Methods of extrapolating the t-expansion series

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(Received 16 February 1988)

We present four new methods in addition to the standard methods of extrapolating the t-expansion series and make a comprehensive comparison of these procedures by applying them to the t series for three quantum systems. We have found that by writing the series as a ratio of decreasing exponentials it is possible to devise methods that are significantly more accurate than the standard methods for low-order series. By studying the function $t(E)$ we have found a procedure that is more accurate than the standard methods for all t-series orders in two of the test systems.

I. INTRODUCTION

The t expansion[1] is a nonperturbative method that calculates ground-state expectation values of many-body systems described by lattice Hamiltonians. The idea behind the method is that for any variational state $|\psi_0\rangle$, the normalized state

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

is a better approximation to the true vacuum for any finite value of t. As long as the initial state $|\psi_0\rangle$ has an overlap with the true ground state, quantities such as

$$O(t)=\langle\psi_t|O|\psi_t\rangle$$

are guaranteed to converge to their true ground-state expectation values in the limit $t\rightarrow\infty$.

Of particular interest is the ground-state energy density

$$E(t)=\frac{\langle\psi_0|He^{-tH}|\psi_0\rangle}{\langle\psi_0|e^{-tH}|\psi_0\rangle} \tag{1.2}$$

which can be written as a power series in the parameter t:

$$E(t)=\sum_{n=0}^{\infty}\frac{(-t)^n}{n!}\langle H^{n+1}\rangle^c=I_1-I_2t+I_3\frac{t^2}{2!}+\cdots .$$

The coefficients $\langle H^{n+1}\rangle^c$ are connected moments of the Hamiltonian and are defined recursively as

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

In order to calculate the limit $E(t\rightarrow\infty)$ for the power series one must know all of the connected moments, which is not possible in any real system. All of the knowledge that we have about the function $E(t)$ is its finite power series

$$E(t)=\sum_{n=0}^{N}\frac{(-t)^n}{n!}I_{n+1} \tag{1.3}$$

and the following information.

(1) $E(t)$ is a monotonically decreasing function. This is because the derivative of Eq. (1.2) is $-(\Delta E)^2$.

(2) $d^2E/dt^2\geq 0$. This can be seen by writing the mass gap (the difference between the first excited state and the ground state) as

$$M(t)=-\frac{g^2}{2}\frac{\partial^2E/\partial t^2}{\partial E/\partial t} ,$$

where g is the coupling constant of the theory.

(3) $E(t)$ rapidly goes to a constant, so dE/dt goes to zero as t goes to infinity.

(4) dE/dt is integrable.

Since we only have a finite power series we know that $E(t)$ will not be well behaved for large values of t. Therefore we must have criteria for knowing what t to trust the series for and a means of extrapolating the series for larger t.

Until recently, the only procedure used to extrapolate the t series were the Padé and D-Padé methods.[1,2] These methods are reliable for series with moderate to high orders of t, but become unreliable for low orders. In fact, the more accurate of the two methods, the D-Padé method, can only be used for series of order greater than 2. This paper examines several new practical procedures for approximating the t-expansion series for large values of t. First we discuss the three quantum-mechanical systems to which the t expansion will be applied. Then we examine in detail the approximation methods and compare the results of each.

II. QUANTUM SYSTEMS

A. The harmonic oscillator

In this test system, we express the partition function explicitly by expanding $|\psi_0\rangle$ in the basis of the energy eigenstates of the system. The partition function $Z(t)$ is defined in terms of the energy as

$$E(t)=-\frac{d}{dt}\ln Z(t)=\frac{-\frac{d}{dt}Z(t)}{Z(t)} . \tag{2.1}$$

Comparing this with Eq. (1.2) gives

$$Z(t)=\langle\psi_0|e^{-Ht}|\psi_0\rangle\ . \tag{2.2}$$

By writing $|\psi_0\rangle=\sum_{n=0}^{N}b_n|n\rangle$ with $H|n\rangle=(n+\frac{3}{2})|n\rangle$ and $b_n^2=e^{-(n+1)^2\gamma}$ we get

$$Z(t)=\sum_{n=0}^{N}e^{-(n+1)^2\gamma}e^{-(n+3/2)t},\quad Z(0)\equiv 1\ . \tag{2.3}$$

Large γ corresponds to the system having a very large probability of being in the ground state; small γ corresponds to the system having nearly equal probability of being in any of the eigenstates. For practical reasons N, the number of states in which $|\psi_0\rangle$ is expanded in terms of, is chosen here to be no bigger than 50. From (2.3) the asymptotic value of the vacuum energy is analytically given as $1\frac{1}{2}$. We applied our methods to this test system by writing $Z(t)$ and $E(t)$ as power series to see how well our methods recover the true vacuum energy.

B. The U(1) one-plaquette lattice gauge theory

The application of the t expansion to lattice gauge theories is discussed in detail in Refs. 1 and 2. For periodic QED in $2+1$ space-time dimensions, the t expansion is used to calculate the vacuum energy

$$E(t)=\frac{\langle\psi_0|He^{-t\bar{H}}|\psi_0\rangle}{\langle\psi_0|e^{-t\bar{H}}|\psi_0\rangle}\ , \tag{2.4}$$

where H is the Kogut-Susskind Hamiltonian:

$$H=\frac{g^2}{2}\left[\bar{H}+\frac{y^2}{2}N_p\right]\ , \tag{2.5}$$

$$\bar{H}=\sum_l E_l^2-\frac{y^2}{4}\sum_p(U_p+U_p^\dagger)\ , \tag{2.6}$$

g is the coupling constant, $y=2/g^2$, and N_p is the number of plaquettes (usually infinite). U_p is the ordered product of the link operators U_l which are elements of the U(1) group. Since E_l are their conjugate variables, the first term of (2.6) is the Casimir operator of the U(1) group on every link. The calculation of $E(t,y)$ is based on the vacuum of the strong-coupling limit so that $E_l|\psi_0\rangle=0$. For $N_p=1$ there are four links to be summed on in (2.6). This model is a particularly good example on which to test our methods because the exact answer may be found by diagonalizing the Hamiltonian in a large basis of strong-coupling states. The weak-coupling limit for the one-plaquette system is $E(g^2=0)=1$. We will analyze the vacuum energy density to order t^8, as calculated by Horn.[3]

C. The SU(2) lattice gauge theory

In $3+1$ dimensions, the Hamiltonian for this model is

$$H=\frac{g^2}{2}\left[\sum_l \mathbf{E}_l^2+x\sum_p(2-\mathrm{tr}U_p)\right]\ , \tag{2.7}$$

where $x\equiv 4/g^4$. The link operators $\mathbf{E}_l$ and U_l are the color-electric field and the SU(2) group elements satisfying

$$[E_l^a,U_{l'}]=\frac{\sigma^a}{2}U_l\delta_{ll'}\ . \tag{2.8}$$

Out of every four links that compose a plaquette one constructs the product $\mathrm{tr}U_p=\mathrm{tr}(U_1U_2U_3^{-1}U_4^{-1})$. The state $|\psi_0\rangle$ is taken to be the ground state of the strong-coupling Hamiltonian so that

$$\mathbf{E}_l|\psi_0\rangle=0\ .$$

Again, we will analyze the series for the vacuum energy density to order t^8 as calculated by Mathews, Snyderman, and Bloom.[4]

III. METHODS AND RESULTS

As stated in the Introduction, these methods are used in conjunction with the t expansion to calculate ground-state energies of quantum-mechanical systems. The Padé, D-Padé, and connected-moment-expansion (CMX) methods have been documented and we include them for completeness and comparison. In this section we apply these various methods to the t-expansion series up to order t^8 for three quantum systems and evaluate the merits of each.

A. Padé method

The standard procedure for extending the range for a series is to express it as a ratio of polynomials with orders L and M,

$$E(t)=\frac{P_L(t)}{Q_M(t)}\ , \tag{3.1}$$

where $L+M$ is less than or equal to the order of $E(t)$. Since we expect $E(t)$ to tend smoothly to its exact value as $t\to\infty$, only diagonal approximants are used. However, if we are satisfied with the computation of $E(t)$ for a finite value of t, then we may use all approximants with $M\geq L$. None of these approximants, including the diagonal Padé, are guaranteed to behave properly for all values of t. The usual criterion used to determine the range in which the Padé calculation can be trusted is that several Padé approximants must agree over this range for a given value of $L+M$. We will refer to this as the Padé criterion. Generally, for a given value of $L+M$ one of the approximants (usually the diagonal Padé) will have a larger range than the others; but with the Padé criterion there is no way of determining this. This is particularly true if there are very few approximants. Also in its stated form, it is difficult to implement the Padé criterion in a machine calculation.

We present a simpler and more accurate cutoff for $E(t)$ and the Padé approximants by trusting the series only to where $dE(t)/dt$ becomes positive or zero for the first time, or when the second derivative of $E(t)$ becomes negative or zero for the first time. Figure 1 represents typical Padé approximants for the energy density t series, and exhibits the general features discussed above. For this di-

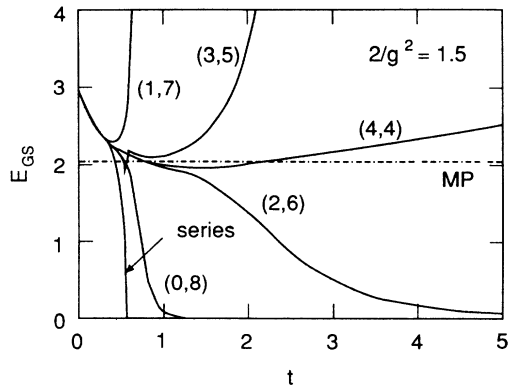

FIG. 1. The vacuum-state energy density for the eighth-order SU(2) series vs the parameter t. L,M refers to the $P_L(t)/Q_M(t)$ approximant. The MP graph is the mean plaquette exact upper bound obtained in Ref. 8. Not shown is that all of the off-diagonal approximant goes to zero for large t.

agram, our new criteria indicate that the largest value we can trust the [4,4] Padé approximant is to $t \approx 1.5$ and that we can only trust the series up to $t \approx \frac{3}{10}$. In general a spurious pole similar to the one in the [3,5] Padé approximant near $t = \frac{7}{10}$ would be mistaken as the cutoff point in a computer program; so when using the cutoff procedure we must avoid values of t near the roots of $Q(t)$ by omitting these points and interpolating the function using smoothly joined parabolas.

In Figs. 2–4 we compare the low- and high-order results of prior extrapolation methods (Padé, D-Padé, and CMX) applied to the harmonic oscillator, U(1), and SU(2) systems for various values of the coupling constant. Wherever there are numerous approximants for a given order, such as in the Padé and D-Padé methods, we present the more accurate results. In all the Padé results we have applied the cutoff procedure to the Padé approximants. To compare the results for no extrapolation, we also include the results of making a cutoff to the series directly. Since it is a Taylor series about $t = 0$, the t series

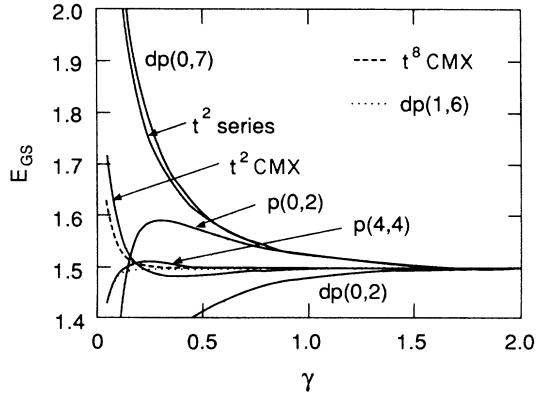

FIG. 2. The first three methods (Padé, D-Padé, and CMX) are applied to the harmonic oscillator. The [4,4] Padé approximant agrees well with the exact answer up to $\gamma = 0.2$, which corresponds to roughly eight coefficients in Eq. (2.3) greater than 10^{-6}. t^n refers to approximating the nth-order series.

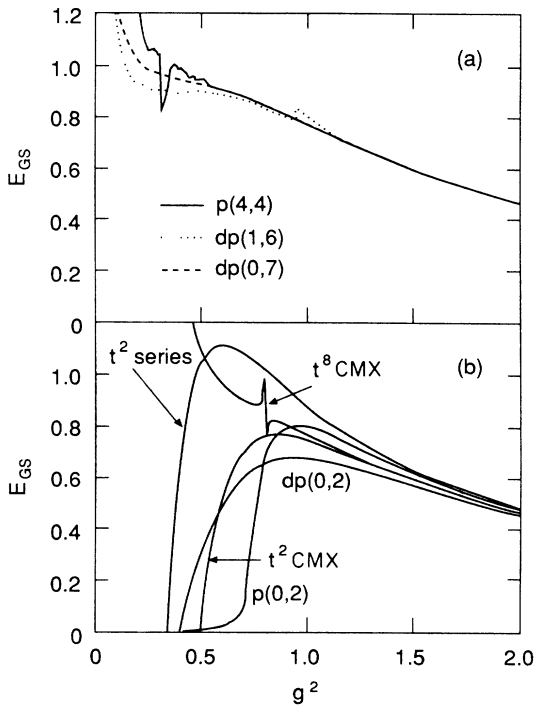

FIG. 3. The results of the first three methods on the U(1) system. The maximum of $dE(y)/dy$ is the cross-over region from strong to weak coupling, and occurs near $g^2 = 1.2$. The bump in the D-Padé [1,6] graph is due to dE/dt not vanishing sufficiently fast for those values of the coupling constant.

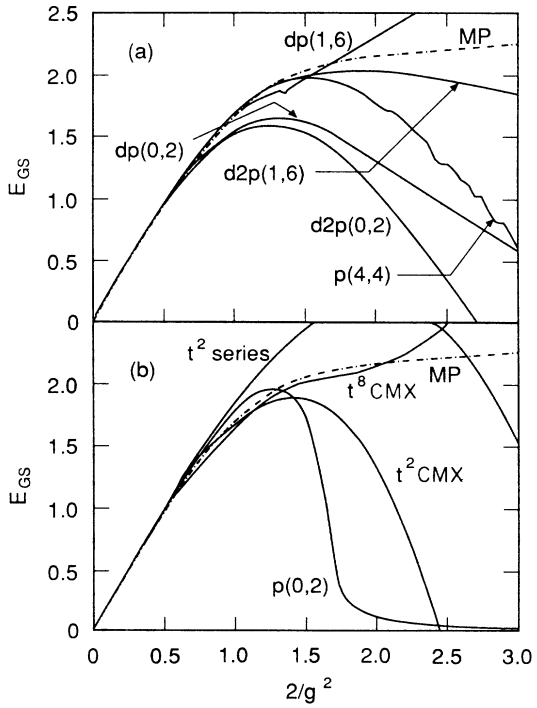

FIG. 4. The results of the first three methods on the SU(2) series. The MP graph has a weak-coupling limit of $\sqrt{6}$. Most of the approximants are in rough agreement with each other up to $y = 1.5$, where $dE(y)/dy$ becomes negative.

is only valid for small t, so we expect the cutoff procedure applied to the t series not to show any drastic improvements for moderate increases in the order. The results verify this. Since the range of the series is extended by the Padé approximants, we expect the cutoff to be closer to the actual ground state. At each order, we have found this to always be true for some values of L and M. This is demonstrated in the diagrams since the Padé results are always more accurate than the direct t-series results. Second-order perturbation theory implies that $dE(y)/dy$ is a monotonically decreasing function and strong-coupling expansions tell us that $dE(\infty)/dy=0$. So $dE(y)/dy$ should be a positive function and we cannot trust $E(y)$ for values of y where its derivative is negative. This means that we should make $E(y)$ be a constant rather than turn down in our diagrams. In the U(1) and SU(2) systems, the cutoff procedure used with the [4,4] Padé approximant produces oscillatory behavior in the weak-coupling regime. This signals the breakdown of the method. Since this occurs past the point where $dE(y)/dy$ becomes negative, it has no effect on the final results.

Our results indicate that it is possible to choose an optimum finite value of t for the Padé approximants to the t series and that the most accurate approximant need not be the diagonal one. We also conclude that the off-diagonal approximants are best for very low orders (t^2,t^3) and near-diagonal approximants are best for higher orders (t^6 to t^8).

B. D-Padé method

The D-Padé method forms Padé approximants to $dE(t)/dt$. It then integrates to find $E(t)$. This method allows the use of $[L,L+M]$ Padé approximants for $M\geq 2$, thereby offering more approximants to be compared for a given value of $L+M$ than in the diagonal Padé case. The D-Padé method yields more accurate results than the diagonal Padé method. See, for example, Figs. 2 and 3(a) where the best Padé results are consistently less accurate than the D-Padé result. This is because our knowledge of the derivative is accurate near $t=0$ and becomes worse for increasing values of t. Hence when $E(t)$ is reconstructed by integration, the effect of the error in the approximation to $dE(t)/dt$ for $t=t_0$ will not show up until the value of t is significantly greater than t_0. So the ground-state energy is of the form

$$E(t)=\int \frac{P_L(\tau)}{Q_M(\tau)}d\tau \ . \tag{3.2}$$

First we write the integrand as

$$\frac{P_L(\tau)}{Q_M(\tau)}=\sum_{i=1}^{m}\frac{P_L(\tau_i)}{Q'_M(\tau_i)(\tau-\tau_i)} \ ,$$

where the τ_i's represent the m roots of $Q_M(\tau)$ and $M\geq L+2$. The integral becomes

$$\int \frac{P_L(\tau)}{Q_M(\tau)}d\tau=\sum_{i=1}^{m}\frac{P_L(\tau_i)}{Q'_m(\tau_i)}\int\frac{1}{\tau-\tau_i}d\tau \ .$$

In general, the integral will have poles along the path of integration as well as complex poles near the real axis, $\tau_i=\gamma_i\pm i\epsilon$. In order for the integral to be defined we express it in terms of the Cauchy principal value as follows:

$$\int\frac{1}{\tau-\tau_i}d\tau=\rho\int\frac{1}{\tau-\gamma_i}d\tau\pm i\pi \ .$$

Since $E(t)$ is the eigenvalue of a Hermitian operator we take the real part of the integral to get

$$E(t)=\sum_{i=1}^{m}\frac{P_L(\gamma_i)}{Q'_M(\gamma_i)}\,\mathrm{Re}[\ln(t-\gamma_i)] \ . \tag{3.3}$$

For a function $f(t,y)$ of more than one variable this method is generalized by forming Padé approximants to $\partial^2 f(t,y)/\partial y\partial t$ in the parameter t. Then we integrate from $t=0$ to $t=\infty$ to form $\partial f/\partial y$ and finally integrate with respect to y to reconstruct $f(y)$. We refer to this specific form of the D-Padé method as a $D2$-Padé approximant. Another advantage of forming a Padé approximant to the derivative of $E(t)$ is that if the derivative of E vanishes quickly enough, then no cutoff is needed in the integration over t. In our calculations, only in the case of the harmonic oscillator does a cutoff of t substantially improve the results.

The denominator of (3.2) must be at least 2 orders higher than the numerator. Therefore, the lowest-order D-Padé approximant one can safely form is the [0,2], which requires up to the t^3 term in the series. As expected for a given order, the approximants with largest $M-L$ values are the most accurate except in the harmonic-oscillator case. There, we have already seen that the derivative does not vanish sufficiently fast.

The first graph in Fig. 4 includes the results of the $D2$-Padé method applied to the SU(2) system. Analogous to the improvement of the D-Padé over the Padé method, by integrating over $y=2/g^2$ as well as t we see that the second derivative with respect to y will generally have the correct sign for a larger value of y in the $D2$-Padé method than in the D-Padé case. This can easily be seen in the $D2$-Padé [1,6] and D-Padé [1,6] graphs. Comparing, for example, the t^8 CMX and t^8 extended CMX (ECMX) results for the SU(2) system in Figs. 4 and 7 below, we see that a similar relationship holds for these two methods. For low orders the $D2$-Padé method shows no improvement over the D-Padé method; however, for higher-order series the $D2$-Padé procedure substantially improves the results for small values of the coupling constant.

C. Connected-moment expansion

The CMX method[5,6] for extrapolating the function for large t is based on expressing $E(t)$ not as a ratio of polynomials but as a set of decreasing exponentials according to the formula

$$E(t)=E(t\to\infty)+\sum_{j=1}^{\infty}A_j\exp(-b_j t), \quad b_j>0 \ . \tag{3.4}$$

To find E_∞, the powers of t on both sides of this equation are equated to get

$$P_1 \equiv I_1 - E_\infty = \sum_{j=0}^{\infty} A_j \ ,$$
$$P_k \equiv I_k = \sum_{j=0}^{\infty} A_j b_j^{k-1}, \quad k>1 \ . \tag{3.5}$$

It is postulated in Ref. 5 that P_1 can be expressed in terms of the other P's as

$$P_1 = \sum_{k=1}^{\infty} W_k(P_2, P_3, \ldots) \tag{3.6}$$

and it is noted that the function S_k defined by

$$S_k \equiv P_k P_{k+2} - P_{k+1}^2 = \sum_{i,j=1}^{\infty} A_i A_j (b_j^2 - b_i b_j)(b_i b_j)^{k-1} \tag{3.7}$$

has the same form as P_k. Hence, S_1 may also be expressed as in Eq. (3.6):

$$S_1 = \sum_{k=1}^{\infty} W_k(S_2, S_3, \ldots) \tag{3.8}$$

or

$$P_1 P_3 - P_2^2 = \sum_{k=1}^{\infty} W_k(P_2 P_4 - P_3^3, P_3 P_5 - P_4^2, \ldots) \ . \tag{3.9}$$

Solving for P_1 gives

$$P_1 = \frac{P_2^2}{P_3} + \sum_{k=1}^{\infty} W_k(P_2 P_4 - P_3^2, P_3 P_5 - P_4^2, \ldots)/P_3 \ . \tag{3.10}$$

Comparing this with (3.6) yields the recursion relation

$$W_1 = P_2^2/P_3 \ , \tag{3.11}$$
$$W_{k+1}(P_2, P_3, \ldots) = P_3^{-1} W_k(P_2 P_4 - P_3^2, P_3 P_5 - P_4^2, \ldots) \ .$$

Substituting P_1 back in the first equation of (3.5) gives

$$E_\infty = I_1 - \frac{I_2^2}{I_3} - \frac{1}{I_3}\frac{(I_4 I_2 - I_3^2)^2}{I_5 I_3 - I_4^2} - \cdots \ . \tag{3.12}$$

This may be written as

$$E_\infty = I_1 - (I_2 \ \cdots \ I_n) \begin{pmatrix} I_3 & \cdots & I_{n+1} \\ \vdots & \ddots & \vdots \\ I_{n+1} & \cdots & I_{2n-1} \end{pmatrix}^{-1} \begin{pmatrix} I_2 \\ \vdots \\ I_n \end{pmatrix} , \tag{3.13}$$

where n is the number of terms in (3.12).

A disadvantage the methods that approximate the series as exponentials have is that if one has an odd-order power series then the last order is not included in the approximation. As indicated by the singularity at $g^2 = 0.8$ in the t^8 CMX result of Fig. 3, the inverse of the matrix in (3.13) will not always exist. If this occurs we must discard the answers in this region.

D. Laplace method

The Laplace method follows the procedure in the harmonic-oscillator system and expands $|\psi_0\rangle$ in terms of the eigenfunctions of the Hamiltonian as

$$|\psi_0\rangle = \sum_{n=0}^{\infty} \sqrt{b_n}\, |n\rangle$$

with $H|n\rangle = \lambda_n |n\rangle$ so that for finite volume V, the partition function is

$$Z(t) = (b_0 e^{-t\lambda_0} + b_1 e^{-t\lambda_1} + \cdots)^V, \quad b_i, \lambda_i > 0 \ . \tag{3.14}$$

From this the energy density is

$$E(t) = \frac{b_0\lambda_0 e^{-t\lambda_0} + b_1\lambda_1 e^{-t\lambda_1} + \cdots}{b_0 e^{-t\lambda_0} + b_1 e^{-t\lambda_1} + \cdots} \ , \tag{3.15}$$

where $0 < \lambda_0 < \lambda_1 < \lambda_2 < \cdots$ so $\lambda_0 V$ is the lowest-lying energy eigenvalue. If we take the Laplace transform of $z(t) = Z(t)^{1/V}$, $G(s) = \int_{-0}^{\infty} e^{-st} z(t)\, dt$ we get

$$G(s) = \frac{b_0}{s+\lambda_0} + \frac{b_1}{s+\lambda_1} + \cdots \ . \tag{3.16}$$

We note that the lowest pole of $G(s)$ corresponds to $-\lambda_0$ and that its residue is positive. We use this knowledge by solving for $z(t)$ in terms of the t-expansion series, $E(t)$ as

$$z(t) = z(0) \exp\left[-\int_0^t E(t')\, dt' \right] \ . \tag{3.17}$$

For small t we may expand this as a Taylor series

$$z(t) = z_0 + z_1 t + \frac{z_2}{2!} t^2 + \frac{z_3}{3!} t^3 + \cdots \ . \tag{3.18}$$

We form $G(s)$ by taking the Laplace transform of (3.18),

$$G(s) = \frac{z_0}{s} + \frac{z_1}{s^2} + \frac{z_2}{s^3} + \cdots \ , \tag{3.19}$$

and define the variable $u \equiv 1/s$ so that

$$G(u) = u(z_0 + z_1 u + z_2 u^2 + \cdots) \ . \tag{3.20}$$

We may write this as a ratio of polynomials by forming a Padé approximant to the terms in parentheses. To know which L, M values should form our Padé approximant we look at (3.16). In terms of u, this is written

$$G(u) = \frac{u[b_0(1+\lambda_1 u)(1+\lambda_2 u)\cdots + b_1(1+\lambda_0 u)(1+\lambda_2 u)\cdots + \cdots]}{(1+\lambda_0 u)(1+\lambda_1 u)(1+\lambda_2 u)\cdots} \ . \tag{3.21}$$

So we see that our Padé approximant should be a $[L,M]=[n-1,n]$ approximant:

$$G(u)=u\frac{P_{n-1}(u)}{Q_n(u)}\ , \tag{3.22}$$

where the order of $Q_n(u)$ (or value of M) corresponds to the number of exponentials to which we are approximating $z(t)$. In order to form the $[n-1,n]$ Padé approximant, we must have coefficients in the t series to order $2(n-1)$. Having written $G(u)$ in this manner, we know that the smallest real negative root of $Q_n(1/u)$ with a positive residue is $-\lambda_0$.

We expect Padé approximants of analytic functions with various singularities to display these singularities but the approximants may also have extraneous poles with nearby zeros known as defects.[7] If the function $f(t)$ is analytic near $t=\alpha$ but has a Padé approximant,

$$g(t)=\frac{P_L(t)}{R_{M-1}(t)(t-\alpha)}$$

with a pole at $t=\alpha$, then the approximant will only agree with the series when its residue is very small at the spurious pole. Therefore, if a pole has a residue that is significantly smaller ($\simeq 10$ times smaller) than the next biggest pole, we discard it and take the next largest pole. Two other characteristics of defects are that they are transient in going from one Padé approximant to the next and they are often associated with successive approximants ($\Delta L=1$ or $\Delta M=1$ or both) being nearly equal.

In Figs. 5–8 we compare the low- and high-order results of the new extrapolation methods (inverse, Laplace, E of F, and ECMX) applied to the harmonic oscillator, U(1), and SU(2) systems for various values of the coupling constant. As with the previous methods, these graphs represent the more accurate results for a given order. For the Laplace method problems occur involving the roots of $Q_n(u)$ for larger n's due to defects, and we know that the results cannot be trusted in these regions. For t series up to order t^{12} in the U(1) system all of the energy

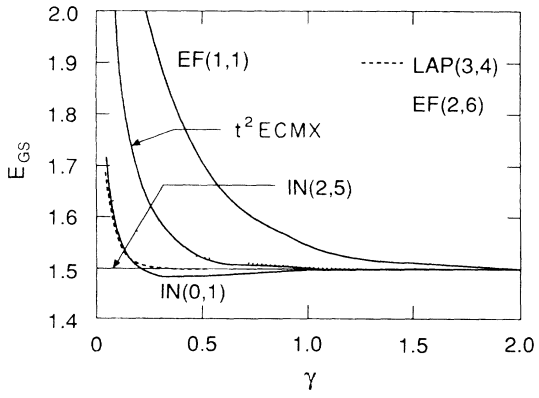

FIG. 5. The new methods (inverse, Laplace, E of F, and ECMX) applied to the harmonic-oscillator series. For the E of F method, the $[L,M]$ means the $[M,L]$ Padé approximant for $F(\delta)$ in Eq. (3.38).

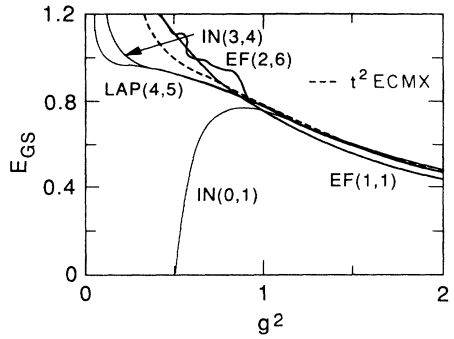

FIG. 6. The new methods applied to the U(1) series. As in the D-Padé, Laplace, and ECMX cases, the inversion method agrees well with the weak-coupling limit of 1.

density results are well behaved. As we increase the order, the results monotonically approach the exact values. For the [6,7] Laplace, the energy density agrees with the exact answer for g^2 as low as $g^2=0.1$, where $E(g^2)=0.9878$.

E. Extended-connected-moment expansion

As in the Laplace method, this method expresses $E(t)$ as a ratio of decreasing exponentials. The difficulty with this approach, as with the CMX and Laplace methods, is finding the b's and λ's so that the Taylor expansion for (3.15) agrees with all orders of the t-expansion series. Once this is achieved, we are assured that $E(t)$ will behave properly as $t\to\infty$. Because of the agreement with the t-expansion series, $E(t)$ will behave properly for small t as well.

There is no loss of generality in defining $b_0=1$ in Eq. (3.15). For convenience we also define

$$N\equiv 1+\sum_{n=1}^{r} b_n,\quad \delta_n\equiv\lambda_n-\lambda_0\ .$$

So that

$$E(t)=\lambda_0+\frac{b_1\delta_1 e^{-t\delta_1}+b_2\delta_2 e^{-t\delta_2}+\cdots}{1+b_2 e^{-t\delta_1}+b_2 e^{-t\delta_2}+\cdots}\ , \tag{3.23}$$

where r is the number of exponentials in the numerator and denominator of (3.23). If we want to express $E(t)$ as

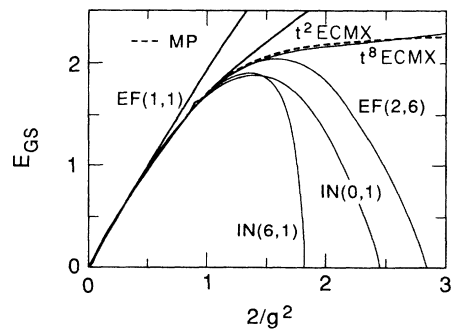

FIG. 7. The new methods applied to the SU(2) series.

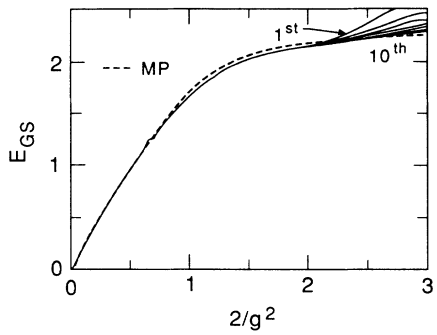

FIG. 8. Ten iterations of the ECMX method applied to the SU(2) series for terms up to t^8 with an initial value of $P_1=I_1-E_{\mathrm{ECMX}(6)}$.

a ratio of n exponentials then we must have $2n+1$ terms in our t-expansion series. It is also clear that the asymptotic value of $E(t\to\infty)$ is λ_0. Now we write $E(t)$ as a power series by expanding the exponentials

$$E(t)=\lambda_0+\frac{S_1-tS_2+\frac{t^2}{2!}S_3+\cdots}{1-tS_1+\frac{t^2}{2!}S_2+\cdots}\ . \tag{3.24}$$

Since the denominator is small we may write

$$E(t)=\lambda_0+\left[S_1-tS_2+\frac{t^2}{2!}S_3+\cdots\right]\times(1-h+h^2-h^3+\cdots)\ , \tag{3.25}$$

where

$$S_n\equiv(b_1\delta_1^n+b_2\delta_2^n+\cdots)/N\ ,$$

$$h\equiv-tS_1+\frac{t^2}{2!}S_2+\cdots\ .$$

To find the b's and λ's we equate the coefficients of the power series in (3.25) with the t-expansion series

$$E(t)=I_1-I_2t+I_3\frac{t^2}{2!}+\cdots\ .$$

We compute out to the second order in t, which corresponds to one exponential in (3.23), and obtain

$$I_1=\lambda_0+S_1,\quad I_2=S_2-S_1^2\ ,\qquad I_3=S_3-3S_1S_2+2S_1^3\ . \tag{3.26}$$

As in the CMX method we define

$$P_1\equiv I_1-\lambda_0,\quad P_n\equiv I_n,\quad n>1\ , \tag{3.27}$$

so that

$$P_1=S_1,\quad P_2=S_2-S_1^2\ ,\qquad P_3=S_3-3S_1S_2+2S_1^2\ . \tag{3.28}$$

These equations may be written as

$$P_1=S_1,\quad g_2\equiv P_2+P_1^2=S_2\ ,\qquad g_3\equiv P_3+3g_2P_1-2P_1^3=S_3\ , \tag{3.29}$$

which have the same structure as Eqs. (3.5) so that we can write

$$\lambda_0=I_1-\frac{g_2^2}{g_3}-\cdots\ . \tag{3.30}$$

Since the g's depend on the unknown P_1, we must solve (3.30) iteratively. In (3.27) we must have an initial estimate of λ_0. Because the answer for the ECMX energy quickly converges for any reasonable initial values, we are free to choose from any of the methods for an initial estimate of λ_0. We will use the lower-order ECMX results. The zeroth-order result is simply the constant term in the t series. So for second order in t we use $P_1=I_1-E_{\mathrm{ECMX}(0)}$ for the first iteration and

$$\lambda_0'=I_1-\frac{g_2(P_1)^2}{g_3(P_1)}\ . \tag{3.31}$$

From this we get $P_1'=I_1-\lambda_0'$,

$$\lambda_0''=I_1-\frac{g_2(P_1')^2}{g_3(P_1')}\ , \tag{3.32}$$

and so forth. This is easily generalized for a t-expansion series with an arbitrary number of terms.

For the t series studies, the Laplace and ECMX methods give the same results. One advantage ECMX has over the Laplace method is that one does not have to deal with the subtle task of finding defects. The problem of finding defects may also be solved by noting that any differences between the Laplace (if we have not searched for defects) and ECMX methods are caused by defects. Figure 8 illustrates the rapid convergence of the ECMX iteration process. The first graph corresponds to the t^6 ECMX results.

F. Inversion method

This method takes advantage of the fact that since $t(E)$ has a much shorter range than $E(t)$, it should be better behaved than $E(t)$. We have already stated that $E(t)$ rapidly decreases to a constant so that its derivative for $t\to\infty$ should be zero. This means that the value of E at which the derivative of $t(E)$ become infinite is the value of $E(t)$ where $dE(t)/dt$ becomes zero. We take this to be $E(t\to\infty)$. We implement this by inverting $E(t)$ thus

$$t(E)=\sum_{n=0}^{N}d_nE^n\ . \tag{3.33}$$

As described in the Padé method section the cutoff t_c for the series $E(t)$ corresponds to the value of t where $dE(t)/dt$ becomes zero for the first time, or when the second derivative of $E(t)$ becomes negative or zero for the first time. So if we take the derivative of t and form a Padé approximant

$$\frac{dt(E)}{dE}=\frac{P_L(E)}{Q_M(E)}\ , \tag{3.34}$$

then the smallest real zero of $Q(E)$ that corresponds to a value of $t(E)$ greater than or equal to t_c is taken to be the

value for $E(t\rightarrow\infty)$.

For the inverse method, the one root of the $[n,1]$ Padé approximant is always a reasonable estimate of the ground-state energy density and, if they exist, the roots of $Q_M(E)$ for larger M are more accurate. In the SU(2) system the results for the t series for order greater than 4 do not improve the low-order results. This is due to the nonexistence of positive real roots less than $E(t=0)$ for large values of y. After varying the application of the inverse method to this system and seeing no change in the results, we conclude that the nonexistence of proper roots for large y is a result of the power series and not the calculation. For the harmonic-oscillator and U(1) systems, the inverse method is more accurate than all of the other methods for high-order series. For these two systems, the inverse method is closer to the exact answers than the CMX, Padé, and D-Padé methods for all of the orders we studied and is comparable to the ECMX/Laplace method for low orders. We have also noted that in all three systems the [0,1] inverse result is the same as the second-order CMX result. It is not completely clear why this is true. The major drawback of the inverse method is that there are more defects and they are harder to detect than in the Laplace method. While the ECMX method may be used as a check for defects in the Laplace method, there is no similar check for the inverse method.

G. E of F

Though this method is not more accurate than the Padé method, we include it for completeness. As with the inversion method we try to improve the behavior of $E(t)$ by expressing the t series as a function of a more compact variable than t. Suppose we define $\delta(t)\equiv 1-Z(t)$ and invert this equation to get

$$t(\delta)=d_0+d_1\delta+d_2\delta^2+\cdots,\quad 0\le\delta\le 1\ . \tag{3.35}$$

Equation (2.1) tells us that

$$E(\delta)=\frac{1}{1-\delta}\frac{1}{\dfrac{dt(\delta)}{d\delta}}\ . \tag{3.36}$$

Therefore if we write the derivative of t as

$$\frac{dt(\delta)}{d\delta}=\frac{1}{1-\delta}F(\delta) \tag{3.37}$$

we are assured that

$$E(\delta)=\frac{1}{F(\delta)}\ , \tag{3.38}$$

where $\delta=1$ corresponds to $t=\infty$. We then extend the range of $E(\delta)$ by forming Padé approximants to it.

The function $E(\delta)$ actually is better behaved than $E(t)$ and the cutoff procedure is really only needed in the U(1) case where improvement is drastic. Figures 5–7 contain graphs of the E of F results. Since $E(\delta)$ has the same general behavior as $E(t)$ we expect the E of F method to have results similar to the Padé method. The t^2 approximants yield inaccurate answers but the results at higher orders are comparable to those obtained with the Padé method. Like the Padé method for higher orders, the near-diagonal approximants are the most accurate. Because of numerous poles in $F(\delta)=Q_L(\delta)/P_M(\delta)$, the cutoff procedure is very difficult to use for U(1) series. As a result, the approximants for $g^2<1.2$ are not well behaved in Fig. 6.

IV. CONCLUSION

We have seen that in the strong-coupling region all of the methods agree. Also, as we increase the order of the t series, the methods generally become more accurate. Through the Laplace and ECMX methods, we have successfully expressed the t series as a ratio of decreasing exponentials by two independent methods and have shown that this ansatz produces very stable results. The ECMX/Laplace method converges rapidly and for, the SU(2) system, essentially requires only three terms in the t series to give the asymptotic value for $E(t)$. It is important to note that all the methods may produce singularities that are inherent to each method. We summarize the results for the three systems by stating that (1) for general orders the inverse and ECMX/Laplace methods are the most accurate, (2) for low orders the E of F method is comparable to the Padé and D-Padé methods which are not as accurate as the CMX, inverse, or ECMX/Laplace methods, and (3) for higher orders the inverse, ECMX/Laplace, and D-Padé methods are the most accurate; the E of F, Padé, and CMX are the least accurate.

Of course these are generalities and should be so treated since the accuracy of the methods will depend on the system to which they are applied. However, we can say that these new procedures provide an excellent complement to the prior methods of extrapolating the t-expansion series, and in some cases greatly surpasses them in accuracy.

ACKNOWLEDGMENTS

The author would like to thank M. Weinstein for many helpful suggestions and for comments on the manuscript, as well as H. R. Quinn and M. Karliner for a number of helpful conversations. This work was supported by the Department of Energy, Contract No. DE-AC03-76SF00515.

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