# BRIEF REPORTS

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## Bound-state eigenvalues for polynomial potentials

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I investigate a recently developed method for obtaining bound-state eigenvalues of anharmonic oscillators, and from it derive useful approaches that converge faster. The method consists of writing the eigenfunction as an exponential of a polynomial times a power series, in which the former factor is properly chosen to simplify the resulting recursion relations for the coefficients of the expansion. I also apply the method to central-field models.

Quantum-mechanical anharmonic oscillators and simple central-field-potential models have received considerable attention for many reasons. In addition to their physical applications, they are interesting as a benchmark for new algorithms to solve the Schrödinger equation. Furthermore, the simplicity of the Schrödinger equation for these models enables one to investigate their mathematical properties in detail, so that one can understand more complicated quantum-mechanical problems. In this respect I mention the remarkable knowledge of perturbation theory resulting from the study of anharmonic oscillators [1].

There is a vast literature on anharmonic oscillators and central-field models. Here I only mention those methods based on a power-series expansion of the wave function [2,3], because they are relevant to the present Brief Report. In particular, I am interested in the approach developed recently by Chhajlany and Malnev [4], which they applied to one-dimensional anharmonic oscillators. In order to discuss this method I write the one-dimensional, time-independent Schrödinger equation as

$$\Psi''(x)+[E-V(x)]\Psi(x)=0 , \tag{1}$$

in which $E$ is the energy, $V(x)$ is the potential-energy function and primes indicate differentiation with respect to $x$. I look for a solution of Eq. (1) of the form $\Psi(x)=u(x)\Phi(x)$, where $\Phi'(x)=-f(x)\Phi(x)$, and rewrite Eq. (1) as a differential equation for $u(x)$:

$$u''-2fu'+(E-V-f'+f^2)u=0 . \tag{2}$$

The form of the function $f(x)$ depends on the form of $V(x)$ as illustrated below. For the sake of concreteness, and to facilitate the discussion of the method, I choose the quartic oscillator for which $V(x)=x^4$. Following Chhajlany and Malnev [4] I consider $V(x)=x^4+\beta^2x^6$. If $f(x)=f_0x+f_1x^3$ and

$$u(x)=\sum_{j=0}^{\infty}u_jx^{2j+p} , \tag{3}$$

the coefficients $u_j$ have to obey the recursion relation

$$(2j+p+1)(2j+p+2)u_{j+1}+[E-f_0(4j+2p+1)]u_j +[f_0^2-f_1(4j+2p-1)]u_{j-1}+(2f_0f_1-1)u_{j-2} +(f_1^2-\beta^2)u_{j-3}=0 , \tag{4}$$

where $j=0,1,\ldots$ and $u_j=0$ if $j<0$. It follows from the indicial equation obtained when $j=-1$ that $u_0\neq0$ provided that either $p=0$ (even states) or $p=1$ (odd states). Chhajlany and Malnev [4] chose $f_0=(2N+p-1/2)^{1/3}$ and $f_1=\beta=1/(2f_0)$ so that Eq. (4) reduces to a three-term recursion relation because the coefficients of $u_{j-2}$ and $u_{j-3}$ vanish for all $j$ values. Furthermore, if one chooses the energy in such a way that $u_N=0$ then $u_{N+1}$ also vanishes and $u_j=0$ for all $j\geq N$. As $N$ tends to infinity $\beta$ tends to zero and $E(x^4+\beta^2x^6)$ approaches $E(x^4)$ from above. The wave function is square integrable because it is a finite polynomial times $\exp(-f_0x^2/2-f_1x^4/4)$. An additional advantage of this method, as pointed out by Chhajlany and Malnev [4], is that one can find upper and lower bounds to the energies of a given quartic-sextic oscillator.

I carried out a numerical investigation using the method of Chhajlany and Malnev [4] and found that it converges rather slowly to the energies of the quartic oscillator. The main reason appears to be that $\beta$ does not

 

approach zero quickly as $N$ increases. Therefore, in order to improve the rate of convergence, I simply set $\beta=0$ in the recursion relation (4) keeping $f_0$ and $f_1$ exactly as above because their choice is perfectly justified in the method of Chhajlany and Malnev [4]. From now on I call this approach case II. Because $f_1\to 0$ as $N\to\infty$, I also tried a case III which is obtained from case II with $f_1=0$. In the latter two cases I obtained the energy from the roots of $u_{N+1}=0$. I refer to the choice made by Chhajlany and Malnev [4] discussed above as case I.

It is worthwhile to compare case III with the method of the Hill determinant proposed by Biswas *et al.* [2] and improved by Banerjee *et al.* [3]. The former authors chose $f_0=1$ for the anharmonic oscillator, finding that the convergence properties of the method deteriorated rapidly as either the quantum number or the coupling parameter increased. Banerjee *et al.* [3] adjusted the value of the scaling parameter $\alpha=f_0/2$ according to the state and value of the coupling constant considered and obtained highly accurate eigenvalues for many states and several problems. In the present case the value of $f_0$ is dictated by the recursion relation, depends on $N$ explicitly, and is apparently independent of the state considered. An appealing feature of the procedure discussed here is that one obtains the value of $f_0$ directly from the recursion relation instead of resorting to external criteria and empirically fitted constants in the expression for the scaling parameter [3].

The power series $u(x)$ in cases II and III does not reduce to a polynomial because the recursion relations for the coefficients $u_j$ have four terms. For this reason one should prove that the resulting wave functions are square integrable. Besides, as the roots of $u_{N+1}=0$ are not exact eigenvalues of a closely related model as in case I, one cannot say beforehand whether they are bounds to the energies of the quartic oscillator.

Table I shows the roots of $u_{N+1}=0$ for the ground state of the quartic oscillator and for the three cases discussed above. I also considered the choice $f_0=1$, and $f_1=\beta=0$ that leads to the method of the Hill determinant [2,3]. It follows that cases II and III converge much faster than case I and that the former become rapidly indistinguishable as expected from the fact that $f_1\to 0$ as $N\to\infty$. Case II provides upper bounds to the energy that are much tighter than those given by case I, but I am presently unable to justify this result. I found the same behavior for all the states considered of this and other models. The only difference is that the velocity of convergence decreases slightly with the quantum number as expected from the following heuristic argument. Since $u_j$ is a polynomial function of $E$ of order $j$ then the root $u_{N+1}=0$ for the $n$th eigenvalue appears for the first time when $N=n-1$ and is thereby further from the convergence limit than the smaller roots that appeared in earlier steps of the convergence process. Because the value of $N$ for a given accuracy depends on the quantum number and $f_0$ depends on $N$ explicitly, one concludes that $f_0$ depends on $n$ indirectly. One may therefore argue that case III is closely related to the method of the Hill determinant proposed by Banerjee *et al.* [3]. As shown in Table I both case II and case III converge faster than the method of the Hill determinant [2,3], which suggests that present choice $f_0\approx N^{1/3}$ is preferable to the prescription in Ref. [3]: $\alpha\approx n^{1/3}$.

To apply case II to a problem with a polynomial potential of order $2k$ one just chooses $f(x)$ to be a polynomial of order $k+1$ or $k+2$ and sets its coefficients so that as many terms as possible in the recursion relation vanish when $j=N$. Case III is simply given by the asymptotic behavior of the coefficients of $f(x)$ in case II as $N$ tends to infinity. In general, one can slightly modify the coefficients of $f(x)$ without much altering the convergence velocity of the method, as shown in case II for the central-field model below.

For illustrative purposes I briefly discuss the anharmonic oscillator with potential-energy function $V(x)=x^2+\lambda x^4$. For case II one finds $f_1=\lambda/(2f_0)$ and $f_0(f_0^2-1)=(2N+p-1/2)\lambda$. The cubic equation for $f_0$ has only one real positive root $f_0\gtrsim[(2N+p-1/2)\lambda]^{1/3}$. When $\lambda=0$ the method yields the exact answer $f_1=0$ and $f_0=1$, so that one reasonably expects accurate results for small values of $\lambda$. For large values of $N\lambda$ one has $f_0\approx(N\lambda)^{1/3}$, which reminds one of the scaling parameter $\alpha\approx(n\lambda)^{1/3}$ proposed in Ref. [3].

Problems that require recursion relations with more terms offer no difficulty other than the consequent enlargement of the polynomial $f(x)$. For instance, to treat the pure sextic oscillator $V(x)=x^6$, one chooses $f(x)=f_0x+f_1x^3+f_2x^5$. According to the rules given above, the coefficients of this polynomial should be

TABLE I. Ground-state energy of the quartic oscillator.

| $N$ | Case I | Case II | Case III | Refs. [2,3] |
|---|---|---|---|---|
| 5 | 1.084 980 850 452 169 | 1.061 914 178 316 474 | 1.071 648 920 792 634 | 1.000 127 603 528 244 |
| 10 | 1.076 878 718 042 57 | 1.060 370 578 598 638 | 1.060 431 975 560 799 | 1.073 514 792 645 938 |
| 15 | 1.073 269 963 666 968 | 1.060 362 131 737 679 | 1.060 361 430 045 079 | 1.057 844 471 312 046 |
| 20 | 1.071 154 053 375 611 | 1.060 362 090 679 441 | 1.060 362 083 913 079 | 1.060 735 617 551 881 |
| 25 | 1.069 737 387 436 911 | 1.060 362 090 485 096 | 1.060 362 090 514 02 | 1.060 363 396 936 691 |
| 30 | 1.068 710 743 276 925 | 1.060 362 090 484 187 | 1.060 362 090 484 709 | 1.060 324 297 550 187 |
| 35 | 1.067 926 388 284 179 | 1.060 362 090 484 183 | 1.060 362 090 484 182 | 1.060 386 166 945 727 |
| 40 | 1.067 304 041 481 431 | 1.060 362 090 484 183 | 1.060 362 090 484 183 | 1.060 350 676 931 148 |
| 45 | 1.066 795 989 946 699 | 1.060 362 090 484 183 | 1.060 362 090 484 183 | 1.060 366 754 261 531 |
| 50 | 1.066 371 937 516 946 | 1.060 362 090 484 183 | 1.060 362 090 484 183 | 1.060 360 408 362 112 |

$f_0=[(4N+2p-1)^2(4N+2p-3)/(20N+10p-7)]^{1/4}$ ,

$f_1=f_0^2/(4N+2p-1)$ ,

and

$f_2=(1-f_1^2)/(2f_0)$

for case II and $f_0=[(4N+2p-1)/5]^{1/2}$, $f_1=(1/5)^{1/2}$, and $f_2=0$ for case III. Here, the velocity of convergence is greater for the latter than for the former, and in both cases $f_0\approx N^{1/2}$ as $N$ tends to infinity. As in the previous example, case II converges from above. The velocity of convergence of the method is remarkably large for this model, though it is smaller than for the quartic oscillator as expected from the stronger singularity of the potential-energy function $V(x)=x^6$ at infinity. The method converges quickly even when $f_0=[(4N+2p-1)/5]^{1/2}$, and $f_1=f_2=0$, which leads to an improved method of the Hill determinant.

The method developed above also applies to three-dimensional models with central-field potentials. After factorizing the angular degrees of freedom one is left with the radial part of the Schrödinger equation, which one can write

$$\Psi''(r)+[2E-2V(r)-l(l+1)/r^2]\Psi(r)=0 , \tag{5}$$

in which $l=0,1,\ldots$ is the angular momentum quantum number. To illustrate the procedure I choose the simple potential $V(r)=r$, for which the Schrödinger equation cannot be solved exactly. In order to apply the method of Chhajlany and Malnev [4] I consider the potential $V(r)=r+\beta^2r^2$ and choose $f(r)=f_0+f_1r$. As before I factorize the wave function as $u(r)\Phi(r)$ in which $\Phi'(r)=-f(r)\Phi(r)$. Under such conditions the coefficients of the expansion

$$u(r)=\sum_{j=0}^{\infty}u_jr^{j+l+1} \tag{6}$$

have to satisfy the recursion relation:

$$(j+2)(j+2l+3)u_{j+2}-2f_0(j+l+2)u_{j+1}+[2E+f_0^2-f_1(2j+2l+3)]u_j+2(f_0f_1-1)u_{j-1}+(f_1^2-2\beta^2)u_{j-2}=0 . \tag{7}$$

In order to reduce (7) to a three-term recursion relation it is necessary that $f_1=2^{1/2}\beta=1/f_0$. If in addition one requires that $f_0$ be a root of $f_0^3+2Ef_0-2N-2l-3=0$ and obtains the energies from the roots of $u_{N+1}=0$, then the expansion (6) reduces to a finite polynomial and the resulting eigenfunctions are square integrable provided $f_0>0$. The latter condition is met for all $N>1$. So far I have described case I. To derive case II one should simply set $\beta=0$ according to the above-mentioned prescription. However, for the sake of simplicity I choose $f_1=1/f_0$, and $f_0=(2N+2l+3)^{1/3}$, the latter coming from the fact that for a given energy value the root of the cubic equation for $f_0$ satisfies $f_0^3/(2N+2l+3)\rightarrow 1$ as $N\rightarrow\infty$. Clearly, this choice is a mixture of what I described as cases II and III, but I will refer to it as case II nonetheless. Case III follows from case II and the condition $f_1=0$, which again leads to the method of the Hill determinant [2,3] with an exponential factor $\exp(-f_0r)$ that depends on the approximation order $N$.

Table II shows the roots of $u_{N+2}=0$ for the three cases discussed above. Again cases II and III converge much faster than case I and cases I and II yield upper bounds to the energy. Furthermore, in this example the equations for cases II and III are simpler than those for case I because in the latter one has to solve the cubic root for $f_0$. Excited states behave exactly in the same way, the only difference being that the larger the radial quantum number the larger the value of $N$ for the same accuracy.

The results above suggest that the approaches termed case II and case III are useful in obtaining highly accurate eigenvalues of the Schrödinger equation with a polynomial potential. Case II is preferable because in the examples considered it converged smoothly from above and in this sense it is an improvement to the method of the Hill determinant which does not exhibit an orderly behavior [2,3]. Furthermore, cases II and III converge faster than the method of the Hill determinant and do not require an empirical fitting of the scaling parameter [3]. However, for case II to be sound theoretically one has to prove rigorously under which conditions it converges from above. On the other hand, case I converges more slowly, but it is constructed in such a way that $E(N)>E(N+1)>E$ (exact) always occurs, at least for the simple examples considered here. In addition to this, case I gives the exact answer for a particular class of problems and enables one to derive upper and lower

TABLE II. Ground-state energy for $V(r)=r$.

| $N$ | Case I | Case II | Case III |
|---|---|---|---|
| 5 | 2.079 180 908 203 125 | 1.913 363 278 357 528 | 1.881 563 508 502 779 |
| 10 | 1.995 303 955 078 125 | 1.857 621 858 328 545 | 1.851 423 063 510 716 |
| 15 | 1.960 924 072 265 625 | 1.855 794 540 395 09 | 1.855 816 542 272 643 |
| 20 | 1.941 705 322 265 625 | 1.855 757 642 573 641 | 1.855 758 809 791 133 |
| 25 | 1.929 246 826 171 875 | 1.855 757 088 496 917 | 1.855 757 046 255 503 |
| 30 | 1.920 428 466 796 875 | 1.855 757 081 566 467 | 1.855 757 081 161 458 |
| 35 | 1.913 814 697 265 625 | 1.855 757 081 490 014 | 1.855 757 081 499 385 |
| 40 | 1.908 636 474 609 375 | 1.855 757 081 489 246 | 1.855 757 081 489 280 |
| 45 | 1.904 461 669 921 875 | 1.855 757 081 489 239 | 1.855 757 081 489 237 |
| 50 | 1.901 011 962 890 625 | 1.855 757 081 489 239 | 1.855 757 081 489 239 |

bounds to the eigenvalues of others [4].

The results obtained in this paper show clearly that the minimum size recursion relation is not necessarily the most efficient way to calculate the eigenvalues. The choices of the parameters in cases II and III are not the best ones. A numerical investigation showed that other values of $f_0$ and $f_1$ led to faster-converging algorithms. However, as I have been unable to develop a systematic procedure to obtain them I believe it is of no value to discuss here such alternative choices. Besides, the gain of convergence speed did not seem to be worth the additional effort required to optimize the values of $f_0$ and $f_1$ in such a numerical way.

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