rangle$, $n \neq 0$ is suppressed relative to the exact ground state $|0\rangle$ by exponential factors of the form $e^{-t(\epsilon_n - \epsilon_0)}$. Clearly, as $t \to \infty$, $|\psi_t\rangle$ converges to the true vacuum, provided that the initial state $|\psi_0\rangle$ has nonzero overlap with $|0\rangle$. The overlap can be very small, but the normalization factor in (1.1) compensates for that. The wavefunction is *contracted* onto the lowest eigenstate of the Hamiltonian.

In the same fashion, the expectation value

$$O(t) \equiv \langle \psi_t |\ \hat{O}\ | \psi_t \rangle$$

of any operator $\hat{O}$ converges to its ground state expectation value as $t \to \infty$. In particular,

$$E(t) \ \equiv \ \frac{\langle \psi_0 |\ H e^{-tH}\ | \psi_0 \rangle}{\langle \psi_0 |\ e^{-tH}\ | \psi_0 \rangle} = \langle \psi_t |\ H\ | \psi_t \rangle \ \to \ E_{GS}$$

For any finite value of t, E_{GS} is an upper bound on the ground state energy, since it is the expectation value of the Hamiltonian in a properly normalized trial wave function.

2. Cluster Expansion

For the sake of definiteness, consider again

$$E(t) \equiv \frac{\langle \psi_0 |\ H e^{-tH}\ | \psi_0 \rangle}{\langle \psi_0 |\ e^{-tH}\ | \psi_0 \rangle}. \tag{2.1}$$

Eq. (2.1) is reminiscent of the expression for the expectation value of a Hamiltonian that one encounters in classical statistical mechanics, the numerator being the quantum mechanical analogue of a partition function. As we shall see, this is a useful analogy and we will be able to use some of the methods familiar from statistical mechanics in order to calculate quantities of interest.

So far, we have seen that E(t) converges to the true vacuum energy as $t \to \infty$. However, in (2.1) H appears in the exponential. In general we do not know how to exponentiate quantum Hamiltonians, so we must devise some systematic approximation procedure which will yield an accurate estimate of $E(t)$. We start

with a power series expansion of the exponential

$$e^{-tH} = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} H^n$$

in both the numerator and denominator of (2.1) . After collecting powers of t, we obtain an expression for $E(t)$:

$$E(t) = \sum_{i=0}^{\infty} a_i \frac{(-t)^i}{i!}$$

where a_i's are defined in terms of moments of H, $\langle\psi_0|\ H^m\ |\psi_0\rangle$.

At this point, it is important to notice that $\langle\psi_0|\ H^m\ |\psi_0\rangle$ scales with the volume V of the system like V^m. On the other hand, $E(t)$ being the expectation value of H in some properly normalized wavefunction, must scale like V. Thus, the a_i's must also scale like V. In order for that to happen, all higher powers of the volume must cancel in the expressions defining a_i's in terms of moments of H.

In fact, the coefficients a_i are the *connected matrix elements* of H:

$$E(t) = \frac{\langle\psi_0|\ He^{-tH}\ |\psi_0\rangle}{\langle\psi_0|\ e^{-tH}\ |\psi_0\rangle} = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} \langle\, H^{n+1}\,\rangle^c \tag{2.2}$$

where, $\langle\, H^{n+1}\,\rangle^c$ is defined recursively,

$$\langle\, H^{n+1}\,\rangle^c = \langle\psi_0|\ H^{n+1}\ |\psi_0\rangle - \sum_{p=0}^{n-1} \binom{n}{p} \langle\, H^{p+1}\,\rangle^c\ \langle\psi_0|\ H^{n-p}\ |\psi_0\rangle$$

Not surprisingly, if we express the series (2.2) in terms of diagram expansion, the connected matrix elements will correspond to connected diagrams.

In analogy with (2.2) we can write the expectation value of any operator O as:

$$\langle OH^m\rangle^c = \langle OH^m\rangle - \sum_{p=1}^{m} \binom{m}{p} \langle OH^{m-p}\rangle^c \langle\psi_0| H^p |\psi_0\rangle \ , \tag{2.3}$$

where $\langle OH^m\rangle$ is defined to be

$$\langle OH^m\rangle = \frac{1}{2^m} \sum_{p=0}^{m} \binom{m}{p} \langle\psi_0| H^p O H^{m-p} |\psi_0\rangle \, . \tag{2.4}$$

3. Padé Approximants

In practice we can calculate the expansion

$$O(t) = \sum_{n=0}^{N} \frac{1}{n!} a_n (-t)^n \tag{3.1}$$

to some finite order N. The question then is how to extract the limiting value of the function $O(t)$ for $t \to \infty$ from its Taylor series expansion around $t = 0$. We know that $O(t) \to const.$ as $t \to \infty$. From (1.2) we expect $O(t)$ to approach its limiting value exponentially in t. We may therefore make use of Padé approximants which are a well known technique for extracting the behavior of a function of the type (3.1) away from the origin of its power series expansion:

Any series of the type $S_N = \sum_{i=0}^{N} a_i x^i$ can be approximated by a ratio of two polynomials:

$$\sum_{i=0}^{N} a_i t^i = \frac{p_0 + p_1 t^1 + p_2 t^2 \ldots + p_L t^L}{q_0 + q_1 t^1 + q_2 t^2 \ldots + q_M t^M} + O(t^{N+1}); \quad N = L + M$$

Such a ratio is referred to as the $[L/M]$ Padé . In principle, if the function which we wish to approximate converges to a constant as $t \to \infty$, in order to reconstruct that behavior we should use the so called *diagonal* Padé , i.e., $L = M$, and watch for convergence of the series , $[M/M] \quad M = 1, 2, 3 \ldots$.

At this point we encounter a generic problem which is common to all functions of the type $O(t) = \langle\psi_t|\ \mathcal{O}\ |\psi_t\rangle$. To illustrate the problem, let us consider the power series for hyperbolic tangent of t:

$$\tanh(t) = t - \tfrac{1}{3}t^3 + \tfrac{2}{15}t^5 - \tfrac{17}{315}t^7 + \tfrac{62}{2835}t^9 - \tfrac{1382}{155925}t^{11} + \tfrac{21844}{6081075}t^{13} - \ldots \qquad (3.2)$$

$\tanh(t)$ goes to a constant as $t \longrightarrow \infty$ and so our first guess would be to use a diagonal Padé . But the series for $\tanh(t)$ contains only *odd* powers of t so that the diagonal Padé does not exists ! We have to use some other method. The method which works very well in practice is the following.

We form non-diagonal $[L/M]$ *D–Padé* approximants to the derivative $\partial O(t)/\partial t$, taking $M \geq L+2$. Such a *D–Padé* goes to zero as $t \longrightarrow \infty$ as expected of $\partial O(t)/\partial t$ and is integrable in t since $M - L \geq 2$. $O(t)$ is then obtained by integrating the Padé with respect to t:

$$O(t) = \int_0^t O'(\tau)_{[L/M]} d\tau \qquad (3.3)$$

In (3.3) the integrand is a ratio of two polynomials, and the denominator may in general have zeros on the positive real axis. In such a case the integrand will have poles along the path of integration. Nevertheless, the integral can still be defined using the *Cauchy principal value*:

$$\int \frac{f(x)}{x - x_0 \mp i\epsilon} dx = P \int \frac{f(x)}{x - x_0} dx \pm i\pi f(x_0)\ . \qquad (3.4)$$

$O(t)$ is an expectation value of a hermitian operator and therefore must be real. Consequently, in what follows we take the real part of the integral:

$$O(t) = P \int_0^t O'(\tau)_{[L/M]} d\tau \qquad (3.5)$$

In our case $M \geq L+2$ and it turns out that the integral in (3.5) can easily be

computed analytically. For our test case, $O(t) = \tanh(t)$ we have,

$$\frac{d}{dt}\tanh(t) = 1 - t^2 + \frac{2}{3}t^4 - \frac{17}{45}t^6 + \frac{62}{315}t^8 - \frac{1382}{14175}t^{10} + \frac{21844}{467775}t^{12} - \ldots \qquad (3.6)$$

Following the procedure described above we can recover the limiting value of $\tanh(t)$ as $t \longrightarrow \infty$ by forming Padés of the series (3.6) and integrating with respect to t from 0 to ∞. The table below shows the results of this integration,

$$\mathcal{P}\int_0^\infty \tanh'(t)_{[L/M]}dt \qquad (3.7)$$

for all possible values of L and M.

M	L					
	0	1	2	3	4	5
2	1.5698					
3	–	–				
4	1.0701	1.0701	0.83143			
5	–	–	–	–		
6	1.0142	1.0142	0.98918	0.98918	1.0409	
7	–	–	–	–	–	–
8	1.0032	1.0032	0.99860	0.99860	1.0018	
9	–	–	–	–		
10	1.0008	1.0008	0.99977			
11	–	–				
12	1.0002					

Empty entries correspond to either $M < L + 2$ or $L + M > 12$. A "–" means that the Padé does not exist.

The convergence of the approximants to the limiting value of 1 is clear. It is also pretty obvious from this exercise that in order to get accuracy of the order of 1% one needs to have at least order of 8 terms in the series.

In practice we have found that yet another enhancement to the usual Padé technique yields very good results. Usually we deal with Hamiltonians of the

form $H = H_0 + \alpha V$. Our choice of $|\psi_0\rangle$ was usually the lowest eigenstate of H_0. Therefore the coefficients in the t power series will be polynomials in α. We are interested in some observable O as function of α: $O(\alpha) = \lim_{t\to\infty} O(\alpha, t)$.

We will proceed as follows: given a series for $O(\alpha, t)$, i.e.

$$O(\alpha, t) = \sum_{i=0}^{N_t} \sum_{j=0}^{N_y} c_{ij}\, t^i \alpha^j \tag{3.8}$$

we differentiate it to obtain

$$\frac{\partial^2 O}{\partial \alpha \partial t}(\alpha, t) = \sum_{i=0}^{N_t} \sum_{j=0}^{N_y} ij\, c_{ij}\, t^{i-1} \alpha^{j-1}. \tag{3.9}$$

Next, we form Padé approximants with respect to the variable t to obtain

$$\bar{O}_{\alpha t}^{[L/M]}(\alpha, t) \tag{3.10}$$

and integrate this with respect to t to obtain

$$\frac{\partial \bar{O}^{[L/M]}}{\partial \alpha}(\alpha) = \int_0^\infty dt'\, \bar{O}_{\alpha t}^{[L/M]}(\alpha, t'). \tag{3.11}$$

Finally, we use this approximation to $\partial O/\partial \alpha$ to reconstruct $O(\alpha)$ by integration,

$$O(\alpha) = \int_0^\alpha d\alpha' \frac{\partial \bar{O}^{[L/M]}}{\partial \alpha}(\alpha') \ . \tag{3.12}$$

We have found that for the class of functions with which we are dealing this is the simplest and best way to proceed.

4. What Has Been Done ?

Obviously, the method as we have discussed it is only partially analytic. In particular, unlike the situation in perturbation theory, we are not expanding in a small parameter and have no control over the rate of convergence of the technique. Also, the use of Padé approximants introduces an element of uncertainty into the result. At present the only thing we know to do is to apply this technique to a variety of problems and see how well it works. The problems which have been discussed to date are:

1. Lattice spin systems in 1+1 dimensions.[1]

   The two dimensional non-linear sigma model exhibits many of the interesting phenomena found in four dimensional gauge theories. Thus the results for lattice Heisenberg model are a good testing ground for the method. For this case the t-expansion was carried out up to t^7, with a rather modest computational effort. The ground state energy was then reconstructed using Padé approximants, as described beforehand. The result was between 0.27% and 0.75% off the exact answer. This should be compared with Anderson's[5] calculation of this quantity in the spin-wave approximation which is on the order of 4%.

   For the two-dimensional Ising model the expansion was carried out up to t^6 and both the ground state energy and the magnetization were reproduced with high accuracy.

2. $SU(2)$–lattice gauge theory in 3+1 dimensions.[2]

   We have computed the vacuum energy density, specific heat, string tension σ, mass of the lowest lying 0^{++}-glueball M and the ratio $R = M^2/\sigma$. Our computations converge best for the energy density, specific heat and R, and these quantities exhibit behavior which agrees with what we expect on general grounds and what is known from Euclidean Monte Carlo calculations. In particular we see a broad lump in the specific heat and determine $\sqrt{R}$ to be $\sqrt{R} = 3.5 \pm .2$, a value which lies in the ballpark of values obtained

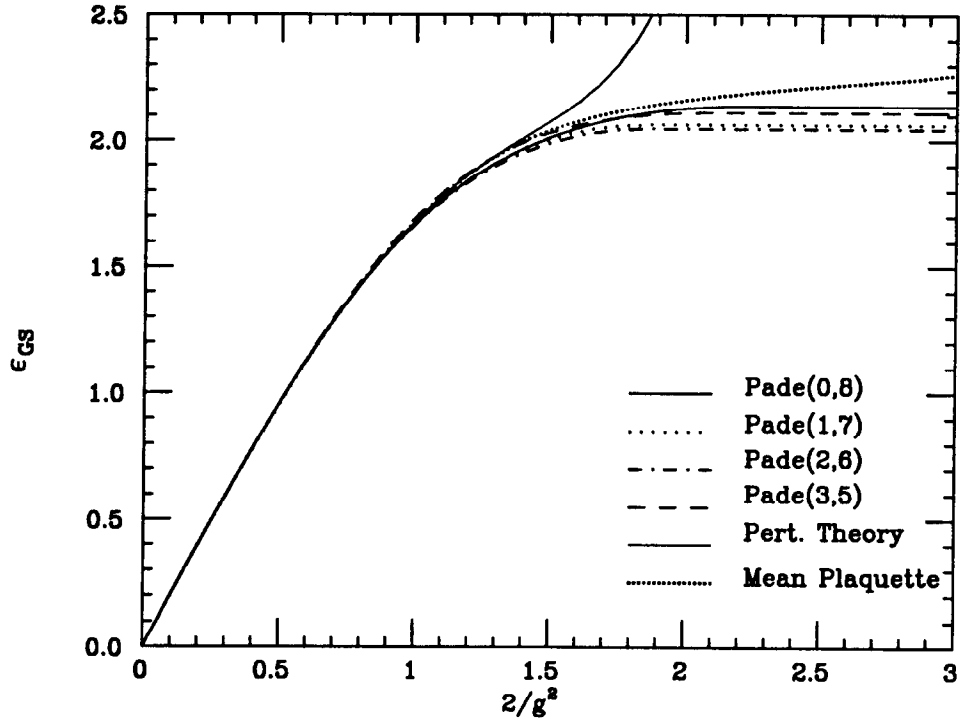

FIG. 1. Curves showing the energy density $\mathcal{E}(y)$ obtained by integrating the corresponding $[L/M]$–Padé approximants to $d\mathcal{E}/dy$. $SU(2)$, D=3+1.

from Monte Carlo calculations. Our previously published results for these quantities are shown in figures 1 to 3.

3. $SU(3)$–lattice gauge theory in 3+1-dimensions.[3]

   The calculation here is much more complicated than for $SU(2)$. The expansion for vacuum energy has been carried out up to t^7. The same series was used to obtain the mass M of the lowest lying 0^{++}-glueball to order t^5. Evaluation of the string tension σ to the same order in allows one to construct the ratio $R = M^2/\sigma$. This yields a dimensional result for M which is consistent with Monte-Carlo analyses. Higher t-series are needed to obtain an accurate estimate for M.

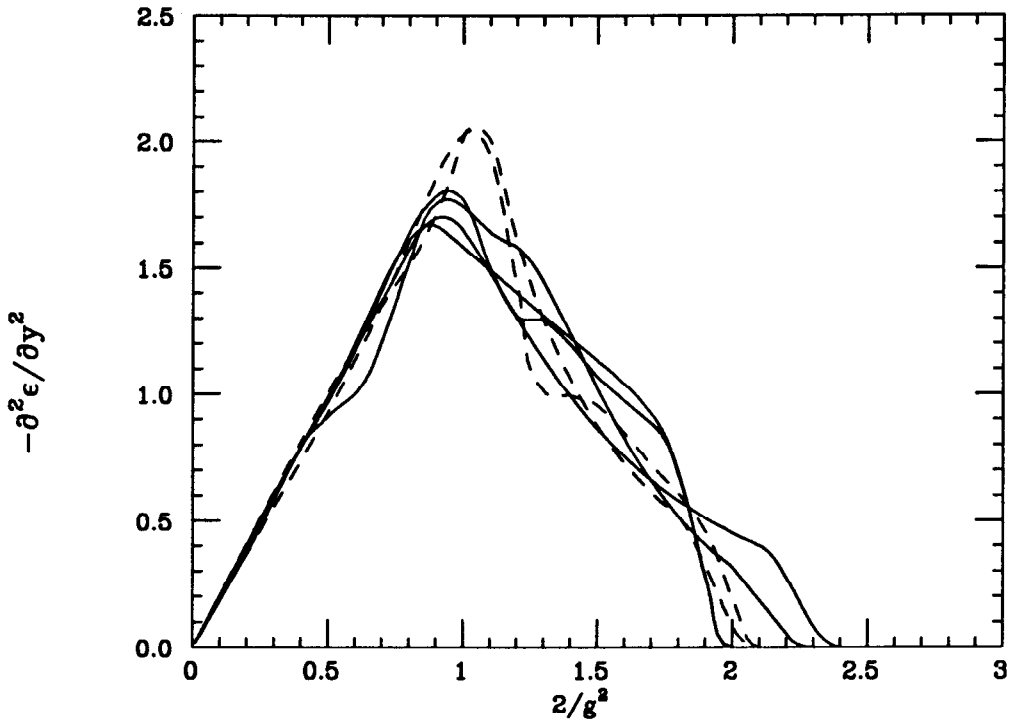

FIG. 2. Plot of "specific heat", $-d^2\mathcal{E}/dy^2$ for various D–Padé approximants.
Continuous lines correspond to $[L/(8-L)]$ Padé-s.
Dashed lines correspond to $[L/(5-L)]$ Padé-s. $SU(2)$, D=3+1.

4. Simple quantum mechanical models like the one plaquette gauge theory.[4] It is important to know how many terms in the t-expansion one needs in order to get results accurate up to a few percent. From the $SU(2)$ pure gauge calculation we learn that we must go beyond t^9. To find out how much farther one needs to go, one can look at an exactly soluble model - one plaquette Hamiltonian:

$$H = \frac{g^2}{2}\left[E_1^2 + E_2^2 + E_3^2 + E_4^2\right] + \frac{2}{g^2}\left[2 - \mathrm{Tr}\, U_{plaq}\right] \qquad (4.1)$$

where $U_{plaq} = U_1 U_2 U_3^\dagger U_4^\dagger$. Comparison of the t-expansion results for this

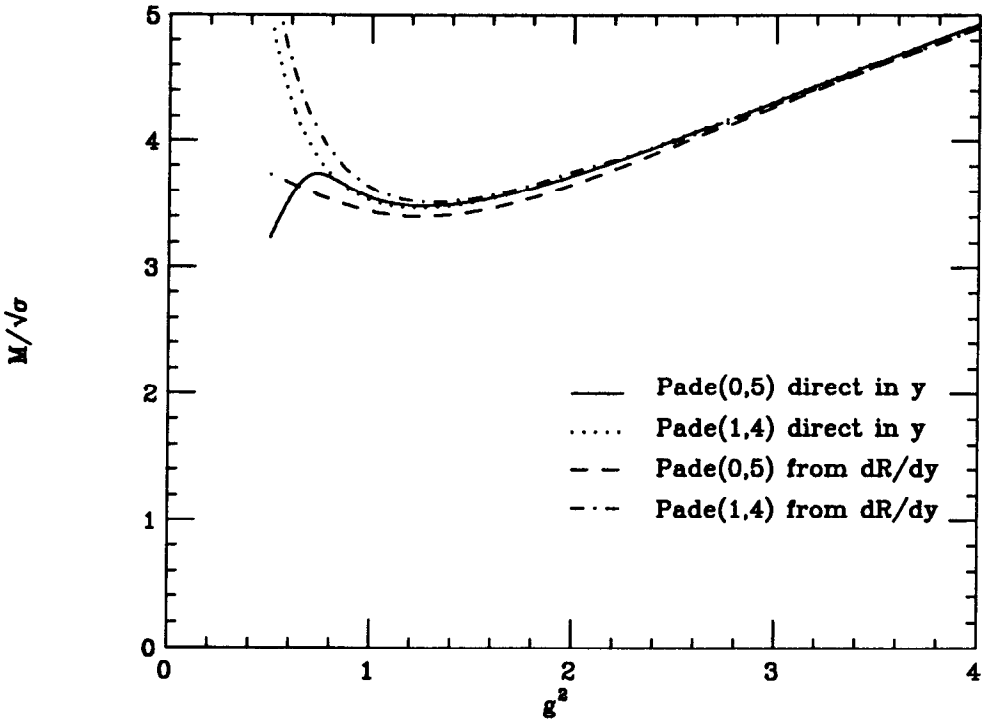

FIG. 3. A plot of the approximants to $\sqrt{R(g^2)} = M/\sqrt{\sigma}$ obtainable from the full series in t. $SU(2)$, D=3+1.

model with the exact answer shows that at order t^9 the ground state energy exhibits the same sort of inaccuracy for $g^2 \leq 1$ as the infinite lattice. To obtain accurate results, with relative errors about 10^{-3}, one needs to carry the expansion up to t^{13}. We therefore expect the infinite lattice calculation to require at least a comparable number of terms in the t series, in order to yield accurate results. The connected matrix elements can probably be computed to such a high order only with the help of computer algebra. Suitable algorithms are currently being studied.

5. bi-state contraction

Here I would like to describe briefly an extension[1] of the formalism, which might possibly facilitate the approach to the weak coupling regime.

Suppose that our Hamiltonian can be written as $H = H_0 + g^2 V$ where g^2 is a coupling constant. In many cases we can diagonalize H exactly in both the $g^2 \to 0$ and $g^2 \to \infty$ limit.

Let $|\psi\rangle$ be the lowest eigenstate of H_0 and $|\chi\rangle$ be the ground state in the strong coupling limit.

For some general value of g^2 we may expand both $|\psi\rangle$ and $|\chi\rangle$:

$$|\psi\rangle = \sum_n c_n |n\rangle , \quad \sum_n |c_n|^2 = 1$$

$$|\chi\rangle = \sum_m d_m |m\rangle , \quad \sum_m |d_m|^2 = 1$$

where

$$H |n\rangle = \epsilon_n |n\rangle$$

Now, in complete analogy with (2.1) , we may define

$$E(t)_{\chi\psi}(t) \equiv \frac{\langle\chi| H e^{-tH} |\psi\rangle}{\langle\chi| e^{-tH} |\psi\rangle} = \frac{\sum_{n=0}^{\infty} d_n^* c_n e^{-\epsilon_n t} \epsilon_n}{\sum_{n=0}^{\infty} d_n^* c_n e^{-\epsilon_n t}} \tag{5.1}$$

From (5.1) it is obvious that as $t \to \infty$ $\quad E_{\chi\psi}(t) \to E_{GS}$. Both $E(t)$ and $E_{\chi\psi}(t)$ converge to the vacuum energy in the formal sense. However, in (5.1) we are performing *simultaneous* expansion around the weak and strong coupling vacua. Thus, for intermediate values of the coupling constant, we have a good reason to expect $E_{\chi\psi}$ to converge more rapidly to the exact value of E_{GS} when only finite number of terms in the t-expansion is taken. On the other hand, the calculation of the higher order terms in this approach is usually more complicated. It remains to be seen whether the trade-off is really there.

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