Bound states of anharmonic potentials

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A procedure based on the exact solutions of multiple-step recursion relations with successive coefficients is shown to provide upper bounds to the bound-state energies of a class of anharmonic-oscillator potentials. Any finite set of energy levels can thereby be estimated to any accuracy. The associated wave functions are guaranteed to be normalizable.

Anharmonic oscillators are of great interest in quantum physics.[1] Their exact solutions for arbitrary couplings are hard to find. This has culminated into the development of many fascinating approximation techniques, some perturbative and some nonperturbative. Among the modern ones, we have, for example, the two-step procedure,[2] the operator method,[3] various $1/N$ expansions for spherically symmetric potentials,[4] the rational function approach[5] and supersymmetric quantum-mechanics-based methods.[6] In addition, one has, of course, the Hill determinant method.[7]

The use of these methods often requires answering two major questions that relate to the normalizability of the wave functions and the convergence of the associated expansions. Such questions are usually hard to answer unambiguously.

This work formulates a technique in which such awkward difficulties simply may not arise. The normalizability of the solutions will be built in and there will be no small parameter expansions whose convergence can be in any doubt. We shall demonstrate that for a class of anharmonic-oscillator Hamiltonians, the given potential function can be enlarged such that the modified Hamiltonian admits a subset of manifestly normalizable solutions. Leach[8] and others[8] have discussed the techniques for realizing such solutions. However, we now observe that such a subset of exact solutions can be made progressively larger by forcing the auxiliary couplings to decrease monotonically. In the process, therefore, the corresponding energy eigenvalues tend monotonically to the energy eigenvalues sought. The attendant wave functions remain always normalizable. It will be ensured that the convergence to the true eigenvalues is from above.

We begin with the problem of the one-dimensional potential

$$V=bx^4, \quad b>0 .$$

To solve this problem, we examine the potential

$$U_1=bx^4+cx^6, \quad c>0 . \tag{1}$$

The associated Schrödinger equation is

$$\psi''+(\varepsilon-x^4-\beta^2x^6)\psi=0 . \tag{2}$$

In Eq. (2) we have used the scales for the quartic oscillator. Let

$$\psi=\exp\left[-\frac{\beta x^4}{4}-\gamma\frac{x^2}{2}\right]v(x) .$$

The parameter γ will be specified shortly. From Eq. (2) we now have

$$v''-2(\beta x^3+\gamma x)v' +[\varepsilon-\gamma+(\gamma^2-3\beta)x^2+(2\beta\gamma-1)x^4]v=0 . \tag{3}$$

Choose

$$2\beta\gamma=1 . \tag{4}$$

Writing $v=\sum_n a_n x^n$ we convert Eq. (3) into the three-step relation

$$(n+3)(n+4)a_{n+4}+[\varepsilon-\gamma(2n+5)]a_{n+2} +[\gamma^2-\beta(2n+3)]a_n=0 . \tag{5}$$

Equation (5) allows v to be a polynomial of degree k provided

$$a_k\neq 0, \quad a_{k+2}=a_{k+4}=0 , \tag{6}$$

with $k=2m$ or $k=2m+1$, $m=0,1,2,\ldots$. Equation (6) immediately gives

$$\gamma^2=\beta(2k+3) , \tag{7}$$

so that

$$\beta^3=\frac{1}{4(2k+3)} . \tag{8}$$

The condition $a_{k+2}=0$ then provides the corresponding energy eigenvalues for the potential U_1. For this purpose the coefficient a_{k+2} is best expressed as a $(m+1)\times(m+1)$ determinant using Eq. (5). Then one easily finds that for $k=2m$ (or $2m+1$) there are $m+1$ exact solutions of even (or odd) parity, respectively. Such

solutions always correspond to the lowest energy states of the given parity. For the remaining solutions v is not a polynomial. These will not interest us here.

As k increases, so does $m+1$—the number of exact solutions. Remarkably, at the same time the tuned sextic coupling β^2 diminishes monotonically as per Eq. (8) and $U_1 \to V$ monotonically. Thus the energy eigenvalues also tend progressively to those of the quartic Hamiltonian from above. The energy spectrum of the quartic potential can thus be ascertained to any desired accuracy. This typical scenario, namely, the increase in k accompanied by a weakening of the auxiliary coupling will be encountered repeatedly in the cases to follow and is indeed the basis of the success of the method.

From a quantitative point of view one notices from Eq. (8) that for $k \cong 100$, the auxiliary coupling $\beta^2 \sim 0.01$. Thus the zeros of approximately a 50×50 determinant can already be expected to provide a good estimate for the low-lying levels of the quartic potential.

In order to get a feeling for the quantitative bounds obtainable let us list some illustrative examples. Consider the case of the ground-state energy ε_0. For $k=0$ we have $v_0=\text{const}$ and $\varepsilon_0=(\frac{3}{2})^{1/3}$ that is about 7.5% above the standard value.[7] For $k=2$, ε_0 is within 5% of the expected result and for $k=4$ we reach the 3% accuracy level. Similar results obtain for the one-node level. Preliminary results indicate that the first bounds for several low-lying levels give roughly similar results. At first glance this seems somewhat surprising, for, one expects the higher levels to be perturbed much more than the lower ones due to the residual sextic coupling. However, the point is that the higher the level, the smaller the residual sextic term for which the first bound is obtained. We may point out also that the zeros of an $n \times n$ determinant give bounds for n levels simultaneously.

Notice that as k grows larger (typically greater than 100) the tuned β^2 values form a quasicontinuum. Thus the problem of a quartic potential perturbed weakly by a sextic term is effectively solved adequately for any small β (typically $\beta \sim 0.1$). In any case the two nearest tuned β values together provide strict upper and lower bounds simultaneously for the energy levels.

Next consider the quartic anharmonic-oscillator potential

$$V(x)=ax^2+bx^4, \quad a>0 .$$

Instead, we first solve the potential $U_2=ax^2+bx^4+cx^6$. Proceeding exactly as before we now have, instead of Eqs. (3) and (5), the equations

$$v''-2(\beta x^3+\gamma x)v' + [\varepsilon-\gamma+(\gamma^2-1-3\beta)x^2+(2\beta\gamma-\lambda)x^4]v=0 \quad (9)$$

and

$$(n+3)(n+4)a_{n+4}+[\varepsilon-\gamma(2n+5)]a_{n+2} + [\gamma^2-1-\beta(2n+3)]a_n=0 . \quad (10)$$

Here, we have used oscillator units so that $V=x^2+\lambda x^4+\beta^2 x^6$ and the parameter γ is chosen such that

$$2\beta\gamma=\lambda . \quad (11)$$

Proceeding as before, polynomial solutions of degree k are obtained if

$$\gamma^2=1+\beta(2k+3) \quad (12)$$

with energies again given by the condition $a_{k+2}=0$.

In Table I we present the first bounds for the ground and first excited states. These are based on the $k=0$ and 1 results, respectively, that lead to the equations

$$\varepsilon_0=\gamma, \quad \gamma^3-\gamma=\tfrac{3}{2}\lambda \quad (13)$$

and

$$\varepsilon_1=3\gamma, \quad \gamma^3-\gamma=\tfrac{5}{2}\lambda . \quad (14)$$

Table I covers the range $\lambda=0.1$ to 100. One sees that just the first step of our procedure that uses only the $v_0 \sim 1$ and $v_1 \sim x$ solutions for U_2 leads to reasonable results. We stress that these results can be improved as much as one pleases by going to larger and larger values of k.

An interesting case is that of weak anharmonicity ($\lambda \sim 0.1$) for which the $k=0$ and 1 results are almost exact and so a useful small parameter expansion in λ for ε_0 and ε_1 can be readily written down from Eqs. (13) and (14), respectively. Such an expansion coincides with the first order of conventional perturbation theory but in contrast it is not beset with any convergence problems.

For the case of strong anharmonicity the $k=4$ and 5 bounds already determine ε_0 and ε_1 correct to about 1%. A detailed numerical compilation of results for this and several other potentials is underway and will be presented elsewhere.

We note that although the existence of the polynomial solutions for the problem of the potential U_2 was formally known earlier,[8] their predictive power was not recognized before.

Next, we consider the full sextic anharmonic-oscillator potential. To solve this problem we introduce the potential

$$U_3=ax^2+bx^4+cx^6+dx^8+ex^{10} . \quad (15)$$

Here, all couplings are positive. Set

TABLE I. First bounds for the ground- and first excited-state energies of the potential $V=x^2+\lambda x^4$ for the range $\lambda=0.1$ to 100 based on the solutions $v=1$ and x, respectively. ε_0 and ε_1 are the results of this calculation and the standard values ε_N are taken from Biswas *et al.* (Ref. 7). The entries in the last column have been suitably rounded off.

λ	ε_0	$\varepsilon_0/\varepsilon_N$	ε_1	$\varepsilon_1/\varepsilon_N$
0.1	1.068	1.003	3.323	1.005
0.2	1.125	1.006	3.574	1.01
0.3	1.176	1.01	3.788	1.015
1.0	1.431	1.03	4.80	1.03
10.0	2.602	1.062	9.114	1.06
100.0	5.376	1.075	19.057	1.07

$$\Psi=\exp\left[\frac{-\alpha x^6}{6}-\frac{\beta x^4}{4}-\frac{\gamma x^2}{2}\right]v(x),\quad \alpha^2\equiv e\ .$$

Selecting the free parameters β and γ suitably, we arrive at a four-term recursion relation with successive coefficients. This makes $v(x)$ a polynomial of degree k provided $a_k\neq 0$ and $a_{k+2}=a_{k+4}=a_{k+6}=0$, which forces the auxiliary couplings d and e to have tuned values that decrease as k increases. With the couplings a, b, and c entirely free, the pure x^6 and ax^2+cx^6 potentials are automatically solved satisfactorily.

To get polynomial solutions for a general potential in the present class of potentials the term with the highest power of x should always be of the form x^{4n+2}, $n=0,1,2,\ldots$. In addition to the dominant asymptotic factor all even subdominant ones should be extracted. The additional parameters so introduced help minimize the size of the recursion relation. A p-step relation requires a coefficient a_k not to vanish but the next $p-1$ coefficients to vanish for a polynomial solution of degree k to materialize. Of the $p-1$ conditions imposed one quantizes the energy and the rest the auxiliary coupling constants. Hence, for example, to solve potentials up to x^8 we must introduce terms up to x^{14}.[9] The problem of such anharmonic oscillators thus reduces effectively to that of solving merely a set of algebraic equations.

Although it is not the purpose of this paper to discuss multiple-well anharmonic potentials in detail, we would like to indicate one interesting fact. If some of the junior couplings are reversed then the full potential can have a double or a multiple-well structure. In such cases too, a partial set of exact solution may be obtained. Consider, for example, the double-well potential

$$v(x)=-x^4+\beta^2x^6\ .$$

Following the procedure leading up to Eq. (8) we now have polynomial solution of degree k, provided

$$2\beta\gamma=-1,\quad \beta^3=\frac{1}{4(2k+3)}\ .$$

For $k=2m$ or $2m+1$, one obtains $(m+1)$ polynomial solutions. The corresponding energies may be positive as well as negative. Several interesting features of the spectrum, especially of the negative branch, can be deduced from these solutions. We shall not go into the details here.

To conclude, some observations are in order. We have seen that for a set of tuned or quantized values of certain coupling constants a subset of solutions splits off from the rest and becomes easily realizable. This is a subset of orthogonal polynomials with appropriate weights. Such subsets (for $k\gg 1$), as we have seen, are well suited to describe the states of the original Hamiltonian. Hence, a detailed study of the properties of such polynomials is a matter of considerable importance.

The fact that an orderly pattern of polynomial solutions emerges for the fine-tuned values of some coupling constants motivates one to speculate that the associated auxiliary Hamiltonians (with potentials $U_1, U_2, \ldots$) develop some deeper symmetry connections that are absent for other arbitrary values of such coupling constants.[10] For large finite k (k being the degree of the polynomial solution) these coupling constants are vanishingly small and form quasicontinuous sets, as we have seen repeatedly. It then means that in any small neighborhood[11] of a given anharmonic-oscillator Hamiltonian there exists a sequence of Hamiltonians which approximate more and more closely the given Hamiltonian and whose subsets of solutions, can be, on account of underlying symmetries, deduced merely by algebraic means. In essence then, even though a given anharmonic Hamiltonian may not be amenable to a direct treatment, a marginally different problem can always be found which is quasi exactly solvable. An excellent knowledge of the original problem thereby obtains without the need to deal with it directly. Inherent in our approach is the reasonable assumption that the energy is not a discontinuous function of the auxiliary coupling constants. For the class of potentials we have studied there is no reason to expect otherwise. The gradual convergence of the predicted energies to known numerical values indicates that this assumption is indeed sound.

Finally, we note that our procedure applies to similar problems in two and three dimensions. Some such three-dimensional problems of considerable interest in atomic and high-energy physics are currently under review.

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[9]The decrease of auxiliary couplings with increasing k holds good for this case also. The structure of the resulting algebraic equations for the cases of higher anharmonicities suggests that this feature continues to remain true.

[10]It is known that a quasi-exactly-solvable (QES) problem could have an association with some underlying symmetry. See, e.g., A. V. Morozov, A. M. Perelomov, A. A. Rosly, M. A. Shifman, and A. V. Turbiner, MIT Preprint No. CTP 1741, 1989 (unpublished). We observe that the dimensions of the representations of the SL(2,R) group correspond to the number of the polynomial solutions for every k for the sextic anharmonic potential in one dimension.

[11]The term neighborhood refers to the parameter space of the auxiliary coupling constants and corresponds to some small domain containing the origin.