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The Hill Determinant: An Application to the Anharmonic Oscillator

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We have calculated the ground-state eigenvalues of the λx^4 anharmonic oscillator nonperturbatively, using the Hill determinant. Our results are in remarkable agreement with those obtained from the Borel-Padé approximants of the perturbation series.

From an exhaustive numerical analysis of the perturbation series for the ground-state energy level of the one-dimensional anharmonic oscillator for which the Hamiltonian is given by

$$H=-\frac{d^2}{dx^2}+x^2+\lambda x^4, \tag{1}$$

Bender and Wu[1] have shown that the power series in λ is divergent for all λ though each term of the series is finite. Further, they show that the energy levels of the system orginally defined for real $\lambda>0$ can be analytically continued into the complex λ plane and that the continuation has an infinite number of branch points with a limit point at $\lambda=0$. Such series are quite common in relativistic quantum mechanics and the usual belief is that they are asymptotic in nature.[2] It is well known in the mathematical literature[3] that such series can often be summed[4] uniquely through the use of such summability techniques as the Stieltjes-Padé or the Borel methods. Simon[5] has recently investigated the anharmonic oscillator with the general anharmonic term λx^{2m} (m an integer >0) and has shown that the pth energy level $E_p^m(\lambda)$ is analytic in a certain region of the λ plane and that the perturbation series is asymptotic to the value $E_p^m(\lambda)$. In particular, he has calculated $E_0^2(\lambda)$ by converting the perturbation series into a series of Padé approximants for various values of λ. In a recent communication, Graffi *et al.*[6] have shown how improved values of the ground-state energy level for arbitrary λ can be obtained by using Padé approximants of the Borel transform of the asymptotic perturbation series. In essence, their method consists in replacing the series $\sum_{n=0}^{\infty} a_n z^n$ by the Borel sum

$$\int_0^\infty e^{-t}\phi(tz)dt, \quad \text{where} \quad \phi(z)=\sum_{n=0}^{\infty}\frac{a_n z^n}{n!}.$$

Within their regions of convergence both series are identical, but for values of z for which the series $\sum_{n=0}^{\infty} a_n z^n$ diverges, the integral representation gives the value of the series provided the integral exists for that z. To facilitate numerical computation, Graffi *et al.* used Padé approximants for $\phi(tz)$.

In this note, we wish to point out that exact values of the energy levels of the anharmonic oscillator can also be obtained without recourse to the standard perturbation series and associated summability techniques. Our approach, essentially based upon solving the Hill determinants in finding eigenvalues, has long been known in the literature of mathematical physics.[7] From our analysis we find the following:

(i) For small λ ($\lambda \ll 0.1$) the ground-state energy is just that predicted by the asymptotic perturbation series.

(ii) For $\lambda \geq 0.1$ our results for the ground-state energy are in remarkable agreement with those obtained from the Padé approximants of the Borel sum of the perturbation series.

(iii) The eigenvalues and eigenfunctions for excited levels can also be obtained within our framework.

(iv) Our method affords a straightforward generalization to the problem with the general anharmonic term of the form λx^{2m}.

We give below an outline of our nonperturbative approach. For simplicity, let us examine the level shifts of the even-parity states and consider the differential equation $H\psi=\epsilon\psi$. We now make the ansatz

$$\psi=e^{-x^2/2}\sum_{n=0}^{\infty}C_n x^{2n}. \tag{2}$$

Substituting this ansatz in the differential equation, we find that the C_n's satisfy the following difference equation:

$$2(n+1)(2n+1)C_{n+1}+C_n(\epsilon-1-4n)-\lambda C_{n-2}=0. \tag{3}$$

The condition that a nontrivial solution for the C_n's exist is given by the vanishing of the following infinite determinant:

$$D=\left|\begin{array}{cccccccccc}
\epsilon-1 & 2 & 0 & 0 & \cdots & & & & & \cdots \\
0 & \epsilon-5 & 12 & 0 & \cdots & & & & & \\
-\lambda & 0 & \epsilon-9 & 30 & \cdots & & & & & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
 & & & & \cdots & -\lambda & 0 & [\epsilon-1-4(n-1)] & 2n(n-1) & \cdots \\
 & & & & \cdots & 0 & -\lambda & 0 & (\epsilon-1-4n) & 2n(n+1) \\
\cdots & & & & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{array}\right| . \qquad (4)$$

This is the well-known Hill determinant of the problem. The eigenvalue condition of the anharmonic oscillator is therefore given by the vanishing of this determinant. It is interesting to note that if D_n stands for the $(n+1)\times(n+1)$ approximant to D, then the D_n's satisfy the following difference equation:

$$D_n=(\epsilon-1-4n)D_{n-1}-16\lambda n(n-1)(n-\tfrac{1}{2})(n-\tfrac{3}{2})D_{n-3}\,. \qquad (5)$$

To facilitate numerical calculation we extract the asymptotic part from D_n, writing

$$D_n=\Gamma(n+2)P_n\,, \qquad (6)$$

whence the P_n's satisfy

$$(n+1)P_n=(\epsilon-1-4n)P_{n-1}-16\lambda(n-\tfrac{1}{2})(n-\tfrac{3}{2})P_{n-3}\,. \qquad (7)$$

This equation (7) is the basis of our numerical analysis for the determination of the eigenvalues. The eigenvalues are the zeros of the D_n, i.e., of P_n in the limit $n\to\infty$. The lowest root of D will correspond to the ground-state energy level, and the various excited energy levels will be given by the sequence of higher roots.[8] To find the energy levels we therefore need to determine the roots of the characteristic polynomials P_n associated with the determinants for large n. Equation (7) affords a very simple procedure for generating characteristic polynomials of all higher degrees. In this connection we would like to point out some interesting properties of our characteristic polynomials P_n:

(i) The characteristic polynomial of any given order has coefficients which alternate in sign, showing that there are no real negative eigenvalues.

(ii) Near the lowest root the derivatives of the characteristic polynomials P_{n-1} and P_{n-3} for large n are of the same sign. Hence from Eq. (7) we can conclude that for sufficiently large n the nth-order characteristic polynomial P_n will have a zero between the zeros of P_{n-1} and P_{n-3}, showing that the lowest root of P_n will stabilize as $n\to\infty$. We illustrate this property in Table I. Similar arguments can be used to establish the stability of all higher roots.

TABLE I. Rate of convergence of ϵ for polynomials of high order (N).

N	$\lambda=0.1$	N	$\lambda=1.0$
38	1.065 285 509 543 767	100	1.392 351 641 522 185
39	1.065 285 509 543 721	101	1.392 351 641 527 460
40	1.065 285 509 543 701	102	1.392 351 641 537 939
41	1.065 285 509 543 722	103	1.392 351 641 526 918
42	1.065 285 509 543 721	104	1.392 351 641 527 298
43	1.065 285 509 543 715	105	1.392 351 641 534 760
44	1.065 285 509 543 717	106	1.392 351 641 529 254
45	1.065 285 509 543 719	107	1.392 351 641 527 879
46	1.065 285 509 543 717	108	1.392 351 641 532 721
47	1.065 285 509 543 717	109	1.392 351 641 530 279

We now search for this stable root numerically by computing successively the lowest zeros of the

TABLE II. Comparison of Hill-determinant eigenvalues ϵ for small λ with Borel-Padé approximants ϵ_B of Ref. 6. The values of ϵ shown indicate the limits of the stable solution.

λ	ϵ_B	N	ϵ
0.1	1.065 285 509 543 70	100	1.065 285 509 543 71
0.2	1.118 292 654 35(85)	100	1.118 292 654 367 03
0.3	1.164 047 157 0(754)	100	1.164 047 157 353 84
0.4	1.204 810 324(767 4)	100	1.204 810 327 372 49
0.5	1.241 854 04(667 82)	100	1.241 854 059 651_{50}^{49}
0.6	1.275 983 5(218 545)	100	1.275 983 566 342 5_9^4
0.7	1.307 748 5(315 493)	100	1.307 748 651 1_{20}^{19}
0.8	1.337 544 9(370 465)	100	1.337 545 208 14_8^7
0.9	1.365 669 2(831 623)	100	1.365 669 825 78_6^2
1.0	1.392 350 (653 679 1)	100	1.392 351 641 5_4^2

TABLE III. Comparison for large λ's.

λ	ϵ_B	N	ϵ
1	1.392 350 (6)	100	1.392 351 6
2	1.607 50(93)	100	1.607 541 3
3	1.769 4(141)	140	1.769 588 8
4	1.902 (6241)	160	1.903 136 9
5	2.017 (2350)	180	2.018 340 6
6	2.118 (5436)	180	2.120 532 9
7	2.209 (7320)	200	2.212 914 2
8	2.292 (8867)	220	2.297 577 8
9	2.369 (4637)	240	2.375 978 5
10	2.440 (5273)	240	2.449 174 0
11	2.506 (8834)	260	2.517 960 8
12	2.56(91603)	280	2.582 955 4
13	2.62(78593)	280	2.644 646 5
14	2.68(33879)	300	2.703 428 6

sequence of polynomials $P_4, P_5, \ldots, P_{100}$, etc. In Tables II and III we give the stabilized value of the lowest energy level for various values of λ, the anharmonicity constant. For small values of λ the stability of the root sets in for comparatively lower-order polynomials and the energy level is correctly given by the first few terms of the Bender and Wu expansion. For higher values of λ we compare our answers with those given by the Padé approximants of the Borel sum of the perturbation series. The agreement of our results with the latter is remarkable, as can be seen from Tables II and III.

For large λ, our energy eigenvalues satisfy the condition that $\epsilon(\lambda)/\lambda^{1/3}$ tends to a finite limit, while the Borel-Padé approximants $\epsilon_B(\lambda)$ have the defect that they become constant. Also, our results always lie within the bounds quoted in Ref. 5.

For completeness we discuss briefly the nature of the ground-state wave function. Defining $R_n = C_{n+1}/C_n$, we find from Eq. (3) that the R_n satisfy

$$2(n+1)(2n+1)R_n = (4n+1-\epsilon) + \lambda(R_{n-1}R_{n-2})^{-1}, \quad (8)$$

which in the limit of large n has the solution

$$R_n \underset{n\to\infty}{\sim} (\lambda/4n^2)^{1/3}. \quad (9)$$

Thus the radius of convergence of our series [Eq. (2)] is infinite and the wave function is an entire function of x.

It is easily checked that for large x the wave function (2) is bounded above and below by[9]

$$x^{1/2}e^{-x^2/2}e^{-(\lambda/4)^{1/2}x^3/3} < \psi(x) < \frac{e^{-x^2/2}}{1-(\lambda/4)^{1/3}x^2}. \quad (10)$$

Moreover, near the origin it behaves like $e^{-x^2/2}$. This establishes the normalizability of the ground-state wave function.

We further note that if one expands the wave function in a normalized Hermite-polynomial basis,[1] the associated difference equation is given by

$$\tfrac{1}{4}[n(n-1)(n-2)(n-3)]^{1/2}a_{n-4} + \tfrac{1}{2}(2n-1)[n(n-1)]^{1/2}a_{n-2} + \tfrac{1}{2}(2n+3)[(n+1)(n+2)]^{1/2}a_{n+2} + \tfrac{1}{4}[(n+1)(n+2)(n+3)(n+4)]^{1/2}a_{n+4} - \left[\frac{\epsilon-1-2n}{\lambda} - \tfrac{3}{4}(2n^2+2n+1)\right]a_n = 0. \quad (11)$$

The resulting Hill determinant is real and symmetric, showing that all the eigenvalues are real. We have calculated the lowest zero of the first few approximants of this determinant. This provides a good check on our earlier results.[10] However, the approximants to the Hill determinant corresponding to Eq. (11) do not satisfy a simple difference equation of the type (5), and numerical computation for large n becomes involved.

Finally, we remark that the Hill-determinant method used above for the anharmonic λx^4 term can easily be extended to the Hamiltonian[11]

$$H = -d^2/dx^2 + x^2 + \lambda x^{2m}. \quad (12)$$

The analogous $(n+1)\times(n+1)$ approximant to the Hill determinant D_n^m for the eigenvalue problem now satisfies the following recurrence relation:

$$D_n^m = (\epsilon - 1 - 4n)D_{n-1}^m - (-1)^m\lambda\,\tilde{a}_n\tilde{a}_{n-1}\cdots\tilde{a}_{n-m+1}D_{n-m-1}^m, \quad (13)$$

where the $\tilde{a}_n$'s are of order n^2. The zeros of D_n^m for $n\to\infty$ are, as before, the various energy levels of the problem.

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[8]The stable roots of the characteristic polynomials P_n for large n are always real, as we are working with a Hermitian Hamiltonian. Complex roots can occur for low n in various successive orders of the determinants. However, we expect that these will never be stable.
[9]Our bounds are consistent with the asymptotic behavior of the wave function found by Loeffel and Martin [J. J. Loeffel and A. Martin, CERN Report No. CERN-TH-1167, 1970 (unpublished)].
[10]Equivalently, the eigenvalues can be obtained from the zeros of the Fredholm determinant associated with the difference equation (11). This equation can be written in the form

$$a_n = \sum_{l=0}^{\infty} \mathcal{G}_{n,l}\, b_l a_l ,$$

where $\mathcal{G}_{n,l}$ is the Green's function of the difference equation. An exact analytic form for $\mathcal{G}_{n,l}$ has been obtained.
[11]We have also investigated mass renormalization in a one-dimensional model Hamiltonian with nonpolynomial interaction.

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Internal-Symmetry Groups and Their Automorphisms*

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It is proposed that outer automorphisms of degenerate internal-symmetry groups must be symmetry operators themselves. In general, however, they are hidden (spontaneously broken) symmetries. Consequences of this proposition are studied. It is found that internal-symmetry groups are not arbitrary but that their intrinsic properties play an important role. The existence of discrete symmetries (such as charge conjugation) follows naturally from assuming the continuous symmetry groups (such as gauge groups). We also find that the enlargement of the isospin symmetry and parity leads directly to the chiral SU(3)×SU(3), so that the existence of an "exact SU(3) limit" is in principle not allowed.

I. INTRODUCTION

Symmetry has always played an important role in physics. Historically the rotational and translational symmetries were the first to be studied. The theory of relativity brought in the Lorentz invariance. With the advent of quantum mechanics, discrete space-time symmetries (parity and time-reversal) came into existence. Finally, the study of elementary-particle physics brought forth a whole new class of symmetries – the internal symmetries, such as the charge conjugation, isospin, unitary spin, and many more "higher symmetries."

The basic difference between space-time (excluding possibly the discrete symmetries) as compared with the internal symmetries seems to lie in that the space-time coordinates are physically measurable quantities, while the corresponding group space of the internal-symmetry groups are fabrications with no physical significance whatsoever.

Thus, the "isospin space" is only introduced to facilitate the comparison of isospin with ordinary spin. The physically important (and meaningful) quantities are the isospin operators. In fact, we need not talk about the isospin space at all. (Of course it may happen in the future that even the isospin space will acquire some physical meaning. For the moment, at least, this is not the case.)

If the only physically meaningful quantities in the internal-symmetry groups are the group elements, then we may expect that the intrinsic group structure plays an important role. In this work we will discuss the restrictions on the internal-symmetry groups which arise from their automorphisms.

In order to facilitate our discussions, it is convenient to first clarify the origin of symmetry operators in physics. This will be done in Sec. II. We will show that there is a one-to-one correspondence between symmetry operators and conventions. Indeed, in the quantum-mechanical sense, each symmetry operator actually carries out a change of convention.

We are then naturally led to ask the question: Is there any convention in our use of internal-symmetry groups? Section IV is devoted to this problem.