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Arbitrarily accurate eigenvalues for one-dimensional polynomial potentials

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Abstract

We show that the Riccati form of the one-dimensional Schrödinger equation can be reformulated in terms of two linear equations depending on an arbitrary function G. When G and the potential (as for anharmonic oscillators) are polynomials the solutions of these two equations are entire functions (L and K) and the zeros of K are identical to those of the wavefunction. Requiring such a zero at a large but finite value of the argument yields low energy eigenstates with exponentially small errors. Approximate formulae for these errors are provided. We explain how to choose G in order to dramatically improve the numerical treatment. The method yields many significant digits with modest computer means. We discuss the extension of this method in the case of several variables.

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1. Introduction

Quantum anharmonic oscillators appear in a wide variety of problems in molecular, nuclear or condensed matter physics. Typically, anharmonic terms appear in expansions about a minimum of a potential, when one tries to incorporate the nonlinear features of the forces responsible for this equilibrium. The most celebrated example is the quartic anharmonic oscillator [1] where a λx^4 term is added to the usual harmonic Hamiltonian. Introducing bilinear couplings among a set of such oscillators leads to a rich spectrum. For instance, multiphonon bound states in one-dimensional lattice models [2]. More generally, one can think about the $\lambda\phi^4$ (or higher powers of ϕ) field theories in various dimensions as systems of coupled anharmonic oscillators.

Anharmonic terms can be treated perturbatively and the perturbative series can be represented by Feynman diagrams. Unfortunately, the coefficients of the series [1, 3] have a factorial growth and the numerical values obtained from the truncated series have an accuracy which is subject to limitations. At fixed coupling, there is an order at which an optimal accuracy is reached. At fixed order, there is a value of the coupling beyond which the numerical values

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are meaningless even as an order of magnitude. In the case of the single-well quartic potential, Padé approximants can be used for the series or its Borel transform. Rigorous proofs of convergence can be established in particular cases [4]. Unfortunately, such a method does not apply to the case of the double-well potential [5] where instanton effects [6, 7] need to be taken into account. It should also be noted that even when Padé approximants converge, the convergence rate may be slow. Strong coupling expansions [8] or variational interpolations [9] sometimes provide more accurate results.

The above discussion shows that finding an expansion which can be used *indiscriminately* for most quantum mechanical problems with polynomial potentials remains a challenging problem. Alternatively, one can use numerical methods. Variational methods are often used to obtain upper and lower bounds on energy levels [10, 11]. These methods are based on rigorous inequalities and are considered superior to methods based on numerical integration [11]. However, the difference between the bounds widens rapidly with the anharmonic coupling and the energy level. Methods based on series expansions in the position variable [12–15] appear to produce more significant digits more easily. However, our understanding of the convergence and numerical stability of these methods seems to be limited to empirical observations. The methods based on series expansions fall into two categories: those based on the evaluations of determinants [12, 14] and those based on boundary conditions at large but finite values of the position [13, 15]. The main goal of this paper is to provide a systematic discussion of the errors associated with this second category of methods and to show how to make these errors arbitrarily small in the most efficient way. With the exception of section 9, we only consider one-dimensional problems. We discuss two types of errors. First, the numerical errors made in calculating the energy which make the wavefunction vanish at some large value of the position $x_{\max}$. Secondly, the intrinsic error due to the finiteness of $x_{\max}$.

The basic elements of the numerical method used hereafter were sketched in [15] and applied to the quartic anharmonic oscillator. We wrote the logarithmic derivative of the wavefunction which appears in the Riccati equation as L/K and showed that these functions were entire. The values of the first ten eigenvalues with 30 significant digits provided for a particular coupling have been used to test new theoretical methods [16]. Two issues were left open in this formulation: first, the basic equations had an interesting invariance which was not understood but could be used to improve the numerical efficiency and secondly, the use of the method for parity non-invariant potentials appeared to be unduly complicated [17].

In section 2, we present a new formulation where these two issues are settled. The basic equations presented depend on an arbitrary *function* denoted by $G(x)$. This freedom can be interpreted as a local gauge invariance associated with the fact that only L/K is physical. The wavefunction is invariant under these local transformations. In section 3, we show how to construct power series for L and K. The complications in the case of parity non-invariant potentials (such as asymmetric double-wells) are minimal. When the potential and the gauge function are polynomials, these series define *entire* function. In other words, it is always possible to construct arbitrarily accurate solutions of the Schrödinger equation for arbitrary E within a given range of the position variable, by calculating enough terms in the expansions of L and K. This allows us to reproduce the asymptotic behaviour of the wavefunction and determine the energy eigenvalues. In section 4, we use the global properties of the flows of the Riccati equation to recall some of the basic results related to the WKB approximation and the Sturm–Liouville theorem. We explain how bifurcations in the asymptotic behaviour of the functions K and L can be exploited to determine the eigenvalues.

It should be noted that the importance of reproducing the proper asymptotic behaviour has been emphasized in variational approaches [18]. It should also be noted that Padé

approximants have been used in conjunction with the Riccati equation in [14], where the quantization condition used was that the approximants give one additional coefficient in the Taylor expansion. This procedure depends only on the coefficients of the expansions used and there is no reference to any particular value of x (as our $x_{\max}$). Consequently, there is no obvious connection between the two approaches.

In the next two sections, we show how to turn the gauge invariance to our advantage. In section 5, the quantitative aspects of the bifurcation are discussed with an exponential parametrization similar to that used to determine Lyapounov exponents in the study of chaotic dynamical system. The exponents are G-dependent. We provide an approximate way of determining the exponents and energy resolution. We explain how our freedom in choosing G can be used to make the bifurcation more violent and improve energy resolution. However, the choice of G also affects the convergence of L and K and consequently the numerical accuracy of the solution of the Schrödinger equation. In section 6, we show in a particular example that for an expansion of L and K at a given order, a judicious choice of gauge can improve the numerical accuracy of an energy level tremendously. We discuss the two principles which allow making optimal choices of G and provide practical methods to determine approximately this optimal choice for the general case. We use these methods to explain some empirical results found in [13].

In section 7, we discuss the error δE on the energy levels due to the finiteness of $x_{\max}$. We propose two approximate formulae valid, respectively, for intermediate and large values of $x_{\max}$ and compatible in overlapping ranges. Note that one can reinterpret the condition that the wavefunction vanishes at $x_{\max}$ as coming from a slightly different problem where the potential becomes infinite at $x_{\max}$. In the path-integral formulation (which can be extended immediately to field theory problems), the fact that the potential becomes infinite at $x_{\max}$ means that paths with values of x larger than $x_{\max}$ are not taken into account. It has been argued [19, 20] that these configurations are responsible for the asymptotic behaviour of the regular perturbative series. In [20], we showed that the perturbative series of several modified problem were convergent. The error formula sets the accuracy limitations of this approach. Some of the methods used in this section could be used for quantum field theory problems.

The anharmonic oscillator can be considered as a field theory with one time and zero space dimensions. It can be used to test approximate methods such as perturbative expansions or semi-classical procedures. An illustrative example is given in [23] where multi-instanton effects were considered and where the splitting of the two lowest levels of a double-well problem was estimated with more than hundred digits. In section 8, we show that our method can be used to reproduce all these digits. Finally, we discuss the generalization of the method to problems with several variables in section 9. For these problems, our ability to reduce the degree of expansion by using optimal gauge functions may be crucial.

2. Basic equations and their gauge invariance

We consider a one-dimensional, time-independent Schrödinger equation $H\Psi = E\Psi$, for a Hamiltonian

$$H = \frac{p^2}{2m} + \sum_{l=1}^{2l} V_j x^j. \tag{1}$$

As is well known, one can re-express the wavefunction in terms of its logarithmic derivative

$$\Psi(x) \propto \exp\left(-\frac{1}{\hbar}\int_{x_0}^{x} \mathrm{d}y\phi(y)\right) \tag{2}$$

and obtain the Riccati form of the equation:

$$\hbar\phi' = \phi^2 + 2m(E - V). \tag{3}$$

It is assumed that $m > 0$ and that the leading power of V is even with a positive coefficient ($V_{2l} > 0$).

Writing $\phi = L/K$, we obtain a solution of equation (3) provided that we solve the system of equations:

$$\hbar L' + 2m(V - E)K + GL = 0 \tag{4}$$

$$\hbar K' + L + GK = 0 \tag{5}$$

where $G(x)$ is an unspecified function. This can be seen by multiplying (4) by K, (5) by L and eliminating GKL by taking the difference. One then obtains the Riccati equation (3) multiplied by K^2. Near a zero of K, one can check that equations (4) and (5) remain valid, namely they impose that ϕ has a simple pole with residue $-\hbar$. This allows the wavefunction to become zero and change sign as the contour goes around the pole on either side.

Equations (4) and (5) are invariant under the *local* transformation

$$\begin{aligned} L(x) &\to Q(x)L(x) \\ K(x) &\to Q(x)K(x) \\ G(x) &\to G(x) - \hbar Q'(x)/Q(x) \end{aligned} \tag{6}$$

where $Q(x)$ is an arbitrary function. It is clear that this transformation leaves ϕ and the wavefunction unchanged. If we choose $G = 0$ and eliminate L using equation (5), we recover the Schrödinger equation for K. Starting from this gauge and making an arbitrary transformation, we find that in general

$$K(x) \propto \Psi(x)\exp\left(-\frac{1}{\hbar}\int_{x_0}^{x} \mathrm{d}y G(y)\right). \tag{7}$$

This shows that when G is polynomial, K is simply Ψ multiplied by an entire function *with no zeros* [21]. This means that the zeros of K and Ψ are identical. In other words, there are no spurious zeros when G is polynomial.

By taking the derivative of equations (4) and (5) and choosing $G(x)$ appropriately, one can obtain the basic equations used in [15]. The explicit form of $G(x)$ is reached by comparing the two sets of equations and integrating one of the differences. The two possibilities are compatible. The resulting integral expression can be worked out easily by the interested reader. The only important point is that the G found that way is in general not polynomial, justifying the spurious zeros found with the original formulation.

3. Solutions in terms of entire functions

The function G can be chosen at our convenience. For instance, we could impose the condition $K = 1$ by taking $G = -L$ and recover the Riccati equation for L. However, the main advantage of equations (4) and (5) is that they are linear first-order differential equations with variables coefficients. It is well known [22] that if we consider these equations for complex x, the solutions inherit the domain of analyticity of the coefficients (provided that this domain is simply connected). If the coefficients are entire functions, there exists a unique entire solution corresponding to a particular set of initial values. In the following, we restrict ourselves to the case where V and G are polynomials.

One can construct the unique solution corresponding to a particular choice of initial values $L(0)$ and $K(0)$ by series expansions. Using $K(x) = \sum_{n=0}^{\infty} K_n x^n$ and similar notation for the other functions, one obtains the simple recursion

$$\begin{aligned} L_{n+1} &= \frac{-1}{\hbar(n+1)} \left(\sum_{l+p=n} (2mV_l K_p + L_l G_p) - 2mE K_n \right) \\ K_{n+1} &= \frac{-1}{\hbar(n+1)} \left(L_n + \sum_{l+p=n} K_l G_p \right). \end{aligned} \tag{8}$$

Given L_0 and K_0, these equations allow us to determine all the other coefficients. For potentials which are parity invariant, and if G is an odd function, L and K can be assigned definite and opposite parities. In this case, we can impose the initial conditions $K_0 = 1$ and $L_0 = 0$ for even wavefunctions and $K_0 = 0$ and $L_0 = 1$ for odd wavefunctions. If the Hamiltonian has no special symmetry, as for instance in the case of an asymmetric double-well, one could leave L_0 indeterminate and fix it at the same time as E using conditions on the wavefunction or its derivative at two different points. These two conditions translate (in good approximation) into two polynomial equations in L_0 and E and can be solved by Newton's method.

The fact that equations (8) determine entire functions provided that V and G are polynomials can be inferred directly from the fact that the coefficients will decrease as $(n!)^{-\kappa}$ for some positive power κ to be determined and in general depending on the choice of G. As we will explain in more detail in section 4, if the leading term in V is $V_{2l}x^{2l}$, one expects from equation (3) that for x large enough

$$\phi(x) \simeq \pm\sqrt{2mV_{2l}}x^l \tag{9}$$

and asymptotically

$$\Psi(x) \propto \exp\left(-\frac{\pm 1}{(l+1)\hbar}\sqrt{2mV_{2l}}x^{l+1} \right). \tag{10}$$

Looking at the general expression for K given in equation (7), one sees that K will have the same asymptotic behaviour provided that the integral of G does not grow faster than x^{l+1}. If this is the case, then $\kappa = 1/(l+1)$. This behaviour is well observed in empirical series.

Note that if G grows faster than x^l, the coefficients decay more slowly and the procedure seems to be less efficient. In the following, we will mostly discuss the case $l = 2$. If we require that G is an odd polynomial growing not faster than x^2, this means that G is homogeneous of degree 1.

4. Quantization from global flow properties

In this section, we use the global properties of the flows associated with the Riccati equation to rephrase some implications of Sturm–Liouville theorem and to justify the asymptotic behaviour given in equation (9). The main goal of this section is to provide a simple and intuitive picture of the bifurcation which occurs when the value of E is varied by a small amount above or below an energy eigenvalue. The main results of this section are summarized in figures 1 and 2.

We consider the solutions of equation (3) obtained by varying E with fixed initial values. It is convenient to introduce an additional parameter s and to rewrite the original equation as a two-dimensional ODE with an s-independent rhs

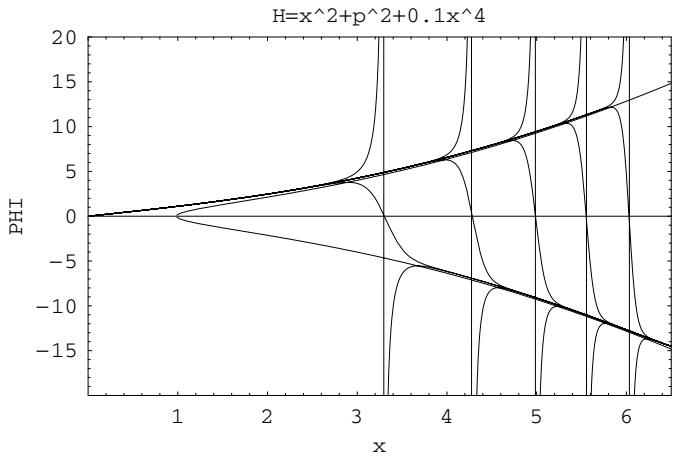

Figure 1. Bifurcations of $\phi(x)$ from the upper part of the WKB curve associated with the ground state energy E_0 for energies $E_0 \pm 10^{-5}$, $E_0 \pm 10^{-10}$, $E_0 \pm 10^{-15}$, $E_0 \pm 10^{-20}$ and $E_0 \pm 10^{-25}$ (from left to right).

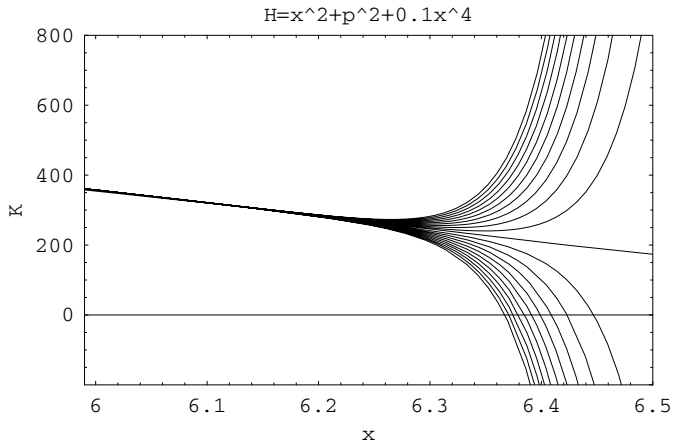

Figure 2. Bifurcations of $K(x)$ from its trajectory for $E = E_0$. The changes in E are $\pm 10^{-30}$, $\pm 2 \times 10^{-30}, \ldots, \pm 10^{-29}$.

$$\hbar\dot{\phi} = \phi^2 + 2m(E - V(x)) \tag{11}$$

$$\dot{x} = 1 \tag{12}$$

where the dot denotes the derivative with respect to s.

The flows in the (x, ϕ) plane have some simple global properties that we now proceed to describe. We consider a solution (phase curve) with initial condition $x = x_0$ and $\phi = \phi_0$ at $s = 0$. We assume that for these values the rhs of equation (11) is > 0. It will become clear later that if such a choice is impossible, a normalizable wavefunction cannot be constructed. With this assumption, the phase curve starts moving up and right as s increases, possibly going through simple poles with residues $-h$. This situation persists unless the rhs of (11) becomes zero. We call the separating curves defined by a zero for the rhs of equation (11), $\phi = \pm\sqrt{2m(V(x) - E)}$, 'WKB curves'. After a phase curve crosses (horizontally) a WKB

curve, it moves right and down. If it crosses the WKB curve again, we can repeat the discussion as at the beginning.

At some point, we reach the 'last' WKB curve (i.e. the farthest right). For x large enough, the potential is dominated by its largest power and the upper (lower) part of this last WKB curve has a strictly positive (negative) slope. For such values of x, if a phase curve crosses the WKB curve, it will do so horizontally and move *inside* the region where the rhs of equation (11) is negative. As s further increases, ϕ decreases, but the phase curve cannot cross the lower part of the WKB curve horizontally which has a strictly negative slope. In the same region, if ϕ has a pole, the curve reappears below the lower part of the WKB curve and will never take positive values again.

In summary, if in the region described above, a phase curve crosses the WKB curve or develops a pole, then it cannot develop a pole again. The other logical possibility is that the phase curve does none of the above. It is thus clear that for fixed E, we can always find an X such that if $x > X$, $\phi(x)$ has no pole. Consequently the two terms involving ϕ in equation (3) cannot grow faster than $2m(E - V)$. Otherwise, $2m(E - V)$ would become negligible and a pole would be necessary. At least one of these two terms needs to match $2m(E - V)$. Inspection of the two possibilities leads to equation (9). Only the positive solution which asymptotically follows the upper WKB curve leads to a normalizable wavefunction.

If we compare two phase curves with identical initial conditions but different E, the curve with larger E initially lies above the other. If the curve with lower E has the first pole at x_1, then that with larger E has the first pole at some $x < x_1$. Remembering that the poles of ϕ produce zeros of Ψ, this rephrases the main idea behind the Sturm–Liouville theorem. An exact energy eigenstate E_n is obtained when the wavefunction has its last zero at infinity. When E is fine-tuned to that value, ϕ follows the upper branch of the WKB curve closely. This trajectory is unstable under small changes in E. If the energy is slightly increased with respect to E_n, ϕ develops a pole and reappears on the lower part of the WKB curve. If the energy is slightly decreased with respect to E_n, ϕ crosses the upper part of the WKB curve and reaches the lower part of the WKB curve. This is illustrated in figure 1 in the case of the ground state of the quartic single-well anharmonic oscillator with $m = 1/2, \hbar = 1, V_2 = 1$ and $V_4 = 0.1$. All the figures in this section and the next two sections have been done with this particular example.

The sensitive dependence on E is also present in the asymptotic behaviour of K. If the energy is slightly increased with respect to E_n, K reaches zero at a finite value of x. If the energy is slightly decreased with respect to E_n, K increases rapidly. This is illustrated in figure 2 for the same example as in figure 1.

We now discuss the initial value ϕ_0. For parity-invariant potentials, one only needs to consider the cases $\phi_0 = 0$ (even Ψ) or $\phi_0 = -\infty$ (odd Ψ) at $x_0 = 0$. For potentials with no reflection symmetry, one needs to ensure that the appropriate behaviour is reached when $x \to -\infty$. This can be implemented in good approximation by requiring that the wavefunction has also a zero at some large negative value $x_{\min}$. For potentials with a reflection symmetry about another point x_1 than the origin, one can impose that the wavefunction ($K(x_1) = 0$) or its derivative ($L(x_1) = 0$) vanish at that point. In all cases, we have an independent condition which allows us to determine ϕ_0.

In summary, for $x_{\max}$ large enough, the condition

$$K(x_{\max}) = 0 \tag{13}$$

provides a sharp upper bound on the energy levels. The lower part of figure 2 makes it clear that as $x_{\max}$ increases, sharper bounds are reached. For potentials that are not parity invariant, an additional condition has to be imposed. In all cases, one obtains polynomial equations

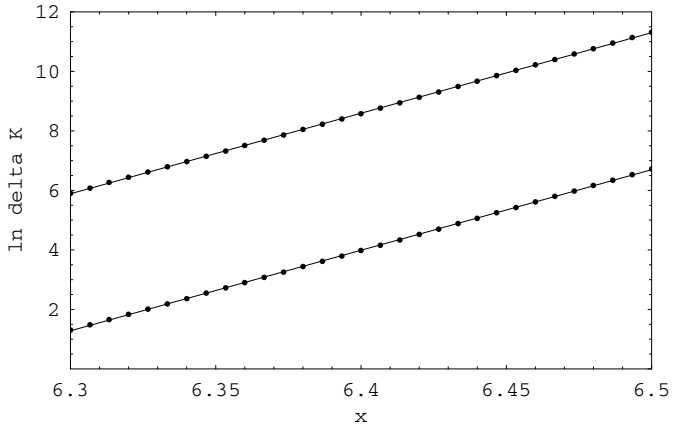

Figure 3. Natural logarithm of $\delta K(x)$ for $E - E_0 = 10^{-30}$ (lower set of point) and $E - E_0 = 10^{-28}$ (upper set of point). Lines are linear fits.

which can be solved for the energy levels given the potential or vice versa using Newton's method. Note also that a sharp lower bound can be found by solving $L(x_{\max}) = 0$. The fact, that in figure 1 a zero of K at $E_0 + \delta$ corresponds to a zero of L at $E_0 - \delta$, suggests that the exact value should be very close to the average of the two bounds.

5. *G*-dependence of the bifurcation

The strength of the bifurcation in K illustrated in figure 2 can be approximately characterized by local exponents. If we consider the departure $\delta K(x)$ from $K(x)$ calculated at some exact energy level E_n, we expect the approximate behaviour

$$\delta K(x) \simeq C(E - E_n)\, \mathrm{e}^{xB}. \tag{14}$$

In other words $\ln(|\delta K(x)|)$ is linear with a slope B independent of the choice of E and an intercept that varies as $\ln(|E - E_n|)$. This situation is approximately realized in the example considered before as shown in figure 3. We have checked in the same example that the sign of the energy difference plays no role. In other words, the same values of C and B can be used above and below E_n.

The exponent B is not uniform. It increases with x and is G-dependent as shown in figure 4. The local values of B have been calculated by fits in regions of width 0.2 with the central value displayed in the horizontal label of figure 4.

The change in B can be understood as follows. If E is changed from E_n to $E_n + \delta E$, then at some point we have a sudden transition from the upper to the lower WKB curve and asymptotically

$$\delta\Psi(x) \propto \delta E \exp\left(+\frac{1}{(l+1)\hbar}\sqrt{2mV_{2l}}x^{l+1}\right). \tag{15}$$

Using equation (7) and expanding about $x_{\max}$, we obtain that, in good approximation

$$B \simeq \frac{1}{\hbar}\left(\sqrt{2mV_{2l}}x_{\max}^{l} - G(x_{\max})\right). \tag{16}$$

As shown in figure 4, this simple expression provides reasonable estimates of B. The slight underestimation comes partly from the fact that equation (16) does not take into account the

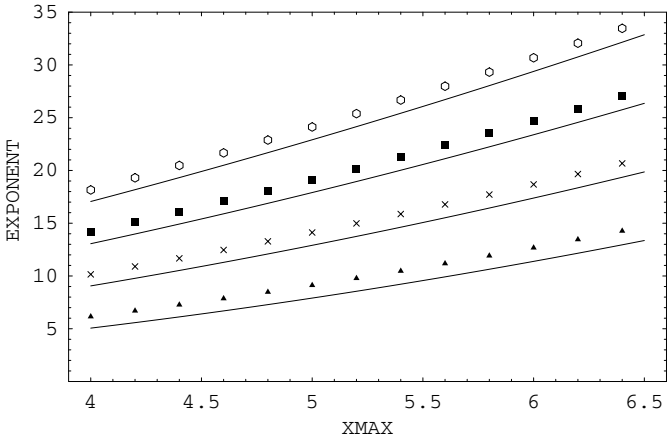

Figure 4. Value of B for various x and for $G = -3x$ (empty hexagons), $G = -2x$ (filled squares) $G = -x$ (crosses) and $G = 0$ (triangles). The continuous lines have been drawn using equation (16).

harmonic term in V. Equation (16) shows that we can increase the strength of the bifurcation near $x_{\max}$ by increasing $x_{\max}$ or $-G(x_{\max})$. This allows us to 'resolve' the energy more accurately. However, at the same time our numerical resolution of $K(x_{\max})$ is affected and we need to take this effect into account. This question is treated in the next section. In general, if we can establish that $K(x_{\max})$ at an energy E very close to E_n, can be calculated with some numerical accuracy δK^{num}, we have the approximate numerical energy resolution

$$\delta E^{\text{num}} \propto \delta K^{\text{num}} \exp\left(+\frac{1}{\hbar}\left(\frac{-1}{l+1}\sqrt{2mV_{2l}}x_{\max}^{l+1} + \int_0^{x_{\max}} \mathrm{d}x\, G(x)\right)\right). \tag{17}$$

6. An optimal choice of G

In this section, we show that from a numerical point of view, the choice of G is important. We discuss the question of an optimal choice, first with an example and then in general. We start with the calculation of the ground state in the case $m = 1/2, \hbar = 1, V_2 = 1$ and $V_4 = 0.1$. We discuss the estimation of the ground state energy using the equation $K(x_{\max}) = 0$ with $x_{\max} = 6$. The fact that we use this finite value for $x_{\max}$ creates an error in the 25th digit (see section 7).

From the discussion in section 3, it is reasonable to limit it to a gauge function of the form

$$G(x) = -ax \tag{18}$$

which, using equation (7), implies that

$$K(x) \propto \Psi(x)\, \mathrm{e}^{\frac{1}{2\hbar}ax^2}. \tag{19}$$

With this restriction, the optimization problem is reduced to the determination of a. As a increases through positive values, the features of Ψ are exponentially amplified, making the bifurcation displayed in figure 2 more violent. Ideally, we would like to take a as large as possible. However, if a is too large, we may need too many coefficients K_n to get a good approximation. If we consider the problem at a given order, the two requirements of sensitivity and accuracy result in a compromise which determines the optimal value of a.

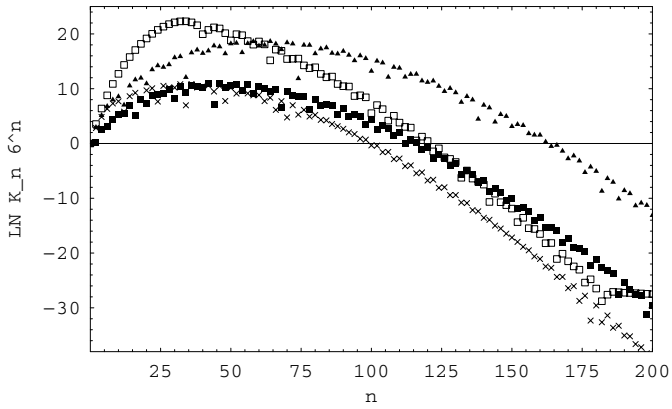

Figure 5. $\ln(|K_n 6^n|)$ versus n, for $G = 0$ (triangles), $G = -x$ (filled squares), $G = -2x$ (crosses) and $G = -3x$ (empty squares).

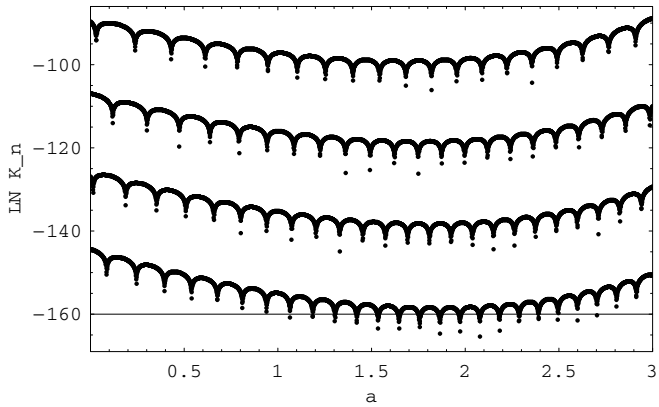

Figure 6. $\ln(|K_n|)$ versus a, for $n = 60$ (upper set), 70 (next set), 80 (next set) and 90 (lower set).

As explained in section 3, the choice of equation (18) guarantees a suppression of the form $(n!)^{\frac{-1}{3}}$ for the coefficients of L and K. However, the choice of a still affects the behaviour of these coefficients significantly as shown in figure 5.

The quantity $K_n x_{\max}^n$ is relevant to decide at which order we need to truncate the series in order to get a good estimate of $K(x_{\max})$. For instance, if we require knowing $K(x_{\max})$ with errors of order 1, we need about 100 coefficients for $a = 2$ but more than 150 for $a = 0$. The corresponding values for $a = 1$ and 3 fall between these two values, indicating that $a = 2$ is close to optimal. This estimate is confirmed by an analysis of the dependence of K_n on a. Sample values are shown in figure 6. We observe rapid oscillations (that we will not attempt to explain) and slowly varying amplitudes which have a minimum slightly below 2. Note that on the logarithmic scale of figure 6, the zeros of K_n give $-\infty$; however, due to the discrete sampling of a, it just generates isolated dots on the graphs. Note also that in figures 5 and 6, the coefficients have been calculated for an accurate value of the ground state energy.

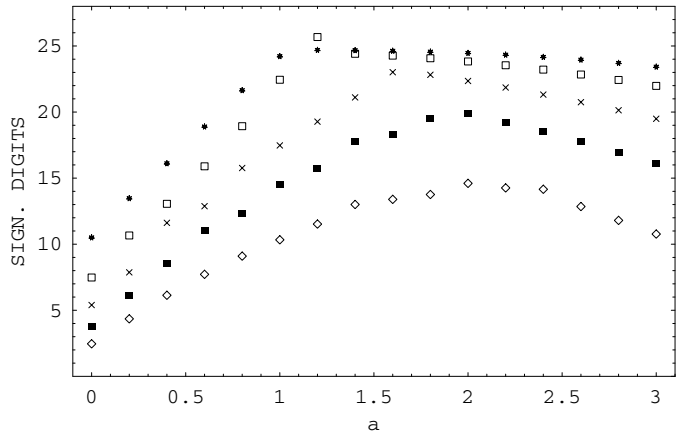

Figure 7. Number of significant digits for E_0 versus a using the condition $K(6) = 0$ with expansions of order 50 (empty diamonds), 75 (filled squares), 100 (crosses), 125 (empty squares) and 150 (stars).

The behaviour of K_n calculated at the value of E sufficiently close to an eigenvalue, can be understood by using the asymptotic form

$$K(x_{\max}) \propto \exp\frac{1}{\hbar}\left(-\frac{1}{l+1}\sqrt{2mV_{2l}}x_{\max}^{l+1} - \int_0^{x_{\max}} \mathrm{d}x\, G(x)\right). \tag{20}$$

We emphasize that the relative sign between the two terms in the exponential is the opposite of that given in equation (17), because we are now on the upper WKB curve. For $a = 0$, equation (20) provides a rough estimate of $K_n x_{\max}^n$. Remembering the minus sign in the parametrization of G (equation (18)), we see that if a is given a small positive value, the argument of the exponential in equation (20) decreases and we can obtain comparable accuracy with less terms in the expansion. Naively, our optimum choice is obtained when the two terms in the exponential cancel. In the general case, this amounts to having

$$\sqrt{2mV_{2l}}x_{\max}^{l+1} \simeq -(l+1)\int_0^{x_{\max}} \mathrm{d}x\, G(x). \tag{21}$$

For the particular example considered here, this cancellation is obtained for $a = (2/3)\sqrt{0.1}x_{\max} \simeq 1.27$. It is clear that when the two terms cancel, the subleading terms neglected in equation (9) should be taken into account. However, in several examples, we found that this simple procedure gives results close to what is found empirically.

We now address the more general question of determining the G-dependence of the number of significant digits that can be obtained from the condition $K(x_{\max}) = 0$ using an expansion of K truncated at a given order. For the example considered before in this section, we see from figure 7 that, for instance for a truncation at order 100, the most accurate answer is obtained for $a \simeq 1.6$. It is worth noting that for this value of a, one gains more than 15 significant digits compared to the $G = 0$ case! This figure also indicates, that as expected, the best possible answer (in the present case, 25 significant digits) can always be achieved by calculating enough coefficients.

Using equation (17) and figure (6), we were able to approximately reproduce the left part of figure 7 ($0 < a < 1$). To give a specific example, at order 100, when one changes a from 0 to 1, δK^{num} becomes four orders of magnitude smaller and the factor $\mathrm{e}^{-(\frac{a}{2\hbar})x_{\max}^2}$ improves the resolution by almost eight orders of magnitude. This approximately accounts for the gain

of 11 significant digits observed in figure 7. A detailed understanding of the figure in the region $1 < a < 2$ is beyond what can be accomplished using the asymptotic form of the wavefunction. However, the naive estimate of equation (21) provides a reasonable estimate of the location of the optimal a.

It should be noted that an ansatz of the form of equation (19) with $a = 1$ has been used in [12] and that the fact that varying a could improve the numerical efficiency was found empirically in [13]. Equation (21) can be used to understand these results. For instance, for $H = p^2 + x^2 + x^8$, we can obtain a very accurate result with $x_{\max} = 2.8$ (see section 7). According to equation (21) the optimal value of a in this case is $a = (2/5)x_{\max}^3 \simeq 8.8$ which is slightly below the value ($\approx$10) suggested in [13]. Note also that equivalently good results can be obtained using $G = -bx^3$.

7. Approximate error formulae

In this section, we discuss the intrinsic error $\delta E = E(x_{\max}) - E(\infty)$ where $E(x_{\max})$ is defined by $\psi(x_{\max}, E(x_{\max})) = 0$, for a given energy level. We emphasize that δE is the error due to the finiteness of $x_{\max}$ independently of practical considerations regarding the numerical estimation of $E(x_{\max})$ which is assumed to be known with an error much smaller than δE in this section. We use the familiar parametrization of the quadratic term of the potential, $V_2 = \frac{1}{2}m\omega^2$ and we restore the dependence on $\hbar$ and m. The error for the ground state of the harmonic oscillator has been estimated in equation (4) of [20]. Using the asymptotic form of the integral in this equation, we obtain

$$\delta E_0^{\text{harm}} \simeq 2\left(\frac{S_0}{\pi\hbar}\right)^{\frac{1}{2}} \mathrm{e}^{-S_0/\hbar} \tag{22}$$

with

$$S_0 = \int_{-\infty}^{+\infty} \mathrm{d}t \frac{1}{2} m((\dot{x}_c(t))^2 + \omega^2(x_c(t))^2) = m\omega x_{\max}^2 \tag{23}$$

and $x_c(t) = x_{\max}\,\mathrm{e}^{-\omega|t-t_0|}$. This corresponds to the semi-classical approximation where the contribution of the large field configurations are obtained by calculating the quadratic fluctuations with respect to $x_c(t)$. The anharmonic corrections can be approximated to the lowest order in the anharmonic couplings by adding a term S_{anh} to S_0 in the exponent of equation (22) with

$$S_{\text{anh}} = \int_{-\infty}^{+\infty} \mathrm{d}t\, V_{\text{anh}}(x_c(t)) \tag{24}$$

and V_{anh} is the anharmonic part of the potential. Our final perturbative estimate is thus

$$\delta E_0 \simeq \delta E_0^{\text{harm}} \exp\left(-\sum_{j=2}^{l}\left(\frac{1}{j\hbar}\right) V_{2j} x_{\max}^{2j}\right). \tag{25}$$

This estimate is accurate if the V_{2j} and $x_{\max}$ are small enough. We expect that for the excited states, the approximate formulae of the form of equation (25) multiplied by a polynomial should hold.

When λ or $x_{\max}$ become too large, equation (25) is not adequate. To obtain a better approximation, we use

$$\frac{\partial}{\partial x_{\max}}\psi(x_{\max}, E(x_{\max})) = 0 \tag{26}$$

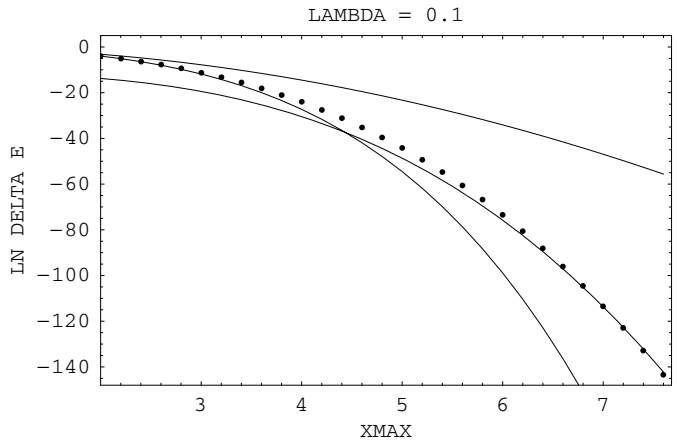

Figure 8. ln (δE_0) as a function of $x_{\max}$ for $\lambda = 0.1$ (black dots). The continuous lines are from top to bottom on the left of the figure: the harmonic case (equation (22)), equation (25) with $V_4 = 0.1$ (fits the dots well on the left of the figure), equation (28) (fits the dots well on the right of the figure).

and the asymptotic behaviour of Ψ. We estimate that $\partial\Psi/\partial E$ is of the order of the non-normalizable WKB solution and as a consequence, δE has the asymptotic form

$$\delta E \simeq P(x_{\max})(\psi(x_{\max}))^2 \tag{27}$$

where P is a polynomial. This form is correct for the ground state of the harmonic oscillator. In the case where the leading term of V is $V_{2l}x^{2l}$, this implies the asymptotic order of magnitude estimate

$$\delta E \approx \exp\left(-\frac{2}{(l+1)\hbar}\sqrt{2mV_{2l}}x_{\max}^{l+1}\right). \tag{28}$$

We have tested the two approximate errors formulae given above (equations (25) and (28)) for the ground state corresponding to $V_{\text{anh}} = \lambda x^4$. We used the numerical values $\hbar = m = \omega = 1$ and $\lambda = 0.1$. The results are shown in figure 8. We see that for small values of $x_{\max}$, the perturbative estimate of equation (25) properly corrects the harmonic result. However when $x_{\max}$ increases, equation (28) gives better results. If the left part of the graph is displayed with a log–log scale, it is approximately linear with a slope close to 3. In figure (8), the proportionality constant not given by equation (28) has been determined by fitting the last five data points on the right of the figure. We conclude that by combining the two approximations it is possible to get a reasonable estimate of the errors on E over a wide range of $x_{\max}$.

We have tested equation (28) for other potentials. For instance, for $H = p^2 + x^2 + x^8$, in order to get 30 significant digits, we estimated that $x_{\max} \simeq 2.8$. We found that the difference between the ground state energy found from the conditions $K = 0$ (upper bound) and $L = 0$ (lower bound) differed in the 30th significant digits.

8. A challenging test

The only practical limitation of the method proposed here is that in some cases the relevant details of the potential appear in widely separated regions, forcing us to calculate a large number of coefficients with many significant digits. A simple example where such problem

may occur is the symmetric double-well with a small quartic coupling where the separation between the wells goes as the inverse square root of the quartic coupling.

In [23], the lowest even and odd energies were calculated for a potential with $m = 1$, $\hbar = 1$, $V_2 = -1/4$, $V_4 = 1/2000$ with 180 significant digits. Remarkably, the authors were able to reproduce the 110 significant digits of the splitting between these two states by calculating instanton effects. We have reproduced the 180 digits of both states using an expansion of order 1700 for K and a value of $x_{\max} = 46$. The calculations were performed with 700 digit arithmetic. The calculation of one level with such a procedure takes less than 2 h with Mathematica on an inexpensive laptop using Pentium3. The computation time increases with the accuracy required. In order to fix the ideas, it takes less than 2 min to reproduce the first 120 digits in the above calculation.

9. The multivariable case

The basic equations presented in section 2 can be extended when the single variable x is replaced by an N-dimensional vector $\vec{x}$. In equation (2), ϕ becomes a vector $\vec{\phi}$ and the integral a line integral. In order to guarantee that the wavefunction is independent of the choice of the line, we require that the curl of $\vec{\phi}$ vanishes. Equation (3) becomes

$$\hbar \vec{\nabla} \vec{\phi} = \vec{\phi} \cdot \vec{\phi} + 2m(E - V). \tag{29}$$

Using $\vec{\phi} = \vec{L}/K$, we write as previously

$$\hbar \vec{\nabla} \vec{L} + 2m(V - E)K + \vec{G} \cdot \vec{L} = 0 \tag{30}$$

$$\hbar \vec{\nabla} K + \vec{L} + \vec{G} K = 0 \tag{31}$$

with $\vec{G}(\vec{x})$ unspecified at this point. These equations imply the multivariable Riccati equation (29) multiplied by K^2. Near a zero of K, these equations imply the same singularity as equation (29). After using equation (31), the condition that ϕ has no curl reads

$$\nabla_i L_{(j)} + G_{(i)} L_{(j)} = \nabla_j L_{(i)} + G_{(j)} L_{(i)}. \tag{32}$$

The parentheses for the vector indices are used in order to distinguish these indices from the order in a power series expansion used later.

The transformation equations (7) can be vectorized trivially with Q treated as a scalar. In the expression of K given by equation (7), the integral becomes a line integral and we require that $\vec{G}(\vec{x})$ has a vanishing curl. This condition is also necessary to establish that different derivatives acting on K commute.

The choice of coordinates to be used depends on the choice of the boundary conditions imposed. If we require Ψ to vanish on a large hypersphere, hyperspherical harmonics should be used. If we require Ψ to vanish on hypercubes (as suggested for lattice problems in [20]) Cartesian coordinates should be used. To fix the ideas, let us consider the case of Cartesian coordinates for two variables x_1 and x_2 with boundary conditions on a rectangle. We expand $K(x_1, x_2) = \sum_{m,n \geqslant 0} K_{m,n} x_1^m x_2^n$ and similar expansions for the two components of $\vec{L}$. The coefficients can be constructed order by order, with the order of $K_{m,n}$ defined as $m + n$. The terms with one derivative yield the higher order terms. For instance, for K, we obtain equations providing $K_{m+1,n}$ and $K_{m,n+1}$ in terms of coefficients of lower order just as in equation (8). A detailed construction shows that if $V(x_1, x_2)$ has no special symmetry, we can determine all the coefficients up to a given order l provided that we supply the values of two coefficients at each intermediate order (for instance $\vec{L}_{m,0}$ for $m \leqslant l$). These coefficients together with E are fixed by the boundary conditions $K(x_{1\min}, x_2) = K(x_{1\max}, x_2) = K(x_1, x_{2\min}) = K(x_1, x_{2\max}) = 0$.

Taking derivatives with respect to the free variables x_1 and x_2, and setting these variables to 0, we obtain an infinite set of conditions. The truncation of this set, together with the truncation of the expansion in the other variable must be studied carefully. If we consider the special case where the problem can be solved by separation of variables, we see that it is important to maintain a uniform accuracy for all the conditions. If all the coefficients have been calculated up to order l, this can achieved in the following way. We retain the order of $l/2$ derivatives of the four conditions in such a way that we get exactly $2l+3$ conditions which can be expanded up to an order close to $l/2$ in the remaining variable. A practical implementation of this program is in progress.

10. Conclusions

In conclusion, we have shown that accurate estimates of the energy levels of arbitrary polynomial potentials bounded from below can be obtained by solving polynomial equations. The fact that the functions L and K are entire guarantees that if we calculate enough terms we will gain proper control of the asymptotic behaviour of the wavefunction. Reaching this goal is in general a difficult task which often requires guesswork and analytical continuations (see e.g. [24]). Here, the convergence of the procedure is guaranteed and the order at which we can terminate the expansion in order to reach a given accuracy can be estimated. In addition, a systematic understanding and control of the errors due to the finite value of $x_{\max}$ have been achieved.

The understanding of the gauge invariance of the basic equations proposed here completely resolves the issues raised from our initial proposal [15]. By varying G, from 0 to $-\phi$, we can interpolate between a situation where K is the wavefunction to another situation where $K = 1$ and $L = \phi$. However, for every other choice of G, only the ratio L/K has a direct physical meaning. By properly choosing G, we can at the same time improve the convergence of K and amplify the bifurcation towards the the non-normalizable behaviour.

The extreme accuracy obtained for two widely separated wells indicates that for reasonably complicated potential, the number of terms that needs to be calculated is not prohibitive. We intend to use this method to test analytical results regarding the role of large configurations in the path-integral and to test semi-classical treatment of potentials with asymmetric wells [6, 7].

The method can be extended in the case of several variables. It remains to be determined if the simultaneous solution of many polynomial equations can be accomplished with a reasonable accuracy. For these problems, the fact that a judicious choice of the arbitrary functions $\vec{G}$ allows us to decrease the order of the expansions may be crucial.

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References

[1] Bender C and Wu T T 1969 *Phys. Rev.* **184** 1231
[2] Wang W Z, Tinka Gammel J, Bishop A and Salkola M 1996 *Phys. Rev. Lett.* **76** 3598

[3] Le Guillou J C and Zinn-Justin J 1990 *Large-Order Behavior of Perturbation Theory* (Amsterdam: North-Holland) and references therein
[4] Loeffel J, Martin A, Simon B and Wightman A 1969 *Phys. Lett.* B **30** 656
Simon B 1970 *Ann. Phys., NY* **58** 76
[5] Brezin E, Parisi G and Zinn-Justin J 1977 *Phys. Rev.* D **16** 408
[6] Coleman S 1985 *Aspects of Symmetry* (Cambridge: Cambridge University Press)
[7] Zinn-Justin J 1989 *Quantum Field Theory and Critical Phenomena* (Oxford: Oxford University Press)
[8] Weniger E 1996 *Phys. Rev. Lett.* **77** 2859
Skala L, Cizek J, Weniger E and Zamastil J 1999 *Phys. Rev.* A **59** 102
[9] Kleinert H 1995 *Phys. Lett.* A **207** 133
[10] Bazley N and Fox D 1961 *Phys. Rev.* **124** 483
Reid C 1965 *J. Chem. Phys.* **43** S186
[11] Payne G and Schlessinger L 1973 *J. Comput. Phys.* **13** 266
[12] Biswas S *et al* 1973 *J. Math. Phys.* **14** 1190
[13] Killingbeck J 1981 *Phys. Lett.* A **84** 95
[14] Fernandez F, Ma Q and Tipping R 1989 *Phys. Rev.* A **39** 1605
[15] Bacus B, Meurice Y and Soemadi A 1995 *J. Phys. A: Math. Gen.* **28** L381
[16] Antonsen F 1999 *Phys. Rev.* A **60** 812
Bietenholz W and Struckmann T 1999 *Int. J. Mod. Phys.* C **10** 531
[17] Oktay B unpublished
[18] Turbiner A 1984 *Sov. Phys.-Ups.* **27** 668
[19] Pernice S and Oleaga G 1998 *Phys. Rev.* D **57** 1144
[20] Meurice Y 2002 *Phys. Rev. Lett.* **88** 141601
Meurice Y 2002 *Nucl. Phys.* B **106** 908
[21] Knopp K 1975 *The Theory of Functions, Part II* (New York: Dover) ch 1 sec 1
[22] Coddington E and Levinson N 1955 *Theory of Ordinary Differential Equations* (New York: McGraw-Hill) ch 3 sec 7
[23] Jentschura U and Zinn-Justin J 2001 *J. Phys. A: Math. Gen.* **34** L253
[24] Bender C and Bettencourt L 1996 *Phys. Rev. Lett.* **77** 4114