PHYSICAL REVIEW D VOLUME 24, NUMBER 10 15 NOVEMBER 1981

Strong-coupling expansion for the ground-state energy in the $|x|^\alpha$ potential

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(Received 18 May 1981)

Using lattice techniques we examine the strong-coupling expansion for the ground-state energy of a $g|x|^\alpha$ ($\alpha > 0$) potential in quantum mechanics. We are particularly interested in studying the effectiveness of various Padé-type methods for extrapolating the lattice series back to the continuum. We have computed the lattice series out to 12th order for all α and we identify three regions. When $\alpha < 2/3$ the lattice series diverges faster than $(2n)!$ and no extrapolation technique appears to work. When $2/3 \leq \alpha \leq 2$ the lattice series diverges roughly like $\Gamma((2/\alpha - 1)n)$; here, diagonal Padé extrapolation schemes give excellent results. When $\alpha \geq 2$ the lattice series has a finite radius of convergence; here, completely-off-diagonal Padé extrapolants work best. As α increases beyond 2 it becomes more difficult to obtain good continuum results, apparently because the sign pattern of the lattice series seems to fluctuate randomly. The onset of randomness occurs earlier in the lattice series as $\alpha \to \infty$.

I. INTRODUCTION

Strong-coupling approximation schemes[1,2] are complicated because they require the introduction of a lattice. Once the lattice (of spacing a) has been introduced it is a relatively routine matter to express the lattice strong-coupling series in terms of diagrams and to evaluate the diagrams. It is difficult, however, to find an extrapolation scheme that accurately and reliably extracts the continuum limit ($a \to 0$) of the lattice series. Various Padé-type extrapolation procedures have been invented to perform this limit.[1-6] These procedures have been tested on quantum-mechanical systems for which the numerical results are already known[2] and then applied to model quantum field theories to obtain new results.[7]

We are interested in the reliability of extrapolation methods. In this paper we study a class of one-dimensional quantum-mechanical potentials and reexamine the various extrapolation procedures currently in use. Specifically, we study the Schrödinger equation[6,8]

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+g|x|^\alpha - E\right)\psi(x)=0\,,\quad \alpha>0 \qquad (1.1)$$

where we have set $\hbar = m = 1$. Using a Lagrangian path-integral formalism we develop a lattice strong-coupling series for the ground-state energy for (1.1) for positive values of α to 12th order (that is, we include all diagrams having 12 or fewer internal lines). Then we compare several methods for extrapolating to the continuum limit.

Our motivation for this project comes from previously published work on the anharmonic oscillator ($\alpha = 4$). It was noted in Ref. 4 that the sequence of extrapolants for the lattice series initially approaches the exact answer, but eventually, starting in 11th order, wanders away from it. We believe that this irregularity in the behavior of the extrapolants is associated with an irregularity in the sign pattern of the lattice strong-coupling series (the lattice series for the anharmonic oscillator alternates in sign until 10th order; the 11th-order term has the same sign as the 10th-order term). This kind of irregularity in the sign pattern (assuming that it persists) suggests the presence of singularities in the complex plane off the negative real axis which could interfere with the convergence of the extrapolants.

By examining the strong-coupling series for the ground-state energy of (1.1) for arbitrary $\alpha > 0$ we have organized our results and obtained a clearer picture of the reliability of the extrapolation procedures currently available. These are our results:

(i) For $0<\alpha<2$, the strong-coupling series has a zero radius of convergence. The coefficients C_n in this series alternate regularly in sign and are empirically found to grow roughly like $[(2/\alpha - 1)n]!$:

$$C_n \sim A n^B \Gamma((2/\alpha - 1)n)[-2\Gamma(3/\alpha)/\Gamma(1/\alpha)]^n\,, \qquad (1.2)$$

where A and B are (unknown) constants. Nevertheless, by Padé techniques one can extract the continuum limit to an apparently unlimited accuracy when $\frac{2}{3} \leq \alpha < 2$. When $0<\alpha<\frac{2}{3}$, C_n grows faster than $(2n)!$ as n increases. Thus, the Carleman condition for the uniqueness of the solution to the moment problem for a Stieltjes series is violated. (Of course we do not *know* that when $0<\alpha\leq 2$ the lattice series is a series of Stieltjes; however, the Padé approximants behave numerically as if it were.) For this case ($0<\alpha<\frac{2}{3}$) we observe that although the Padé extrapolants converge beautifully they converge to the wrong limit.

(ii) For $\alpha>2$ the lattice series has a finite radius of convergence. The series exhibits an alternating-sign pattern for the first N_α terms, after which the pattern seems to become irregular. As α increases from 2, N_α decreases monotonically from ∞ at $\alpha=2$ to 5 at $\alpha=\infty$. As α increases it becomes more difficult to extract the continuum limit.

(iii) The special case $\alpha=2$ (the harmonic oscillator) forms a boundary between the above two regions and is also the one case in which we have been able to sum the strong-coupling expansion analytically and to obtain the exact answer. Extrapolation procedures give the exact answer when $\alpha=2$.

(iv) The case $\alpha=\infty$ (the square-well) is interesting because the vertices are expressible in terms of Bernoulli numbers and the resulting lattice series is a sequence of rational numbers. This model is also noteworthy as an example for which the strong-coupling-expansion methods outlined in Refs. 2 and 4 work very poorly. The extrapolation techniques defined in these references give a sequence some of whose elements are complex. Conventional Padé approximants appear to be better because they give real positive extrapolants. However, this sequence of extrapolants is irregular up through 12th order and only comes within 25% of the correct answer.

In Sec. II we review the derivation of the lattice strong-coupling series. We discuss in Sec. III the behavior of the coefficients of the resulting lattice strong-coupling series for various values of α. Finally, in Sec. IV we compare several different extrapolation procedures for the lattice strong-coupling series of Sec. III.

II. DERIVATION OF THE LATTICE STRONG-COUPLING SERIES

For a general one-dimensional potential $V(x)$ we derive the strong-coupling expansion for the ground-state energy from the vacuum functional $Z[J]$ in the presence of an external source J. In Euclidean space

$$Z[J]=\int \mathfrak{D}\phi \exp\left\{-\int dt[\dot{\phi}^2/2+V(\phi)+J\phi]\right\}. \tag{2.1}$$

Following Ref. 2 we replace the kinematical term in this path integral by a functional differential operator and obtain

$$Z[J]=\exp\left[\tfrac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx\,dy\,D^{-1}(x,y)\frac{\delta}{\delta J(x)}\frac{\delta}{\delta J(y)}\right]P[J], \tag{2.2}$$

where

$$D^{-1}(x,y)=\delta''(x-y). \tag{2.3}$$

The remaining path integral $P[J]$ is an infinite product of ordinary integrals on a lattice having lattice spacing a:

$$P[J]=\prod\int_{-\infty}^{\infty}\frac{d\phi_i}{(2\pi a)^{1/2}}\exp[-aV(\phi_i)-J_i\phi_i a]. \tag{2.4}$$

Here the symbol ϕ_i means the function $\phi(x)$ evaluated at the ith lattice point.

For a potential of the form

$$V(\phi)=g|\phi|^\alpha \tag{2.5}$$

it is easy to express each of the integrals in (2.4) as a series in inverse powers of g:

$$P[J]=\prod_i F(J_i)/(2\pi a)^{1/2}, \tag{2.6}$$

where

$$\begin{aligned}F(J)&=\int_{-\infty}^{\infty}dx\,e^{-Jxa-ag|x|^\alpha}\\&=F(0)\sum_{n=0}^{\infty}\frac{J^{2n}a^{2n(1-1/\alpha)}g^{-2n/\alpha}\Gamma((2n+1)/\alpha)}{(2n)!\Gamma(1/\alpha)}\end{aligned} \tag{2.7}$$

and

$$F(0)=2(ag)^{-1/\alpha}\Gamma(1+1/\alpha). \tag{2.8}$$

Note that the integral in (2.7) ceases to exist when $\alpha<1$. Nevertheless, the series coefficients in (2.7) continue to exist for all $\alpha>0$ and, in effect, provide a continuation[9] of the strong-coupling expansion coefficients to values of α less than 1. Although the strong-coupling lattice series exhibits different types of behavior in three regions of α ($0<\alpha<\frac{2}{3}$, $\frac{2}{3}\le\alpha\le 2$, $\alpha>2$), we do not observe any change in the behavior of the lattice series at $\alpha=1$.

The Feynman rules for the diagrams of the lattice strong-coupling expansion are read off from (2.2) and (2.7):

$$\text{for every line } D^{-1}(x,y), \tag{2.9a}$$

$$\text{for a } 2n\text{-point vertex } V_{2n}=\left(\frac{d}{dJ}\right)^{2n}\ln F[J]\bigg|_{J=0}. \tag{2.9b}$$

In addition, associated with every diagram is a symmetry number. The techniques for computing the symmetry numbers and evaluating diagrams have already been discussed in Ref. 2.

The first few vertices are

$$V_2 = xa^2\Gamma(3/\alpha)/\Gamma(1/\alpha)\,,$$
$$V_4 = x^2a^5[\Gamma(5/\alpha)/\Gamma(1/\alpha) - 3\Gamma^2(3/\alpha)/\Gamma^2(1/\alpha)]\,,$$
$$V_6 = x^3a^8[\Gamma(7/\alpha)/\Gamma(1/\alpha) - 15\Gamma(5/\alpha)\Gamma(3/\alpha)/\Gamma^2(1/\alpha) + 30\Gamma^3(3/\alpha)/\Gamma^3(1/\alpha)]\,,$$
$$V_8 = x^4a^{11}[\Gamma(9/\alpha)/\Gamma(1/\alpha) - 28\Gamma(3/\alpha)\Gamma(7/\alpha)/\Gamma^2(1/\alpha) - 35\Gamma^2(5/\alpha)/\Gamma^2(1/\alpha) + 420\Gamma^2(3/\alpha)\Gamma(5/\alpha)/\Gamma^3(1/\alpha) - 630\Gamma^4(3/\alpha)/\Gamma^4(1/\alpha)]\,.$$

Here x is a dimensionless quantity,

$$x = a^{-(2+\alpha)/\alpha}g^{-2/\alpha}\,, \qquad (2.10)$$

defined so that a disappears from the final expressions for the energy in Eq. (2.15).

Here are some special cases:

(i) When $\alpha=\infty$ the vertices can be expressed simply in terms of Bernoulli numbers:

$$V_{2n} = 2^{2n-1}B_{2n}x^na^{3n-1}/n\,. \qquad (2.11a)$$

(ii) When $\alpha=2$ all the vertices V_{2n} vanish except for $V_2 = xa^2/2$.

(iii) When $\alpha=1$

$$V_{2n} = x^na^{3n-1}(2n)!/n\,. \qquad (2.11b)$$

The rationale for strong-coupling calculations is this: We develop the lattice strong-coupling expansion for the fixed-a, large-g domain in which x is a small parameter. We then seek to estimate by extrapolation the value of the analytically continued strong-coupling series for $a\to 0$ $(x\to\infty)$.

To calculate the ground-state energy we note that $Z[0]$, the vacuum persistence functional at vanishing external source, is equal to e^{-E_0T}, where T is the volume of space and E_0 is the ground-state energy. Thus,

$$E_0 = -\frac{1}{T}\ln Z[0] = \lim_{a\to 0}\left\{-\frac{1}{a}\ln[F(0)/(2\pi a)^{1/2}] - (\text{the sum of all connected diagrams having no external legs})/T\right\}. \qquad (2.12)$$

We have evaluated by hand all diagrams up through 6 internal lines and by computer all diagrams up through 12 internal lines.[10]

A dimensional argument shows that the ground-state energy E_0 for the Schrödinger equation (1.1) is proportional to a fractional power of g:

$$E_0 = \epsilon(\alpha)g^{2/(\alpha+2)}\,, \qquad (2.13)$$

where $\epsilon(\alpha)$ is a dimensionless number.[11] To facilitate the extrapolation to zero lattice spacing we remove the logarithm in (2.12) by taking a derivative with respect to g [note that $g\,d/dg = -(2/\alpha)x\,d/dx$]:

$$\alpha g\frac{dE_0}{dg} = \frac{2\alpha}{\alpha+2}\epsilon(\alpha)g^{2/(\alpha+2)} = g^{2/(\alpha+2)}\lim_{x\to\infty}x^{\alpha/(\alpha+2)}\left(1+\sum_{n=1}^{\infty}x^nC_n\right). \qquad (2.14)$$

The derivation of the leading term on the right-hand side of (2.14) makes use of (2.8), (2.10), and (2.12). One can show that the nth term in the series will have the form C_nx^n by evaluating and summing all vacuum graphs having n internal lines. Thus, we have the dimensionless continuum ground-state energy $\epsilon(\alpha)$ expressed as the zero lattice-spacing $(x\to\infty)$ limit of the lattice strong-coupling expansion:

$$\epsilon(\alpha) = \frac{\alpha+2}{2\alpha}\lim_{x\to\infty}x^{\alpha/(\alpha+2)}\left(1+\sum_{n=1}^{\infty}x^nC_n\right). \qquad (2.15)$$

This is the basic equation that we study in this paper.

III. DISCUSSION OF THE LATTICE STRONG-COUPLING SERIES

In the preceding section we showed that the dimensionless ground-state energy $\epsilon(\alpha)$ of the Schrödinger equation

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + |x|^\alpha - \epsilon(\alpha)\right]\psi(x) = 0 \qquad (3.1)$$

can be expressed as the limit of the lattice strong-coupling series in (2.15). We have computed the first 12 coefficients in explicit analytic form as functions of α. Here are the first five coefficients for arbitrary α:

$$C_1 = -2\Gamma(3/\alpha)/\Gamma(1/\alpha)\,,$$
$$C_2 = 2\Gamma(5/\alpha)/\Gamma(1/\alpha)\,,$$
$$C_3 = -[\Gamma^2(1/\alpha)\Gamma(7/\alpha) + 3\Gamma(1/\alpha)\Gamma(3/\alpha)\Gamma(5/\alpha) - 4\Gamma^3(3/\alpha)]/\Gamma^3(1/\alpha)\,,$$
$$C_4 = [\Gamma^3(1/\alpha)\Gamma(9/\alpha) + 8\Gamma^2(1/\alpha)\Gamma(3/\alpha)\Gamma(7/\alpha) + 10\Gamma^2(1/\alpha)\Gamma^2(5/\alpha) - 42\Gamma(1/\alpha)\Gamma^2(3/\alpha)\Gamma(5/\alpha) + 21\Gamma^4(3/\alpha)]/[3\Gamma^4(1/\alpha)]\,,$$

$$C_5 = -[\Gamma^4(1/\alpha)\Gamma(11/\alpha) + 15\Gamma^3(1/\alpha)\Gamma(3/\alpha)\Gamma(9/\alpha) + 60\Gamma^3(1/\alpha)\Gamma(5/\alpha)\Gamma(7/\alpha) - 90\Gamma^2(1/\alpha)\Gamma^3(3/\alpha)\Gamma(7/\alpha) - 160\Gamma^2(1/\alpha)\Gamma(3/\alpha)\Gamma^2(5/\alpha) + 210\Gamma(1/\alpha)\Gamma^3(3/\alpha)\Gamma(5/\alpha) - 36\Gamma^5(3/\alpha)]/[12\Gamma^5(1/\alpha)].$$

The complexity of these coefficients C_n continues to increase with n so we also display the series in Eq. (2.15) for several specific choices of α.

Notice that in the following series the coefficients C_n will be rational numbers only when $1/\alpha$ is an integer or a half-odd integer. For these cases we list, in the examples that follow, the exact rational form of the coefficients. For other values of α the listed values of the coefficients depend upon the accuracy of the numerical evaluation of the Γ functions. (For the special examples $\alpha = \frac{1}{4}$ and $\alpha = \frac{1}{8}$ only the approximate forms are given because the rational forms require integers with hundreds of digits):

$$\epsilon(\tfrac{1}{8}) = \tfrac{17}{2} \lim_{x\to\infty} x^{1/17}(1.0 - 1.025\,873\,7\times10^{19}x + 8.094\,397\,6\times10^{42}x^2 - 2.519\,127\,7\times10^{69}x^3 + 5.624\,858\,4\times10^{97}x^4 - 3.485\,048\,4\times10^{127}x^5 + 3.274\,768\,8\times10^{158}x^6 - 3.072\,412\,8\times10^{190}x^7 + 2.118\,349\times10^{223}x^8 - 8.490\,813\,3\times10^{256}x^9 + 1.644\,271\,4\times10^{291}x^{10} - 1.324\,368\,7\times10^{326}x^{11} + 3.920\,147\,3\times10^{361}x^{12} - \cdots), \qquad (3.2)$$

$$\epsilon(\tfrac{1}{4}) = \tfrac{9}{2} \lim_{x\to\infty} x^{1/9}(1.0 - 1.330\,56\times10^{7}x + 4.054\,836\,7\times10^{16}x^2 - 1.815\,215\times10^{27}x^3 + 5.740\,973\,3\times10^{38}x^4 - 8.391\,153\,8\times10^{50}x^5 + 4.308\,690\,1\times10^{63}x^6 - 6.420\,531\,5\times10^{76}x^7 + 2.412\,113\,4\times10^{90}x^8 - 2.051\,021\,5\times10^{104}x^9 + 3.624\,27\times10^{118}x^{10} - 1.241\,918\,2\times10^{133}x^{11} + 7.793\,395\,8\times10^{147}x^{12} - \cdots), \qquad (3.3)$$

$$\epsilon(\tfrac{1}{2}) = \tfrac{5}{2} \lim_{x\to\infty} x^{1/5}(1 - 240x + 725\,760x^2 - 6\,350\,745\,600x^3 + 120\,922\,357\,248\,000x^4 - 4\,321\,357\,624\,627\,200\,000x^5 + 261\,318\,398\,832\,231\,579\,648\,000x^6 - 24\,758\,001\,241\,899\,464\,180\,367\,360\,000x^7 + 3\,467\,174\,428\,686\,216\,667\,014\,105\,661\,440\,000x^8 - 686\,113\,651\,251\,773\,224\,133\,321\,019\,831\,091\,200\,000x^9 + 185\,121\,667\,331\,531\,093\,557\,728\,660\,599\,212\,710\,297\,600\,000x^{10} - 66\,153\,128\,876\,623\,411\,508\,633\,878\,019\,212\,439\,193\,649\,152\,000\,000x^{11} + 30\,565\,246\,093\,405\,286\,095\,413\,946\,705\,792\,041\,733\,359\,327\,510\,528\,000\,000x^{12} - \cdots), \qquad (3.4)$$

$$\epsilon(\tfrac{2}{3}) = 2 \lim_{x\to\infty} x^{1/4}\Big(1 - \frac{105x}{4} + \frac{135\,135x^2}{32} - \frac{173\,166\,525x^3}{128} + \frac{1\,429\,736\,497\,875x^4}{2048} - \frac{4\,348\,647\,012\,504\,375x^5}{8192} + \frac{36\,899\,922\,214\,229\,673\,375x^6}{65\,536} - \frac{209\,453\,201\,904\,396\,013\,318\,125x^7}{262\,144} + \frac{12\,298\,364\,126\,266\,132\,301\,701\,111\,875x^8}{8\,388\,608} - \frac{113\,475\,898\,356\,688\,322\,826\,658\,215\,271\,875x^9}{33\,554\,432} + \frac{2\,572\,219\,107\,417\,797\,820\,871\,446\,728\,741\,878\,125x^{10}}{268\,435\,456} - \frac{35\,130\,413\,968\,925\,927\,062\,636\,428\,231\,732\,122\,671\,875x^{11}}{1\,073\,741\,824} + \frac{2\,276\,087\,413\,255\,141\,413\,171\,683\,611\,101\,573\,688\,772\,109\,375x^{12}}{17\,179\,869\,184} - \cdots\Big), \qquad (3.5)$$

$$\epsilon(1) = \tfrac{3}{2} \lim_{x\to\infty} x^{1/3}(1 - 4x + 48x^2 - 832x^3 + 17\,968x^4 - 455\,904x^5 + 13\,189\,632x^6 - 427\,449\,600x^7 + 15\,337\,993\,536x^8 - 604\,283\,926\,144x^9 + 25\,969\,690\,820\,608x^{10} - 1\,210\,844\,480\,455\,680x^{11} + 60\,960\,214\,854\,542\,848x^{12} - \cdots), \qquad (3.6)$$

$$\epsilon(\tfrac{3}{2}) = \tfrac{7}{6} \lim_{x\to\infty} x^{3/7}(1.0 - 1.47\,697\,629x + 4.10\,327\,375x^2 - 13.7\,985\,443x^3 + 51.3\,826\,146x^4 - 204.585\,909x^5 + 855.578\,156x^6 - 3718.65\,738x^7 + 16\,683.0315x^8 - 76\,887.362x^9 + 362\,757.133x^{10} - 1\,747\,495.45x^{11} + 8\,577\,625.3x^{12} - \cdots). \qquad (3.7)$$

Note that for the examples quoted above with $0<\alpha<2$, the numerical coefficients C_n in the series grow rapidly with increasing n. We have done a rough fit to the growth of C_n for various values of $0<\alpha<2$ and have arrived at the empirical formula in (1.2), which appears to account for the most rapidly varying component of the asymptotic behavior of C_n for large n. We do not have a good guess for the dependence of A and B on α. Equation (1.2) implies that when $0<\alpha<2$ the series in (2.15) has a zero radius of convergence. Nevertheless, one can treat the series as a formal representation of the ground-state energy and extract information from it by using Padé approximants. This procedure will be discussed in the next section.

The choice $\alpha=2$ corresponds to the harmonic oscillator and the resulting series is

$$\epsilon(2)=\lim_{x\to\infty} x^{1/2}(1-x+\tfrac{3}{2}x^2-\tfrac{5}{2}x^3+\cdots).$$

It is easy to see that the full series for this case can be written as

$$\epsilon(2)=\lim_{x\to\infty} x^{1/2}\sum_{n=0}^{\infty}\frac{(-1)^n(2n)!}{n!\,n!}\left(\frac{x}{2}\right)^n=\lim_{x\to\infty} x^{1/2}\frac{1}{(1+2x)^{1/2}}=\frac{1}{\sqrt{2}}. \tag{3.8}$$

This is, so far as we know, the only case for which the strong-coupling series can be summed exactly.

A few more examples are given below for $\alpha>2$:

$$\begin{aligned}\epsilon(3)=\tfrac{5}{6}\lim_{x\to\infty} x^{3/5}(1.0&-0.746\,564\,44x+0.673\,957\,504x^2-0.613\,756\,98x^3+0.548\,324\,8x^4-0.477\,344\,63x^5\\&+0.403\,976\,37x^6-0.331\,720\,967x^7+0.263\,560\,4x^8-0.201\,727\,305x^9+0.147\,674\,08x^{10}\\&-0.102\,125\,083x^{11}+0.065\,176\,011x^{12}-\cdots),\end{aligned} \tag{3.9}$$

$$\begin{aligned}\epsilon(4)=\tfrac{3}{4}\lim_{x\to\infty} x^{2/3}(1.0&-0.675\,977\,93x+0.5x^2-0.352\,540\,683x^3+0.232\,495\,094x^4-0.142\,706\,048x^5\\&+0.080\,878\,922x^6-0.041\,513\,005\,3x^7+0.018\,405\,315\,7x^8-0.006\,082\,864\,17x^9\\&+0.000\,335\,225\,368x^{10}+0.001\,765\,920\,3x^{11}-0.002\,080\,732\,32x^{12}+\cdots),\end{aligned} \tag{3.10}$$

$$\begin{aligned}\epsilon(5)=\tfrac{7}{10}\lim_{x\to\infty} x^{5/7}(1.0&-0.648\,766\,264x+0.435\,649\,686x^2-0.268\,712\,066x^3+0.149\,584\,465x^4\\&-0.074\,353\,69x^5+0.032\,072\,78x^6-0.011\,005\,417\,1x^7+0.001\,967\,428\,01x^8\\&+0.001\,058\,075\,43x^9-0.001\,516\,159\,68x^{10}+0.001\,135\,723\,5x^{11}-0.000\,652\,063\,566x^{12}+\cdots),\end{aligned} \tag{3.11}$$

$$\begin{aligned}\epsilon(6)=\tfrac{2}{3}\lim_{x\to\infty} x^{3/4}(1.0&-0.636\,849\,925x+0.405\,577\,805x^2-0.231\,239\,712x^3+0.115\,773\,294x^4-0.049\,863\,399x^5\\&+0.017\,328\,481\,4x^6-0.003\,701\,166\,9x^7-0.000\,753\,357\,273x^8+0.001\,484\,098\,54x^9\\&-0.001\,085\,152\,02x^{10}+0.000\,573\,323\,9x^{11}-0.000\,229\,402\,24x^{12}+\cdots),\end{aligned} \tag{3.12}$$

$$\begin{aligned}\epsilon(8)=\tfrac{5}{8}\lim_{x\to\infty} x^{4/5}(1.0&-0.629\,268\,5x+0.380\,815\,08x^2-0.199\,770\,2x^3+0.088\,575\,922x^4-0.031\,747\,426\,4x^5\\&+0.007\,722\,888\,5x^6+0.000\,182\,488\,064x^7-0.001\,651\,320\,37x^8+0.001\,225\,622\,06x^9\\&-0.000\,602\,026\,02x^{10}+0.000\,207\,858\,828x^{11}-0.000\,032\,877\,5x^{12}+\cdots).\end{aligned} \tag{3.13}$$

The limiting value $\alpha\to\infty$ corresponds to the infinite square well. The lattice strong-coupling series is

$$\begin{aligned}\epsilon(\infty)=\tfrac{1}{2}\lim_{x\to\infty} x\bigg(1&-\frac{2x}{3}+\frac{2x^2}{5}-\frac{184x^3}{945}+\frac{206x^4}{2835}-\frac{536x^5}{31\,185}-\frac{215\,668x^6}{212\,837\,625}+\frac{1552x^7}{405\,405}-\frac{2\,943\,058x^8}{1\,206\,079\,875}\\&+\frac{7\,353\,163\,432x^9}{7\,795\,859\,096\,025}-\frac{5\,465\,896\,763\,564x^{10}}{32\,157\,918\,771\,103\,125}-\frac{2\,922\,973\,616x^{11}}{39\,952\,040\,821\,875}\\&+\frac{263\,787\,817\,794\,533\,716x^{12}}{3\,028\,793\,579\,456\,347\,828\,125}+\cdots\bigg).\end{aligned} \tag{3.14}$$

For $\alpha\geq 2$, the first 12 coefficients C_n suggest that these lattice strong-coupling series have finite radii of convergence which seem to increase with increasing α.

Notice that in each of the examples quoted above, the first few terms of the series have signs alternating like $(-1)^n$. For $\alpha=2$ this pattern persists for all values of n, and we believe that this is also true for $0<\alpha<2$. For $\alpha>2$, however, only the first few terms exhibit this simple alternating pattern and after some critical value $n=N_\alpha$ the pattern is broken. N_α decreases with increasing α: $N_2=\infty$, $N_4=10$, $N_5=8$, $N_6=7$, $N_8=6$, and $N_\infty=5$. From the analytic forms of the coefficients $C_n(\alpha)$ we have calculated the numerical values of $C_n(\alpha)$ as functions of α. As already remarked, for $0<\alpha\leq 2$ the sign of $C_n(\alpha)$ is the same as that of $(-1)^n$ so we write

$$C_n(\alpha)=(-1)^n K_n(\alpha)$$

and display in Table I the smallest value of α, $\alpha=\alpha_n$ at which $K_n<0$. (For $n=1,2,3,4,5$, $K_n>0$.) We summarize these results as follows:

(i) For any value of α, the first five terms in the lattice strong-coupling series (2.15) will alternate according to $C_n \propto (-1)^n$.

(ii) For $\alpha<3.45$ (the $|x|^3$ oscillator, for example), the first 12 terms (at least) will alternate in sign.

(iii) For $\alpha>27.8$ [in particular, for the square-well series in Eq. (3.14)] only the first five terms in the series oscillate.

We belabor the issue of the sign pattern of the coefficients C_n because we believe it relates to the effectiveness of the extrapolation procedures that will be discussed in Sec. IV. Recall that the lattice strong-coupling series is derived in a regime such that the expansion parameter x given in Eq. (2.10) is small and the series (2.15) can be presumed to converge or to be asymptotic. Then Eq. (2.15) is an expansion for a function $f(x)$ (analytic, we hope) with finite limit [the value $\epsilon(\alpha)$] as $x\to\infty$.

More precisely, let us remember that $\epsilon(\alpha)$ has the form

$$\epsilon(\alpha)=\frac{\alpha+2}{2\alpha}\lim_{x\to\infty}[xf(x)]^{\alpha/(\alpha+2)}\,.$$

If $f(x)$ has a pole on the negative real axis, and if this is the nearest singularity to the origin, then this singularity should dominate the large-n terms

TABLE I. α_n, the smallest value of α for which the sign of the coefficient C_n in Eq. (2.15) fails to obey the rule $(-1)^n$.

n	α_n
6	27.8
7	7.82
8	5.56
9	4.58
10	4.05
11	3.65
12	3.45

in the series (2.15) and asymptotically the terms will alternate in sign. The harmonic-oscillator result in Eq. (3.8) is an example. The more complicated sign pattern exhibited by the lattice strong-coupling series for the $\alpha>2$ oscillators indicates that $f(x)$ has a more elaborate singularity structure and that it will not be easy to extract accurate information by extrapolation.

Because we have only 12 terms in the series it is not possible to make definite statements about the singularities and the radius of convergence; indeed, we cannot even be sure that $f(x)$ is analytic at $x=0$. [For $\alpha<2$ the radius of convergence is zero so it must be presumed that $f(x)$ is not analytic at the origin.]

From the values in Table I, it seems likely that, as α is increased, the extrapolants will become increasingly unreliable.

The coefficients $C_n(\alpha)$ are combinations of Γ functions with varying signs. This leads to oscillatory behavior in α, with a very slow approach to the asymptotic square-well values.

IV. EXTRAPOLATION TO ZERO LATTICE SPACING

The fundamental question is this: How well does Eq. (2.15) predict the value of $\epsilon(\alpha)$, the ground-state energy of the $|x|^\alpha$ oscillator for coupling strength equal to one? Recall that

$$\epsilon(\alpha)=\frac{\alpha+2}{2\alpha}\lim_{x\to\infty}x^{\alpha/(\alpha+2)}\left[1+\sum_{n=1}^{\infty}x^nC_n(\alpha)\right]. \quad (2.15)$$

Because $\epsilon(\alpha)$ is finite, the function represented by $1+\sum_{n=1}^{\infty}x^nC_n$ must behave like $x^{-\alpha/(\alpha+2)}$ for large x. We therefore begin by raising (2.15) to the power $(\alpha+2)/\alpha$:

$$\epsilon^{(\alpha+2)/\alpha}=\left(\frac{\alpha+2}{2\alpha}\right)^{(\alpha+2)/\alpha}\lim_{x\to\infty}x\left(1+\sum_{n=1}^{\infty}x^nd_n\right), \quad (4.1)$$

where the coefficients d_n are easily determined in terms of C_n.

One reasonable extrapolation scheme to apply to Eq. (4.1) is to convert the formal power series $1+\sum d_nx^n$ into a $P_N^{N-1}(x)$ Padé approximant and then to take the limit as $x\to\infty$ of the expression $xP_N^{N-1}(x)$. By construction, this limit exists for all N, and thus one obtains a sequence of approximants defined by

$$\epsilon_{\text{Padé}}^{2N-1}\equiv\frac{\alpha+2}{2\alpha}\left[\lim_{x\to\infty}xP_N^{N-1}(x)\right]^{\alpha/(\alpha+2)}. \quad (4.2)$$

The superscript $2N-1$ indicates that all the terms up through x^{2N-1} are used to construct the approximant.

Another method for extrapolating the series was introduced in Ref. 2. The technique proposed there by Bender, Cooper, Guralnik, and Sharp

(BCGS) was to construct the extrapolants $\epsilon_{\rm BCGS}^{(N)}$ defined by

$$\epsilon_{\rm BCGS}^{N} \equiv \frac{\alpha+2}{2\alpha}\,[D_N^{(N)}]^{-\alpha/(N\alpha+2N)}\,, \qquad (4.3)$$

where $D_N^{(N)}$ is the coefficient of x^N in $(1+\sum_1^\infty x^n d_n)^{-N}$. The extrapolants generated by this technique have been discussed elsewhere.[2,4] We have also explored variants of this technique; we describe some in the Appendix.

The two extrapolation schemes described above produce sequences of extrapolants that we hope converge or come very close to the answer $\epsilon(\alpha)$. We find three separate behaviors for these extrapolants depending on whether $0<\alpha<\frac{2}{3}$, $\frac{2}{3}\leq\alpha\leq 2$, or $\alpha>2$. In Table II we give the results of both procedures described above applied to the cases of $\alpha=\frac{1}{2}$, $\frac{2}{3}$, 1, $\frac{3}{2}$, 4, 6, 8, ∞ and compared to the exact values.[11,12] We observe that when $\alpha<\frac{2}{3}$ the $\epsilon_{\rm Pad\acute{e}}^{2N-1}$ extrapolants converge beautifully but to the wrong answer. We believe that this happens because the coefficients C_n grow with n faster than $(2n)!$, which violates the Carleman condition for Stieltjes series.[13] When $0<\alpha<2$ the extrapolants $\epsilon_{\rm Pad\acute{e}}^{2N-1}$ are monotonic and apparently converging toward the correct answer. Indeed, repeated Richardson extrapolation[13] gives the correct answer to three significant figures. For example, when $\alpha=1$, the first-order Richardson extrapolants,

$$R_N^{(1)} \equiv (N+1)\epsilon_{\rm Pad\acute{e}}^{2N+1} - N\epsilon_{\rm Pad\acute{e}}^{2N-1}\,, \qquad (4.4)$$

of the $\epsilon_{\rm Pad\acute{e}}^{2N-1}$ in Table III are $R_1^{(1)}=0.774\,94$, $R_2^{(1)}=0.789\,98$, $R_3^{(1)}=0.795\,03$, $R_4^{(1)}=0.797\,53$, $R_5^{(1)}=0.799\,06$. Performing repeated first-order Richardson extrapolations of this sequence,

$$R_N^{(k)} \equiv (N+1)R_{N+1}^{(k-1)} - NR_N^{(k-1)} \qquad (4.5)$$

TABLE II. The P_N^{N-1} Padé extrapolants and the BCGS extrapolants for the ground-state energy of the $|x|^\alpha$ oscillator calculated from the lattice strong-coupling expansions in Eqs. (3.4)–(3.7). N is the order of perturbation theory. The exact results are taken from Ref. 11 (see also Ref. 12). When a complex number arises in a BCGS extrapolant no higher extrapolants are given.

	$\alpha=\frac{1}{2}$		$\alpha=\frac{2}{3}$		$\alpha=1$		$\alpha=\frac{3}{2}$	
N	Padé	BCGS	Padé	BCGS	Padé	BCGS	Padé	BCGS
1	0.605 49	0.605 49	0.624 79	0.624 79	0.655 19	0.655 19	0.686 52	0.686 52
2						0.786 84		0.717 04
3	0.638 95	complex	0.675 44	complex	0.715 06	0.716 96	0.721 44	0.725 34
4						complex		0.730 59
5	0.653 27		0.698 47		0.740 04		0.731 68	0.733 24
6								0.735 19
7	0.661 49		0.712 30		0.753 79		0.735 99	0.736 42
8								0.737 42
9	0.666 92		0.721 79		0.762 53		0.738 28	0.738 12
10								0.738 73
11	0.670 84		0.728 82		0.768 62		0.739 55	0.739 18
12								0.739 56
Exact	0.922 45		0.878 94		0.808 61		0.743 88	

	$\alpha=4$		$\alpha=6$		$\alpha=8$		$\alpha=\infty$	
N	Padé	BCGS	Padé	BCGS	Padé	BCGS	Padé	BCGS
1	0.743 10	0.743 10	0.753 66	0.753 66	0.757 33	0.757 33	0.750 00	0.750 00
2		0.697 79		0.693 16		0.690 17		0.684 65
3	0.666 00	0.685 05	0.659 02	0.679 80	0.660 72	0.678 69	0.700 93	0.711 47
4		0.680 68		0.678 56		0.682 01		0.800 27
5	0.686 96	0.679 45	0.724 31	0.682 47	0.762 02	0.692 95	0.973 42	complex
6		0.679 51		0.689 07		0.710 00		
7	0.476 39	0.680 04	0.378 92	0.697 29	0.330 14	0.734 74	0.364 23	
8		0.680 63		0.706 34		0.773 72		
9	0.676 36	0.681 03	0.722 50	0.715 29	0.787 48	0.867 01	0.990 20	
10		0.681 15		0.722 51		complex		
11	0.670 29	0.680 94	0.688 35	0.725 58	0.717 38		0.957 04	
12		0.680 43		0.722 41				
Exact	0.667 98[a]		0.680 70		0.704 05		$\pi^2/8=1.2337$	

[a]This number is given wrong in Refs. 2 and 4. In the notation of these references the correct value for $4gdE/dg$ is 0.561 073 and not 0.569 473.

gives even better results: $R_1^{(2)} = 0.805\,02$, $R_2^{(2)}$ $0.805\,13$, $R_3^{(2)}$ $0.805\,01$, $R_4^{(2)} = 0.805\,18$. If we compare these results with the exact answer $\epsilon(1) = 0.808\,61$ taken from Ref. 10 we get a relative error of 0.4%.

The BCGS extrapolants are ineffective when $\frac{2}{3} \leq \alpha < 2$; they form a sequence that eventually becomes complex and is therefore not useful.

When $\alpha = 2$ the strong-coupling series may be summed exactly, as is pointed out in Sec. III; the $a \to 0$ ($x \to \infty$) limit then gives the exact answer $1/\sqrt{2}$.

When $\alpha > 2$, the BCGS extrapolants at first decrease toward the correct answer until they reach a minimum and then increase away from the exact answer again (eventually to become complex). Thus, the BCGS extrapolants in the $\alpha > 2$ regime behave in a manner reminiscent of the partial sums of an asymptotic series. If we did not know the correct answer, our best estimate of the correct answer would have to be the value of the extrapolant at the first minimum reached. This value in the BCGS approximants provides a better estimate of the answer than the Padé approximants (which are not as smooth and well behaved, and tend to jump around irregularly): when $\alpha = 4$, the relative error is 1.7%, for $\alpha = 6$ it is 0.4%, for $\alpha = 8$ it is 4.5%; however, for $\alpha = \infty$ the error is 55%.[14] The poor result at $\alpha = \infty$ occurs because the sign pattern of the strong-coupling lattice series becomes irregular before the extrapolants have a chance to converge.

ACKNOWLEDGMENTS

We are greatly indebted to R. Roskies for his computer evaluation of the lattice diagrams in 7th through 12th order. We are also indebted to the MIT Laboratory for Computer Science for allowing us the use of MACSYMA for algebraic manipulation. LMS is grateful for the hospitality of the Department of Physics, Washington University. This work was supported in part by the U. S. Department of Energy and in part by the National Science Foundation.

APPENDIX

We have considered several extrapolation schemes other than those used in the body of this paper and checked their utility by applying them to the most ill-behaved case, the square-well series, $\alpha = \infty$, in Eq. (3.14). (a) One can first square the series and then construct the P_n^{n-1} Padé approximants. The resulting sequence of extrapolants, 0.685, 0.672, 0.931, 0.933, 0.926, 0.925, comes fairly close to the desired result. (b) Another plausible procedure consists of first exponentiating the lattice series in Eq. (3.14) to produce a series beginning with 1, constructing the diagonal Padé approximants $P_n^n(\infty)$, and taking the logarithm of this limit. Again there results a series of extrapolants that come close (this time to within 2%) to the exact answer, before veering off. These extrapolants are 0.972 96, 0.693 00, 1.2200, 1.2200, 0.951 01, 0.933 93.

Note that the extrapolants from both these Padé techniques are very irregular and are therefore impossible to extrapolate to a limit and at best only come close to the correct result before turning away. The primary criticism of these procedures, however, is that if the answer were not known ahead of time it would be difficult to determine from these very irregular approximants. We have discovered a class of extrapolation schemes that produces a monotonic and very regular sequence of approximants with an unambiguous limit. The drawback is that the limit of these approximants is not equal to the answer to the problem, and we do not yet know the relation between the two quantities. The motivation for this new procedure is simple. If we raise the series in Eq. (3.14) to the $2n$th power, the first n coefficients will all be positive. This fact suggests the following variation on the BCGS procedure:

TABLE III. Richardson extrapolants [see (4.5)] of the Padé extrapolants in Table II. The exact values for $\epsilon(\alpha)$ are also shown.

	$\alpha=\frac{1}{2}$			$\alpha=\frac{2}{3}$			$\alpha=1$		$\alpha=\frac{3}{2}$
N	$R_N^{(1)}$	$R_N^{(2)}$	$R_N^{(3)}$	$R_N^{(1)}$	$R_N^{(2)}$	$R_N^{(3)}$	$R_N^{(1)}$	$R_N^{(2)}$	$R_N^{(1)}$
1	0.672 41	0.691 40	0.697 83	0.726 09	0.762 99	0.781 57	0.774 94	0.805 02	0.756 36
2	0.681 90	0.694 62	0.699 68	0.744 54	0.772 28	0.788 09	0.789 98	0.805 13	0.752 16
3	0.686 14	0.696 31	0.700 77	0.753 79	0.777 55	0.791 99	0.795 03	0.805 01	0.748 92
4	0.688 68	0.697 42		0.759 73	0.781 16		0.797 53	0.805 18	0.747 44
5	0.690 43			0.764 01			0.799 06		0.745 90
Exact		0.922 45			0.878 94		0.808 61		0.743 88

Raise the series to the $-2n$ power, take the nth coefficient of the resulting series, and finally take the $-1/2n$ root. (More generally we could raise the series to the kn power, pick off the coefficient of x^{kn}, and take the $-1/kn$ root. Here, however, we discuss only the $k=2$ case.) The extrapolants produced by this procedure are 0.433 01, 0.385 01, 0.365 44, 0.354 36, 0.347 11, 0.341 92, 0.338 01, 0.334 93, 0.332 43, 0.330 36, 0.328 61, 0.327 12. These extrapolants are smooth and well behaved in contrast with those listed in Table II. The difficulty with this technique is that we do not know how to predict the relation between the limit of this sequence and the limit of the original function. In sample problems to which we have applied this method the relation appears to depend in a complicated way upon the singularity structure of the function.

Surely the lattice series in Eq. (3.14) must contain an enormous amount of information about its true value at $x=\infty$. We are dismayed that after computing the energy to 12th order in perturbation theory, it is so difficult to extract its zero-lattice-spacing limit.

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[9]One can avoid introducing such nonexistent integrals by not using functional differentiation. Instead, one fixes the number of lattice points at n and explicitly evaluates the n-fold multiple integral representing Z. Dividing the logarithm of the resulting expression by n gives a polynomial in x [see Eq. (2.10)] plus an expression that vanishes as $n\to\infty$. The polynomial agrees with the strong-coupling expansion Eq. (2.15).

[10]We thank R. Roskies for providing us with his computer calculation of the vacuum diagrams in orders seven through twelve.

[11]A table of $\epsilon(\alpha)$ may be found in J. F. Barnes, H. J. Brascamp, and E. H. Lieb, in *Studies in Mathematical Physics*, edited by E. H. Lieb, B. Simon, and A. S. Wightman (Princeton University Press, Princeton, New Jersey, 1976). We have taken the $\alpha=8$ result from Table VII of F. T. Hioe, D. MacMillan, and E. W. Montroll, J. Math. Phys. 17, 1320 (1976). (The corresponding entry in their Table V is in error.)

[12]Reference 11 treats the equation $(-d^2/dx^2+x^\alpha-E_{\mathrm{BBL}})\psi=0$, which differs from Eq. (1.1) by a factor of 2 in the derivative term. Therefore, the exact ground-state energies given in Table II are $2^{-\alpha/(2+\alpha)}E_{\mathrm{BBL}}$. Reference 11 does not give an exact result for $\alpha=\frac{2}{3}$. We obtained the value in Table II by interpolation.

[13]For a discussion of the Carleman condition and Richardson extrapolation see C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978).

[14]Ader *et al.* (see Ref. 8) examined the strong-coupling expansion for the x^{2k} potential. Their calculation, however, was only through fifth order in the lattice strong-coupling series. Consequently, they did not observe the different behaviors exhibited by the strong-coupling series for the three different regions of the parameter $\alpha=2k$: $0<\alpha<\frac{2}{3}$, $\frac{2}{3}\le\alpha\le 2$, $2<\alpha$. Furthermore, because the first sign irregularity appears in sixth order, they did not observe this phenomenon.