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FAST TRACK COMMUNICATION

Finding gaps in a spectrum

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Abstract
We propose a method for finding gaps in the spectrum of a differential operator. When applied to the one-dimensional Hamiltonian of the quartic oscillator, a simple algebraic algorithm is proposed that, step by step, separates with a remarkable precision all the energies even for a double-well configuration in a tunnelling regime. Our strategy may be refined and generalized to a large class of 1D-problems.

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1. Introduction

Obtaining some physically interesting piece of information on a spectrum of a differential operator is generically a difficult problem. For systems in low dimension, say one or two, though numerical approaches can usually compute the spectrum to a high precision, very few is usually known when demanding the standard criterions of rigour of mathematical physics.

The aim of the present communication is to propose a method for finding gaps in the spectrum of a differential operator. We will mainly focus on the stationary one-dimensional non-magnetic Schrödinger equation with a smooth potential $V(x)$ defined on the whole real axis,

$$-\frac{1}{2}\frac{\mathrm{d}^2\varphi}{\mathrm{d}x^2} + V\varphi = E\varphi, \tag{1}$$

but it can be easily understood that our ideas, which will be explained in the first part of this communication (section 2), can be extended to a wider family of ordinary differential equations. For the sake of definiteness, in the second part (section 3) we will illustrate more concretely our method on the quartic oscillator (11) where the numerical 'exact' spectrum will serve us as a touchstone. We will show that we are able to obtain gaps in the energy spectrum, i.e. intervals where there is no eigenenergy, with purely algebraic manipulations involving no integrals. An algorithm is explicitly constructed in the case of the quartic oscillator—but it remains robust under any kind of smooth perturbations—and provides more and more

non-trivial gaps. As far as we know, in the huge mathematical physics literature (Bender and Orszag (1978), Voros (1983) for instance and their references) on the quartic oscillator no such gaps have been found. We will present strong evidence that, for still unknown reasons, this algorithm allows us to resolve all the eigenenergies with a surprising precision even though, remaining stuck to the simplest means, we are far from having exhausted all the possibilities that our method offers. Actually, some very subtle information on the spectrum can be gained since we can find a gap in between the tunnelling doublets, i.e. when the energies are below the height of the intermediate barrier in a double-well configuration.

2. Guideline of the method

2.1. General strategy

The key idea of our method is to construct, for a given integer $N \geqslant 1$, a real function $J_N(\varphi', \varphi, x, E)$ from a possible real square-integrable solution φ of (1) with energy E (the prime stands for the derivative $\mathrm{d}/\mathrm{d}x$) such that

$$\text{(i)} \quad \frac{\mathrm{d}}{\mathrm{d}x}(J_N(\varphi'(x), \varphi(x), x, E)) = (\varphi(x))^N F_N(x, E),$$

$$\text{(ii)} \quad \lim_{|x|\to+\infty} J(\varphi'(x), \varphi(x), x, E) = 0.$$

The real function F_N of both the spatial coordinate x and the energy E is *φ-independent* and is constructed from the potential V and its derivatives. An example of J_N is given by equation (2) and some F_N's are given by (5)–(8). Condition (i) is the cornerstone of our method and, before justifying how it can be obtained (we will see that condition (ii) is not so restrictive), let us first explain how gaps in the spectrum may be obtained.

When conditions (i) and (ii) are simultaneously fulfilled, an immediate consequence is that the integral $\int_{-\infty}^{+\infty}(\varphi(x))^N F_N(x, E)\,\mathrm{d}x$ vanishes. This implies that if E is truly an eigenenergy, the function $x \mapsto (\varphi(x))^N F_N(x, E)$ should change its sign. If N is even, we obtain a φ-independent condition: *for any fixed energy $x \mapsto F_N(x, E)$ must change its sign on the real axis*. We will see that for such a one-dimensional problem, and for a given N, we still can choose F_N in a wide continuous set of smooth functions on the real axis. A forbidden value of E (i.e. E cannot be an eigenenergy) is obtained if we are able to construct an F_N that remains positive on the whole x-axis. Once this property is achieved, it remains stable under small perturbations within the set of F_N's, and we obtain a whole interval where no eigenenergy can exist.

When N is odd, *a priori* some non-trivial information can be extracted for the ground state only, if there is any. Indeed, it is known that its wavefunction can be chosen positive for any Schrödinger equation of the form (1) with a nonsingular potential (see for instance (Reed and Simon (1978), XIII.12)) whereas all the excited eigenfunctions do change their sign. No gap can be found but one can use this strategy to find upper and lower bounds on the ground state energy even in a multidimensional situation. The differential method presented in (Mouchet 2005) corresponds to $N = 1$.

2.2. Obtaining condition (i) and determination of F_N

In order to obtain condition (i), let us start with J being a homogeneous polynomial of degree N with respect to its first two variables (φ', φ):

$$J_N(\varphi'(x), \varphi(x), x, E) = \sum_{n=0}^{N} a_n(x, E)(\varphi'(x))^{N-n}(\varphi(x))^n. \tag{2}$$

The smooth functions $\{a_n\}_{n\in\{0,\dots,N\}}$ will be constructed in order to get condition (i): equation (1) allows us to eliminate φ'' from the total derivative of J_N and then the systematic cancellation of the coefficients of $(\varphi')^{N-n}$ for $N-n>0$ leads to the relations

$$\forall n\in\{0,\dots,N-1\},\qquad a_{n+1}=-\frac{1}{n+1}a_n'-\frac{N-n+1}{n+1}2(V-E)a_{n-1}, \tag{3}$$

(to get a unified expression, we define $a_{-1}\equiv 0$) with

$$F_N(x,E)=a_N'(x,E)+2(V(x)-E)a_{N-1}(x,E). \tag{4}$$

The recurrence relation (3) uniquely determines all a_n's and F_N from a_0, which remains a free smooth function. For instance, we have

$$F_1=-a_0''+2(V-E)a_0, \tag{5}$$

$$F_2=\frac{1}{2}a_0'''-4(V-E)a_0'-2V'a_0, \tag{6}$$

$$F_3=-\frac{1}{6}a_0^{(iv)}+\frac{10}{3}(V-E)a_0''+\frac{10}{3}V'a_0'+(V''-6(V-E)^2)a_0, \tag{7}$$

$$F_4=\frac{1}{24}a_0^{(v)}-\frac{5}{3}(V-E)a_0'''-\frac{5}{2}V'a_0''+\left(-\frac{3}{2}V''+\frac{32}{3}(V-E)^2\right)a_0' +\left(-\frac{1}{3}V'''+\frac{32}{3}V'(V-E)\right)a_0. \tag{8}$$

The only condition on a_0 is that it must not increase too rapidly when $|x|\to+\infty$ in order to get condition (ii). From the standard semiclassical analysis (Messiah (1991), for instance chapter VI), we know that if a bound state of V exists, its wavefunction decreases exponentially as $\exp\left(-\left|\int^x\sqrt{2(V(x')-E)}\,\mathrm{d}x'\right|\right)$ when $|x|\to+\infty$; therefore, the ansatz (2) will vanish at infinity as soon as $|a_0|$ becomes negligible compared to $|\varphi|$. The condition

$$|a_0(x)|\ll\exp\left|\int^x\sqrt{2(V(x')-E)}\,\mathrm{d}x'\right|\qquad\text{when}\quad|x|\to+\infty \tag{9}$$

is sufficient and not too demanding.

We do not loose generality with the form (2). In fact any smooth function $J(\varphi',\varphi,x,E)$ will inevitably lead to the hierarchy of functions $\{F_N\}_{N\geqslant 1}$. To understand this, consider one monomial $c(\varphi')^n\varphi^m$, where c is a function of x, in the Taylor expansion of $\frac{\mathrm{d}}{\mathrm{d}x}J(\varphi',\varphi,x,E)$ with respect to (φ',φ) once φ'' has been substituted by $2(V-E)\varphi$. This monomial can be written as

$$\begin{aligned}c(\varphi')^n\varphi^m&=-\frac{1}{m+1}(c(\varphi')^{n-1})'\varphi^{m+1}+\frac{1}{m+1}\frac{\mathrm{d}}{\mathrm{d}x}(c(\varphi')^{n-1}\varphi^{m+1})\\&=-\frac{1}{m+1}[c'(\varphi')^{n-1}\varphi^{m+1}+2(n-1)(V-E)c(\varphi')^{n-2}\varphi^{m+2}]\\&\quad+\frac{1}{m+1}\frac{\mathrm{d}}{\mathrm{d}x}(c(\varphi')^{n-1}\varphi^{m+1}).\end{aligned} \tag{10}$$

By using this type of identity an adequate number of times we can systematically absorb all the powers of φ' in a total derivative while keeping the homogeneity in (φ',φ). This procedure can be pursued until we obtain $c(\varphi')^n\varphi^m$ of the form $\tilde{c}\varphi^{n+m}+\frac{\mathrm{d}}{\mathrm{d}x}(j(\varphi',\varphi,x,E))$ where $\tilde{c}$

and j are smooth functions. A redefinition of $J \to J - j$ for each monomial of degree $n+m = N$ leads to condition (i). Rather than the starting point (2), we could have started from $J_N(\varphi', \varphi, x, E) = a_0(\varphi')^N$ and, working modulo a total derivative, repetitions of procedure (10) would have led to condition (i). For small N, it can been checked that F_N thus obtained are also given by (5)–(8).

3. Application to the quartic oscillator and generalizations

To illustrate the efficiency of our approach, in this section we will consider a quartic potential, which can always be reduced in appropriate units to

$$V(x) \stackrel{\text{def}}{=} \frac{s}{2}x^2 + \frac{1}{4}x^4, \tag{11}$$

for s real. The associated energy spectrum is purely discrete and bounded from below by the minimum $\min(V)$. The energies can been computed numerically without any difficulty by diagonalizing the Hamiltonian in the standard basis of the eigenstates of a harmonic oscillator. They are given by the continuous black lines in figure 1. For large positive s, the bottom of the spectrum $\{E_n | n = 0, 1, 2, \ldots\}$ tends to the harmonic spectrum $(n + 1/2)\sqrt{s}$. For $s < 0$, we get a double-well configuration where the central barrier reaches its maximum at 0. When s decreases from 0, we observe the pairing of the energies (E_{2n}, E_{2n+1}) into doublets that characterize tunnelling from one well to the other. For $s \leqslant s_0 \simeq -2.0481$ the two first states E_0 and E_1 are both negative, therefore below the energetic barrier, and $1/(E_1 - E_0)$ represents the tunnelling oscillation period (recall that we are working in units where $\hbar = 1$) of a state initially localized in one well and constructed from a linear combination of the symmetric/antisymmetric eigenstates associated with E_0 and E_1, respectively. As $-s$ increases, a standard semiclassical analysis shows that $E_1 - E_0$ behaves like $2^{11/4}|s|^{5/4}\exp(-|2s|^{3/2}/3)/\sqrt{\pi}$ for large $-s$ (Garg (2000), section 5, for instance). This exponentially small splitting is a highly non-trivial piece of spectral information to obtain by approximate methods. Nevertheless, we will show that for a given positive or negative s, we actually can exhibit a gap between E_0 and E_1.

For simplicity, and in order to keep the computation tractable with elementary algebraic manipulations, we will work with $N = 2$ and take a_0 of the form

$$a_0(x) = P(x)\,\mathrm{e}^{-\lambda x^2/2}, \tag{12}$$

where λ is real (not necessarily positive, see (9) and P is a real polynomial in x. (To lighten the notations we leave the E-dependence implicit. Note that P may depend on λ as well) Condition (9) is largely satisfied. From expression (6), we have $F_2(x) = Q(x)\exp(-\lambda x^2/2)$ where Q is the polynomial,

$$\begin{aligned} Q(x) = {} & P'''(x) - 3\lambda x P''(x) - (2x^4 + (4s - 3\lambda^2)x^2 + 3\lambda - 8E)P'(x) \\ & + (2\lambda x^5 - (\lambda^3 - 4s\lambda + 4)x^3 + (3\lambda^2 - 8E\lambda - 4s)x)P(x), \end{aligned} \tag{13}$$

that must change its sign if E is an eigenenergy. To find a forbidden value for the energy we construct an even Q and therefore start from an odd P:

$$P(x) = \sum_{m=0}^{M} p_m x^{2m+1}. \tag{14}$$

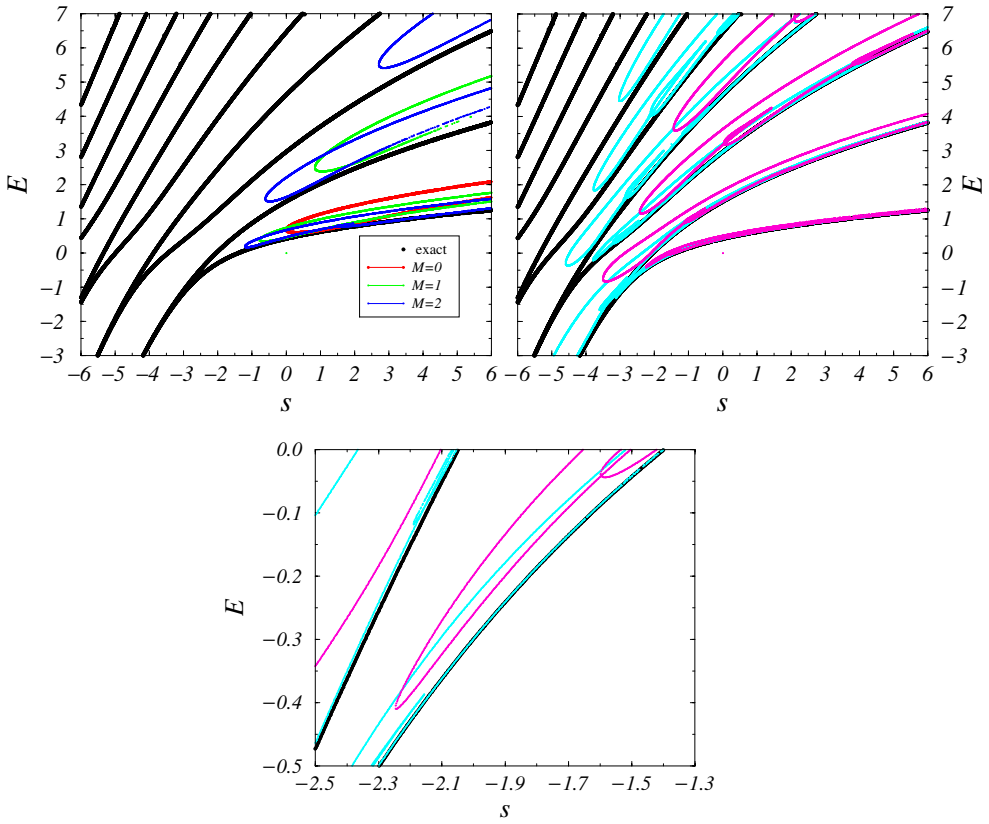

Figure 1. The black thick lines stand for the exact spectrum of the Hamiltonian $p^2/2+sx^2/2+x^4/4$. On the upper left panel are the boundaries of the gaps that are given by the solutions of (18) for $M = 0$ (red, the equation of the curve is obtained by cancelling (17)), $M = 1$ (green), $M = 2$ (blue). The gaps on the upper right panel are obtained for $M = 7$ (magenta) and $M = 15$ (cyan). For a given M, no gap can be found for a too small value of s but we can see that for a given value of s all the lowest energies can be separated by a gap for a large enough M. The boundaries of the gaps converge to the exact spectrum when M increases. For instance, for $M = 15$ and $s > 0$, the lowest gap is very thin and can hardly be distinguished from the ground state E_0. In some cases, equations (18) provide two disconnected gaps in between two successive energies. As can be seen in the panel below, for $M = 7$ and $M = 15$, even the doublet (E_0, E_1) can be separated in a tunnelling regime (i.e. when they are both negative).

(This figure is in colour only in the electronic version)

Then

$$Q(x) = \sum_{m=0}^{M+3} q_m x^{2m}, \tag{15}$$

where the coefficients $\{q_m\}$ are expressed in terms of $\{p_m\}$ via the recurrence relation

$$\begin{aligned} q_m = {} & (2m+3)(2m+2)(2m+1)\,p_{m+1} - (2m+1)(3\lambda(2m+1) - 8E)\,p_m \\ & + (2m(3\lambda^2 - 4s) - 8E\lambda)\,p_{m-1} - (\lambda^3 - 4s\lambda + 4m - 2)\,p_{m-2} + 2\lambda p_{m-3}, \end{aligned} \tag{16}$$

for $m \in \{0, \ldots, M+3\}$ (we define $p_m = 0$ for $m < 0$ or $m > M$). The simplest way to control the sign of Q is to reduce it to a polynomial of degree two in x^2: $Q(x) = x^{2M+2}R(x)$ where

$R(x) \stackrel{\text{def}}{=} (q_{M+3}x^4 + q_{M+2}x^2 + q_{M+1})$. This can be done if we choose p's in order to cancel all q_m for $m \leqslant M$. For $m \in \{0, \ldots, M-1\}$, equations (16) determine uniquely all p's up to a common factor p_0 that can be taken to one without loss of generality: p_n is a polynomial in (E, λ) of degree at most n. From equation (16) written for $m = M$, the condition $q_M = 0$ imposes an algebraic relation of degree at most $(M+1)$ between E and λ that implicitly defines λ as a function of E (several branches are possible in general). After eliminating λ, the discriminant of R appears as a function $\Delta_M(E, s)$ of E and s only. For a given s, all the values of E, where $\Delta_M < 0$, are forbidden. The boundaries of the gaps are given by the zeroes of $E \mapsto \Delta_M(E, s)$. For instance, when $M = 0$ we have

$$\Delta_0(E, s) = 65536E^6 - 73728E^4 s - 41472E^3 + 20736E^2 s^2 + 7776Es + 6561. \tag{17}$$

For a given value of s, the real roots of this polynomial define intervals of forbidden values of E. The degree of the polynomial $\Delta_M(E, s)$ increases with M.

We can generalize and reformulate these algebraic manipulations to any kind of polynomial potential of even degree $\deg V$ (not necessarily symmetric). With the choice (12), the expression (6) shows that $F_2\, \mathrm{e}^{\lambda x^2/2}$ is a polynomial $Q(x, \lambda, E)$ of degree $\deg V + \deg P + 1$ in x. For any (λ, E) the coefficients of P can be chosen to cancel all the coefficients of $x \mapsto Q(x, \lambda, E)$ but the $(\deg V + 2)$ th higher powers. The cancellation of the coefficient $q(\lambda, E)$ of $x^{\deg P}$ allows the factorization $Q(x, \lambda, E) = x^{\deg P+1} R(x, \lambda, E)$ where the degree of $x \mapsto R(x, \lambda, E)$ is precisely $\deg V$. Now, if $\deg P$ is odd and $x \mapsto R(x, \lambda, E)$ has no root of odd multiplicity for a given couple (λ, E) such that $q(\lambda, E) = 0$, we are sure that E cannot be an eigenvalue. In the (x, λ, E)-space, the two equations $q(\lambda, E) = 0$, $R(x, \lambda, E) = 0$ define generically a curve $\mathcal{C}$ (possibly made of disjoint smooth pieces) that can be parameterized by x, namely $(E(x), \lambda(x))$, where the Jacobian $J = |\partial_\lambda q \partial_E R - \partial_\lambda R \partial_E q|$ does not vanish. The projection of $\mathcal{C}$ on the E-axis defines some intervals outside which no eigenenergy can be found. The borders of these intervals are the projections of some points (not necessarily of all points) of $\mathcal{C}$ where the tangent is normal to the E-axis. Using the implicit function theorem these points are to be found among the solutions of $0 = \mathrm{d}E/\mathrm{d}x = -\partial_\lambda q \partial_x R/J$. To sum up, the boundaries of the gaps are to be found from the solutions—if there are any—of the three equations

$$q(\lambda, E) = 0, \qquad R(x, \lambda, E) = 0, \qquad \partial_\lambda q(\lambda, E) \partial_x R(x, \lambda, E) = 0. \tag{18}$$

The boundaries obtained above for the quartic potential using the zeroes of the discriminants Δ_M are included in the solutions of (18) since they cancel simultaneously q, R and $\partial_x R$ but some others boundaries may be obtained if $\partial_\lambda q$ vanishes instead of $\partial_x R$. Determining which values represent boundaries of gaps from all the solutions of (18) may require some global analysis that can be pursued numerically. The larger the M, the larger the degree of the algebraic equations to solve and the more gaps are expected to be found. For the quartic oscillator, the numerical results are shown for several values of M in figure 1 and table 1 illustrates the precision of our method.

Let us also consider the even potential $V(x) = x^6$. The polynomial R is now of third degree in the variable x^2. As explained above, a necessary condition to obtain the boundaries of the gaps for a given positive integer M is to solve simultaneously the three equations (18). The last step consists in verifying that the polynomial $R(x)$ does not have real roots of odd multiplicity. The results obtained are qualitatively similar to those showed above for the quartic oscillator (see table 2).

Table 1. Comparison between the exact energies $\{E_n \mid n = 0, 1, 2, \ldots\}$ (given in the upper table) and the gaps for $s = -2.3$ and several values of M. The two lowest energies (E_0, E_1), being negative though below the central barrier, form a tunnelling doublet. There are two gaps between (E_0, E_1) for $M = 15$ and one gap for $M = 16$. The last line sums up the best bounds when comparing the gaps obtained for each M up to 16. We did not retain the lowest bounds that are below the trivial bound min V.

n	0	1	2	3	4	5	6
E_n	−0.5012	−0.2549	0.9606	2.1003	3.5281	5.1202	6.8609

M	$E_0 < \cdots < E_1$	$E_1 < \cdots < E_2$	$E_2 < \cdots < E_3$	$E_3 < \cdots < E_4$	$E_4 < \cdots < E_5$	$E_5 < \cdots < E_6$
$\leqslant 4$	–	–	–	–	–	–
5	–	[0.0399, 0.4582]	–	–	–	–
6	–	[−0.1108, 0.4359]	–	–	–	–
7	–	[−0.1836, 0.3908]	[1.1734, 1.4748]	–	–	–
8	[−0.4614, −0.4281]	[−0.2001, 0.3408]	[1.0601, 1.5156]	–	–	–
15	[−0.4994, −0.4865]	[−0.2414, 0.0507]	[0.9845, 1.2930]	[2.1214, 2.3143]	[3.7509, 4.3535]	[5.3268, 6.0726]
	[−0.4835, −0.4336]			[2.3789, 2.7014]		
16	[−0.5006, −0.4369]	[−0.247, −0.24]	[0.9903, 1.2652]	[2.1318, 2.3167]	[3.6068, 3.7792]	[5.3426,6.0835]
		[−0.2325, 0.0206]		[2.3307, 2.6590]	[3.9847, 4.3128]	
$\bigcup_{M=0}^{16}$	[−0.5006, −0.4211]	[−0.2497, 0.4582]	[0.9726, 1.5156]	[2.1214, 2.8710]	[3.6068, 4.4028]	[5.3268,6.0835]

Table 2. Comparison between the exact energies $\{E_n \mid n = 0, 1, 2\}$ (given in the left table) and the gaps for $V(x) = x^6$.

n	0	1	2
E_n	0.6807	2.5797	5.3948

M	$E_0 < \cdots < E_1$	$E_1 < \cdots < E_2$
0	–	–
1	[0.967, 1.041]	–
2	[0.736; 1.122]	–
3	[0.710, 1.081]	[3.016, 3.624]
4	[0.715, 1.036]	[2.724, 3.702]
5	[0.723, 0.995]	[2.674, 3.642]

4. Conclusions

From what precedes it is clear that our method is not specific to the quartic potential but can be adapted straightforwardly to many other situations. We also let for future investigations the cases $N > 2$.

This method can also be applied to a spectral problem with different boundary conditions. For, say, Dirichlet boundary conditions equation (ii) is replaced by the vanishing of J_N at the two points where the function φ vanishes.

Even though our method cannot provide a rigorous proof of the existence of an eigenenergy in a given range, it offers some precise clues where some possible energies may lie, specially if some convergence behaviour is observed, as it appears in the case of the quartic oscillator. Therefore, we are able to obtain this way a substantial piece of physical information.

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