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Simple procedure to compute accurate energy levels of an anharmonic oscillator

L. Gr. Ixaru
Institute of Physics and Nuclear Engineering, Division of Fundamental Physics, P.O. Box 5206, Bucharest, Romania
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A procedure based on the piecewise perturbation treatment of the Schrödinger equation is developed. The procedure is shown to be convergent for any bounded perturbation. A simple way to construct the algorithm is also developed, which can be used for any potential of polynomial form. Our procedure is further particularized for the anharmonic-oscillator potential $v(x)=m^2x^2+2\lambda x^{2\alpha}$ ($\lambda>0$ and integer $\alpha\geq 2$) and applied to produce highly accurate numerical values for its energy levels. The experimental results also show that this procedure exhibits almost equal efficiency for all relevant values of the principal quantum number n, mass parameter m^2, coupling λ, and anharmonicity α.

I. INTRODUCTION

It is well known that for the anharmonic-oscillator problem, i.e.,

$$\psi_n''=[v(x)-E_n]\psi_n,$$
$$v(x)=m^2x^2+2\lambda x^{2\alpha},\quad x\in(-\infty,+\infty), \tag{1.1}$$
$$\lim_{x\to\pm\infty}\psi_n(x)=0,$$

with integer $\alpha\geq 2$, the perturbation theory, in which m^2x^2 is taken as the reference potential and $2\lambda x^{2\alpha}$ as a perturbation, diverges for all positive λ no matter how small. This fact, which has first been proved in Ref. 1 for the case $\alpha=2$, has stimulated many efforts to search for alternative procedures for accurate computation of the problem (1.1).

Reid,[2] for instance, performed variational calculations based on the harmonic-oscillator basis to obtain the first 25 eigenvalues of Eq. (1.1) with $m^2=0$, $\alpha=2$, and $\lambda=\frac{1}{2}$ to 12 significant figures. Biswas *et al.*[3] were able to compute the first eight eigenvalues for $m^2=1$, $\alpha=2$, and various λ in the range $0>\lambda\geq 50$ by using the Hill determinant method. Hioe and Montroll[4] and Hioe *et al.*[5] considered the problem for various values of α. For each α they first delimited three regimes of the values of the quantum number n and the anharmonicity constant λ, called the near harmonic, near pure anharmonic, and boundary layer regime, respectively, and next devised suitable procedures in each of the three regimes. Banerjee *et al.*[6] used an appropriately scaled basis for the eigenfunctions to obtain the eigenvalues as the zeros of some function of energy which is constructed by means of some recurrence procedure. In the case of quartic anharmonicity $\alpha=2$, which is discussed there in great detail, the recursion formula is very simple, so that the computation of a single step in the recurrence procedure is carried out very fast indeed. Nevertheless, since the number of steps is roughly proportional to n, this procedure becomes less and less efficient with increasing n. Finally, note the approach of Caswell[7] who tried to revigorate the standard perturbative approach by replacing the original parameters m^2 and λ by some "effective" parameters M^2 and Λ, and then transformed the perturbation series in the original coupling λ into one in the effective coupling Λ. He tested his procedure on low-lying levels ($n\leq 10$) from various values of α and λ, with good results. A novelty in Ref. 7 is that it also gives numerical results for the double-well anharmonic-oscillator problem, i.e., of the same form as in Eq. (1.1) but with negative m^2.

All the procedures mentioned above have in common the capability of being successful for low-lying energy levels. When n increases some of these methods (Refs. 2, 3, and 6) become less and less efficient, while the behavior of the method of Ref. 7 at large n is not yet investigated. As for the approach developed in Refs. 4 and 5, this is probably uniformly efficient for any n, but this is achieved at the expense of actually choosing between three different algorithms, each valid in a certain regime of values of n and λ.

In this paper we devise an alternative procedure which consists of a *unique* algorithm and which exhibits almost equal efficiency for all relevant values of n, m^2, α, and λ. Our procedure is based on the perturbation theory *but not* with m^2x^2 as the reference potential and $2\lambda x^{2\alpha}$ as a perturbation. We use instead a piecewise perturbation technique in which the reference potential is adjusted at will.

Procedures based on this idea have been investigated intensively in the last decade, but with particular emphasis upon their numerical aspects; see Ref. 8 for a review paper. The main novelties brought by the present paper refer to the mathematical conditions under which the piecewise perturbation technique is convergent and also to the manner of constructing the expressions of the perturbative corrections. All these are treated in

Sec. II. In fact, in Sec. IIA, it is shown that the piecewise perturbation technique based upon the constant reference potential (which we prefer to use, due to its simplicity) is convergent under the very relaxed condition that the perturbation is bounded. In Sec. IIB we give a new, general, and simple-to-use procedure for obtaining the formulas of the piecewise perturbative corrections in any order. We show namely that these corrections are some linear combinations of elementary functions, viz., sin, cos, sinh, or cosh. We also show that in the case when the potential is a polynomial in x each correction consists of a *finite* number of terms with polynomial coefficients.

The potentialities of such a procedure to solve the anharmonic-oscillator problem, as well as some related practical aspects, are discussed in Sec. III.

In Sec. IV we report on numerical results from several test cases. The sample covers most of the relevant situations, viz., λ between 0.01 and 100, $\alpha = 2$, 3, and 4, m^2 positive or negative, and n between zero and 10 000. We find out that the computer time needed to compute the eigenenergy E_n with some preset relative error is practically independent of the values of m^2, α, and λ, but slightly increases with n to approach values which are approximately as large as the ones required by the standard WKB method, see Fig. 2.

II. THE PIECEWISE PERTURBATION THEORY

Consider the Schrödinger equation

$$\psi''(x) = [v(x) - E]\psi(x), \quad x \in (\alpha \geq -\infty, \beta \leq +\infty), \quad (2.1)$$

and suppose that the interval (α,β) can be divided into three intervals (α,a), $[a,b]$, and (b,β), so that in the extreme intervals (α,a) and (b,β) the solution can be calculated with sufficient accuracy by some asymptotic procedure such as the WKB method, for instance. The solution on the whole (α,β) is the sequence of the piecewise solutions on the three subintervals, properly matched at their mesh points a and b.

The actual problem then is the solution on $[a,b]$. For sake of simplicity we introduce the current variable $\delta = x - a$ and denote $h = b - a$. Then, the Eq. (2.1) on $[a,b]$ reads

$$y''(\delta) = [V(\delta) - E]y(\delta), \quad \delta \in [0,h], \quad (2.2)$$

where $y(\delta) = \psi(a+\delta)$ and $V(\delta) = v(a+\delta)$.

Specifically, our aim is to construct the two linear independent solutions u and v of Eq. (2.2) which obey the initial conditions: $y(0) = 1$, $y'(0) = 0$ for u, and $y(0) = 0$, $y'(0) = 1$ for v. (Note that the Wronskian of u and v is equal to unity.) In fact, once u and v are known, the further treatment of Eq. (2.2) reduces to some simple algebraic manipulations. For instance, if we have to solve the initial-value problem associated with Eq. (2.2) in which the values of $y(0)$ and $y'(0)$ are given, the solution and its derivative at any δ can be written in simple matrix form

$$\begin{pmatrix} y(\delta) \\ y'(\delta) \end{pmatrix} = \begin{pmatrix} u(\delta) & v(\delta) \\ u'(\delta) & v'(\delta) \end{pmatrix} \begin{pmatrix} y(0) \\ y'(0) \end{pmatrix}, \quad (2.3)$$

while when the initial conditions are specified at the point h, one has

$$\begin{pmatrix} y(\delta) \\ y'(\delta) \end{pmatrix} = \begin{pmatrix} u(\delta) & v(\delta) \\ u'(\delta) & v'(\delta) \end{pmatrix} \begin{pmatrix} v'(h) & -v(h) \\ -u'(h) & u(h) \end{pmatrix} \begin{pmatrix} y(h) \\ y'(h) \end{pmatrix}. \quad (2.4)$$

The same is also true in the case of two-point boundary problems. Indeed, when the Strum-Liouville conditions $A_0 y(0) + B_0 y'(0) = 0$, $A_1 y(h) + B_1 y'(h) = 0$ ($|A_0| + |B_0| \neq 0$, $|A_1| + |B_1| \neq 0$) are imposed, then the eigenvalues of Eq. (2.2) are given by the roots against E of some linear combinations of the propagators u and v and of their derivatives u' and v', each taken at h. If, for instance, $B_0 = B_1 = 0$, then the eigenvalues are simply the roots of $v(h)$.

To construct the propagators u and v we make use of perturbation theory. We assume that $V(\delta)$ is a real, integrable function of δ on $[0,h]$ and that E is a real parameter. There is, however, no difficulty in extending our approach in the complex case.

A real constant potential $\bar{V}$ is taken as the reference potential of our perturbation scheme. As for the actual value of this constant, there is no serious restriction because, as we will see in Sec. IIA below, the scheme is convergent for any finite $\bar{V}$ provided $V(\delta)$ is bounded. Nevertheless, if $\bar{V}$ is chosen such as it fits the given $V(\delta)$ on $[0,h]$, the procedure becomes more efficient, in the sense that fewer perturbative corrections must be retained in the perturbation series for u and v to obtain them with the desired accuracy. Accordingly, we adopt for $\bar{V}$ the following recipe[8]:

$$\bar{V} = \frac{1}{h}\int_0^h V(\delta)\,d\delta. \quad (2.5)$$

Now we present details concerning the perturbation scheme. First we recall that the propagators $\bar{u}(\delta)$ and $\bar{v}(\delta)$ of the constant potential $\bar{V}$ are[8]

$$\bar{u}(\delta) = \xi(F,\delta) \equiv \begin{cases} \cos(|F|^{1/2}\delta) & \text{if } F \leq 0, \\ \cosh(F^{1/2}\delta) & \text{if } F > 0, \end{cases} \quad (2.6a)$$

and

$$\bar{v}(\delta)=\eta_0(F,\delta)\equiv\begin{cases}|F|^{-1/2}\sin(|F|^{1/2}\delta) & \text{if } F<0,\\ \delta & \text{if } F=0,\\ F^{-1/2}\sinh(F^{1/2}\delta) & \text{if } F>0,\end{cases} \tag{2.6b}$$

where $F=\bar{V}-E$.

Each of the propagators u and v, which we look for, can be written as a perturbation series

$$p(\delta)=p_0(\delta)+p_1(\delta)+p_2(\delta)+\cdots, \tag{2.7}$$

where the kth correction $p_k(\delta)$, $k=1,2,\ldots$, is the solution of the equation

$$p_k''=Fp_k+\Delta V(\delta)p_{k-1},\quad p_k(0)=p_k'(0)=0, \tag{2.8}$$

with $\Delta V(\delta)\equiv V(\delta)-\bar{V}$. Here p means either u or v according to the starting quantity in the set (2.8): if $p_0(\delta)=\bar{u}(\delta)$, then $p\equiv u$, while if $p_0(\delta)=\bar{v}(\delta)$, then $p\equiv v$.

A. Convergence of the perturbation series (2.7)

We prove now that the series (2.7) is uniformly and absolutely convergent if the perturbation ΔV is bounded, i.e., $|\Delta V(\delta)|\leq C$ on $[0,h]$.

We start with the identity $V(\delta)-E=F+\Delta V(\delta)$. As the perturbative procedure takes F as reference coefficient and $\Delta V(\delta)$ as a perturbation, the validity of the whole approach depends actually on the ratio of these two contributions, $\sigma=\Delta V/F$. Accordingly, the most unfavorable situation for the convergence of the perturbation series (2.7) would occur when $F=0$, i.e., when $E=\bar{V}$. We prove below that even in this case the series is convergent.

Consider in detail the case $p=u$. The Eq. (2.8) reads

$$u_k''=\Delta V(\delta)u_{k-1},\quad u_k(0)=u_k'(0)=0, \tag{2.9}$$

with $u_0(\delta)=\xi(F=0,\delta)=1$. For the proof we use the following auxiliary equation:

$$u_k^{C\,\prime\prime}=Cu_{k-1}^C(\delta),\quad u_k^C(0)=u_k^{C\,\prime}(0)=0,\quad C\geq 0,$$

with the same starting quantity $u_0^C(\delta)=u_0(\delta)=1$. It has the solution $u_k^C(\delta)=C^k\delta^{2k}/(2k!)$, i.e., the series

$$u^C(\delta)=u_0^C(\delta)+u_1^C(\delta)+u_2^C(\delta)+\cdots \tag{2.10}$$

is uniformly convergent for any $C\geq 0$; its sum is actually $u^C(\delta)=\cosh(C^{1/2}\delta)$. Now choose $C=\max|\Delta V(\delta)|$ on $[0,h]$ and verify that each u_k^C is an upper bound for $|u_k(\delta)|$ of Eq. (2.9). For $k=1$, we have

$$|u_1(\delta)|=\left|\int_0^\delta d\delta_2\int_0^{\delta_2}\Delta V(\delta_1)\,d\delta_1\right|\leq\left|\int_0^\delta d\delta_2\int_0^{\delta_2}|\Delta V(\delta_1)|\,d\delta_1\right|\leq\left|\int_0^\delta d\delta_2\int_0^{\delta_2}C\,d\delta_1\right|=u_1^C(\delta),$$

for $k=2$ we have

$$|u_2(\delta)|=\left|\int_0^\delta d\delta_2\int_0^{\delta_2}V(\delta_1)u_1(\delta_1)\,d\delta_1\right|\leq\left|\int_0^\delta d\delta_2\int_0^{\delta_2}|\Delta V(\delta_1)||u_1(\delta_1)|\,d\delta_1\right|\leq\left|\int_0^\delta d\delta_2\int_0^{\delta_2}Cu_1^C(\delta_1)\,d\delta_1\right|=u_2^C(\delta)$$

and so on; this completes the proof for the convergence of u. The same procedure can be repeated word by word for v. The only differences are that the starting quantity is $v_0(\delta)=\eta_0(F=0,\delta)=\delta$, and the analog of Eq. (2.10) is $v^C=\sinh(C^{1/2}\delta)/C^{1/2}$.

B. Construction of the perturbative corrections

We introduce the following functions:

$$\eta_1(F,\delta)=[\delta\xi(F,\delta)-\eta_0(F,\delta)]/F,$$
$$\eta_s(F,\delta)=[\delta^2\eta_{s-2}(F,\delta)-(2s-1)\eta_{s-1}(F,\delta)]/F,$$
$$s=2,3,\ldots. \tag{2.11}$$

Some properties of the functions $\xi,\eta_0,\eta_1,\eta_2,\ldots$, are listed below.

(i) Differentiation with respect to δ:

$$\frac{\partial\xi(F,\delta)}{\partial\delta}=F\eta_0(F,\delta),$$
$$\frac{\partial\eta_0(F,\delta)}{\partial\delta}=\xi(F,\delta), \tag{2.12}$$
$$\frac{\partial\eta_s(F,\delta)}{\partial\delta}=\delta\eta_{s-1}(F,\delta),\ s=1,2,\ldots.$$

(ii) Differentiation with respect to F:

$$\frac{\partial\xi(F,\delta)}{\partial F}=\tfrac{1}{2}\delta\eta_0(F,\delta),$$
$$\frac{\partial\eta_s(F,\delta)}{\partial F}=\tfrac{1}{2}\eta_{s+1}(F,\delta),\quad s=0,1,2,\ldots. \tag{2.13}$$

(iii) The series expansion of η_s in powers of $Z\equiv F\delta^2$ reads

$$\eta_s(F,\delta)=2^s\delta^{2s+1}\sum_{q=0}^{\infty}g_{sq}Z^q/(2q+2s+1)! \tag{2.14}$$

with

$$g_{sq}=\begin{cases}1 & \text{if } s=0,\\ (q+1)(q+2)\cdots(q+s) & \text{if } s>0.\end{cases}$$

(iv) The asymptotic behavior of η_s, which is actually valid when $Z\gg\frac{1}{4}s^2(s+1)^2$, is

$$\eta_s(F,\delta)\sim\begin{cases}\delta^{2s+1}\xi(F,\delta)/Z^{(s+1)/2} & \text{for odd } s,\\ \delta^{2s}\eta_0(F,\delta)/Z^{s/2} & \text{for even } s.\end{cases}\tag{2.15}$$

Now proceed with the construction of the kth correction p_k to the propagator p. To this aim we assume that the inhomogeneous term in Eq. (2.8) is a linear combination of the functions ξ and $\eta_0,\eta_1,\eta_2,\ldots,\eta_S$, viz.,

$$\Delta V(\delta)p_{k-1}(\delta)=Q(\delta)\xi(F,\delta)+P_0(\delta)\eta_0(F,\delta)+P_1(\delta)\eta_1(F,\delta)+\cdots+P_S(\delta)\eta_S(F,\delta),\tag{2.16}$$

where $Q,P_0,P_1,P_2,\ldots,P_S$ are *polynomials* in δ.

Now search for p_k of the form

$$p_k(\delta)=C_0(\delta)\eta_0(F,\delta)+C_1(\delta)\eta_1(F,\delta)+\cdots,\tag{2.17}$$

and show that this sum has a finite number of terms and that the coefficients $C_s(\delta)$, $s\geq 0$ are polynomials in δ. In fact, differentiate Eq. (2.17) twice with respect to δ [use Eq. (2.12)] and form $p_k''-Fp_k$. One gets

$$p_k''-Fp_k=2C_0'\xi(F,\delta)+(C_0''+2C_1'\delta+2C_1)\eta_0(F,\delta)+\cdots+[C_s''+2C_{s+1}'\delta+2(s+1)C_{s+1}]\times\eta_s(F,\delta)+\cdots.\tag{2.18}$$

This should be equal to $\Delta V(\delta)p_{k-1}(\delta)$. Then, upon identifying the coefficients of $\xi,\eta_0,\eta_1,\eta_2,\ldots$ of the expressions (2.18) and (2.16), one gets

$$2C_0'(\delta)=Q(\delta),\quad C_s''+2[C_{s+1}'\delta+(s+1)C_{s+1}]=P_s,\quad s=0,1,2,\ldots,S\tag{2.19a}$$

and

$$C_s''+2[C_{s+1}'\delta+(s+1)C_{s+1}]=0,\quad s=S+1,S+2,\ldots.\tag{2.19b}$$

These equations can be solved iteratively; for C_0 one simply gets

$$C_0(\delta)=\tfrac{1}{2}\int_0^\delta Q(\delta_1)\,d\delta_1,\tag{2.20a}$$

while for $C_1(\delta),C_2(\delta),\ldots$, we get

$$C_s(\delta)=\tfrac{1}{2}\delta^{-s}\int_0^\delta \delta_1^{\,s-1}M_{s-1}(\delta_1)\,d\delta_1,\tag{2.21a}$$

where

$$M_s(\delta)=\begin{cases}P_s(\delta)-C_s''(\delta) & \text{if } s=0,1,2,\ldots,S,\\ -C_s''(\delta) & \text{if } s=S+1,S+2,\ldots.\end{cases}\tag{2.21b}$$

These can be particularized at once for the case when $Q,P_0,P_1,\ldots,P_S$ are polynomials in δ.

Let us denote the degree of a polynomial A by the corresponding lower case character a. The Eq. (2.20a) implies that $C_0(\delta)$ is a polynomial whose degree is $c_0=q+1$. In turn, $M_0(\delta)$ is also a polynomial, viz., $M_0(\delta)=\sum_{i=0}^{m_0}(M_0)_i\delta^i$, with $m_0=\sup(p_0,c_0'')=\sup(p_0,q-1)$, so that $C_1(\delta)$ which results from Eq. (2.21a) is a polynomial of the same degree, viz.,

$$C_1(\delta)=\sum_{i=0}^{m_0}(C_1)_i\delta^i\quad\text{with}\quad(C_1)_i=\frac{1}{2(i+1)}(M_0)_i.\tag{2.20b}$$

The iteration goes on to higher s with the formulas

$$C_s(\delta)=\sum_{i=0}^{m_{s-1}}(C_s)_i\delta^i\quad\text{with}\quad(C_s)_i=\frac{1}{2(i+s)}(M_{s-1})_i.\tag{2.20c}$$

The degree of the polynomial M_{s-1} is $m_{s-1}=\sup(p_{s-1},c_{s-1}'')=\sup(p_{s-1},c_{s-1}-2)$ for $s\leq S+1$, but $m_{s-1}=c_{s-1}''=c_{s-1}-2$ for $s>S+1$. The latter implies $c_{S+2}=c_{S+1}-2$, $c_{S+3}=c_{S+1}-4$, and so on. Thus, upon denoting the integer part of $\frac{1}{2}c_{S+1}$ by $\bar{S}$, it results that $C_s(\delta)=0$ for any $s>S+\bar{S}+1$, i.e., the last term in the sum (2.17) is $C_{S+\bar{S}+1}(\delta)\eta_{S+\bar{S}+1}(F,\delta)$.

Up to this point we have shown that if $\Delta V(\delta)p_{k-1}(\delta)$ is of the form (2.16) then $p_k(\delta)$ results in the form (2.17) with a finite number of terms, and also that the coefficients are polynomials in δ which can be calculated by Eqs. (2.20a)–(2.20c). The only remaining question is whether the ansatz (2.16) is valid. The answer is positive provided $V(\delta)$ is a polynomial in δ. In fact, for $k=1$, Eq. (2.16) consists of a single term. This is the first term, with $Q(\delta)=\Delta V(\delta)$ (which is a polynomial as V is) for $p=u$, and the second term, with $P_0(\delta)=\Delta V(\delta)$ for $p=v$. This guarantees that p_1 will be of the form (2.17). In turn, ΔVp_1 will also be of the form (2.16), and so on.

As an illustration of how to apply our procedure we take a simple example. Consider the potential

$$V(\delta)=V_0+V_1\delta+V_2\delta^2,\quad \delta\in[0,h],$$

with constant V_0, V_1, and V_2, for which we search for the first-order correction to u.

To this aim, first form $\overline{V}$ by Eq. (2.5) and ΔV. These read

$$\overline{V}=V_0+\tfrac{1}{2}V_1h+\tfrac{1}{3}V_2h^2,$$

$$\Delta V(\delta)=V_1(\delta-\tfrac{1}{2}h)+V_2(\delta^2-\tfrac{1}{3}h^2).$$

Next form $\Delta V(\delta)p_0(\delta)$, see Eq. (2.16). As $p_0(\delta)$

$=\bar{u}(\delta)=\xi(F,\delta)$, see Eq. (2.6a), the right-hand side (RHS) in Eq. (2.16) contains only the first term and $Q(\delta)=\Delta V(\delta)$. Then, Eq. (2.20a) gives directly

$$C_0(\delta)=\tfrac{1}{4}V_1(\delta^2-\delta h)+\tfrac{1}{6}V_2(\delta^3-\delta h^2)\,.$$

Now form $M_0(\delta)=-C_0''(\delta)=-\frac{1}{2}[\Delta V(\delta)]'=-\frac{1}{2}V'(\delta)$, i.e., $m_0=1$, $(M_0)_0=-\frac{1}{2}V_1$, and $(M_0)_1=-V_2$. The Eq. (2.20b) then leads to

$$C_1(\delta)=-\tfrac{1}{4}V_1-\tfrac{1}{4}V_2\delta\,.$$

This is the last nonvanishing coefficient in the RHS of Eq. (2.17). Thus the formula of the first-order correction is

$$u_1(\delta)=[\tfrac{1}{4}V_1(\delta^2-\delta h)+\tfrac{1}{6}V_2(\delta^3-\delta h^2)]\eta_0(F,\delta)$$
$$-\tfrac{1}{4}(V_1+V_2\delta)\eta_1(F,\delta)\,.$$

To summarize, the results of this section are that the proposed piecewise perturbation procedure is convergent provided $\Delta V(\delta)$ is bounded, and that the procedure becomes particularly practical if the potential $V(\delta)$ is a polynomial in δ. Clearly, the anharmonic-oscillator potential automatically meets this condition. Yet, our procedure remains suitable also for any other well-behaved $V(\delta)$. In this case an extra stage is necessary, in which this $V(\delta)$ is approximated by a polynomial. This can be achieved easily through some standard fitting procedure such as, for instance, the least-squares procedure.

III. THE ANHARMONIC OSCILLATOR

Our task is now to convert the anharmonic-oscillator problem (1.1) into a form which is suitable for the piecewise perturbation theory. This is achieved in two stages.

The first stage is the reduction of the domain $(-\infty,+\infty)$ to $[0,+\infty)$. To achieve it we start from the remark that the eigensolution ψ_n of the problem (1.1) is either symmetric (for even n) or antisymmetric (for odd n) with respect to x. Therefore, the eigenvalues of the original problem (1.1) are identical with the ones of the same Eq. (1.1) on the half-axis $[0,+\infty)$, if in the latter case the following conditions are imposed at the origin; $\psi_n(0)=0$ for odd n, and $\psi_n'(0)=0$ for even n.

The second stage is to find a suitable value for the cutoff point b. As this b must guarantee that the errors of the eigenvalues obtained are within some preset level, we choose the following procedure. We introduce two auxiliary potentials which underestimate and overestimate the given $\upsilon(x)$ on $[0,+\infty)$. These are

$$\upsilon^{\rm low}(x)=\begin{cases}\upsilon(x), & 0\le x\le b\\ \upsilon(b), & x>b\,,\end{cases}$$
$$\upsilon^{\rm up}(x)=\begin{cases}\upsilon(x), & 0\le x\le b\\ \infty, & x>b\,,\end{cases}\qquad(3.1)$$

see Fig. 1. Their eigenvalues $E_n^{\rm low}$ and $E_n^{\rm up}$ are obviously the lower and upper bounds, respectively, for the eigenvalues E_n of $\upsilon(x)$ which we look for. The problem is then reduced to the computation of these $E_n^{\rm low}$ and $E_n^{\rm up}$. Specifically, let us assume that we want to compute the energy spectrum under some $E_{\rm max}$. A natural condition for b is that this should lay somewhere in the classically forbidden region, i.e., $b>X$, where X is the turning point corresponding to $E_{\rm max}$, that is the positive root of the algebraic equation $\upsilon(X)=E_{\rm max}$.

To locate b more precisely we are helped by qualitative estimates emerging from the WKB approach. In fact, if one assumes that this approach works well enough around b, a simple relationship between $E_n^{\rm up}$ and $E_n^{\rm low}$ exists, namely,

$$E_n^{\rm up}-E_n^{\rm low}\sim P(E_n^{\rm low})\,,\qquad(3.2)$$

where $P(E)=\exp(-2\int_X^b[\upsilon(x)-E]^{1/2}dx)$. This relationship provides us with a practical way to compute the suitable b in terms of the desired accuracy in the results.

In conclusion, $E_n^{\rm low}$ and $E_n^{\rm up}$ are the eigenvalues of the problem

$$\psi_n''=[\upsilon(x)-E_n]\psi_n\,,\quad x\in[0,b]\,,\qquad(3.3)$$

i.e., with the same $\upsilon(x)$. The difference is in the boundary conditions. In fact, the conditions at the origin are the same for the two cases, namely, $\psi_n(0)=0$ for odd n and $\psi_n'(0)=0$ for even n, while at b one should impose $\psi_n(b)=0$ for $E_n^{\rm up}$ but $\psi_n'(b)+k_n\psi_n(b)=0$ for $E_n^{\rm low}$, with $k_n=[\upsilon(b)-E_n]^{1/2}$.

The problem (3.3) is manifestly suitable for the piecewise perturbation procedure, and two alternative versions might be equally used. One of them would be to take the whole $[0,b]$ as a single interval [i.e., $b=h$, under the notation in Eq. (2.2)]. Such a way seems to be particularly useful when

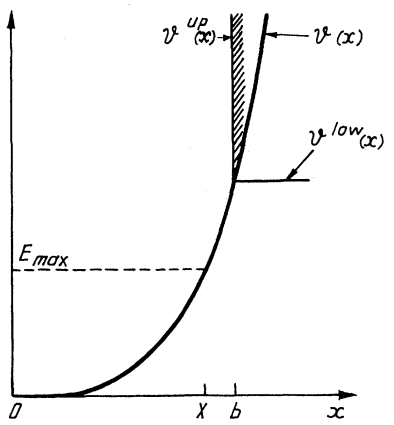

FIG. 1. The anharmonic-oscillator potential $\upsilon(x)$ and its two approximations $\upsilon^{\rm up}(x)$ and $\upsilon^{\rm low}(x)$.

one is interested mainly in obtaining approximate but closed formulas for the eigenvalues. However, in this paper we are more interested in the computation of eigenvalues with high numerical accuracy and this would imply a rather large number of perturbative corrections to generate the propagators u and v. Another version is then suggested which consists of partitioning $[0, b]$ in several (N, for example) elementary intervals. In each interval the algorithm (2.7) with a preset (but *small*) number of corrections is used. These piecewise solutions are finally matched at the mesh points to obtain the solution over the whole $[0, b]$. This was our preferred version. The number of corrections has been fixed at two. The step sizes of the elementary intervals are adjusted automatically in terms of the desired accuracy, as explained in Ref. 9.

IV. NUMERICAL RESULTS

Our computations have been carried out on a computer (IBM 370/135) in double precision arithmetic, i.e., with sixteen decimal figures in the mantissa. We measure the accuracy in eigenvalues by p, which is the number of exact figures after the decimal point (ADP figures). The maximal p is limited by the word length of the computer used. In fact, the computation involves the difference $v(x) - E$. Then, if p_V is the integer part of $\log_{10}[\sup|v(x)|]$ on $[0, b]$, the maximal p available is $p_{\max} = 16 - p_V$.

The program proceeds as follows:

(a) It reads the input values of m^2, λ, α, $n_{\max}$, $E_{\max} = E_{n_{\max}}$, and p_{input} (this is the maximal number of ADP figures achieved by the data of the tables compared). All these are taken from Refs. 5 and 7, see below.

(b) Next, it computes b from the condition $P(E_{\max}) = 10^{-16}$, and p_V.

(c) Now $p_{\max} = 16 - p_V$ is compared with p_{input}. There are three cases; $p_{\max} \geq p_{\text{input}} + 2$, $p_{\max} = p_{\text{input}} + 1$, and $p_{\max} \leq p_{\text{input}}$. The value of p is accordingly set as $p_{\text{input}} + 2$, $p_{\text{input}} + 1$, and $p_{\max}$, respectively.

(d) The partition of $[0, b]$ is chosen such as to ensure the computation of the eigenvalues with p exact ADP figures.

(e) Now the program computes E_n^{low} and E_n^{up} for each $n = 0, 1, 2, \ldots, n_{\max}$. Next, it examines how many figures are identical in E_n^{low} and E_n^{up}. In all cases investigated, full coincidence has been observed in all p ADP figures. This ensures that E_n searched for is correct within the same accuracy.

(f) The execution goes back to (a) with newer parameters, if any.

In Table I the following tables of eigenvalues have been checked out with our procedure: Table III of Ref. 4 ($m^2 = 1$, $\alpha = 3$, $n_{\max} = 5$, and 29 values for λ between 0.0001 and 20 000 i.e., a total of 174 eigenvalues); Table IV of Ref. 5 ($m^2 = 1$, $\alpha = 4$, $n_{\max} = 3$, and the same 29 values for λ, i.e., 116 eigenvalues); Table II of Ref. 7 ($m^2 = 1$, $\alpha = 2$, $n_{\max} = 10$, and five values for λ between 0.01 and 100, i.e., 55 eigenvalues); Table IV of Ref. 7 ($m^2 = -1$, $\alpha = 2$, $n_{\max} = 10$, and four values for λ between 0.1 and 100, i.e., 44 eigenvalues). To preserve the same scaling as in these tables, the eigenvalues of our Eq. (3.3) are finally divided by two. Note also that all eigenvalues are measured from the bottom of the potential; this is particularly relevant for the case $m^2 = -1$.

By the value assigned to p, our results are typically more accurate by two figures than the results of these tables. The only exception takes place for the case $\lambda = 0.01$ of Table II (Ref. 7) for which $p_{\text{input}} = 15$ while $p_{\max} = 14$. As for the practical efficiency of our procedure, note that the number N of steps of the partition which resulted from stage (d) is of about 30 for $p = 5$ and about 200 for $p = 14$. It does not depend significantly on the values of m^2, α, or λ.[10] The central-processor-unit (CPU) time to compute the propagators u and v (with two corrections included) in each elementary interval, namely τ_{elem}, is about 5 msec.

As for the computational effort per eigenvalue, namely τ, this is given by the product $NI\tau_{\text{elem}}$, where I is the number of iterations on energy required by the shooting procedure to locate each eigenvalue with the desired precision. Typically, the values of I are $I = 4$ and $I = 7$ for $p = 5$ and $p = 14$, respectively. Thus the estimated values of τ are $\tau \simeq 0.6$ sec and $\tau \simeq 7$ sec, respectively, and these are in good agreement with the experimental timings.

From the total of 389 eigenvalues checked out, 41 have been found in error. Some of the errors are manifestly misprints while the others are systematic, namely the ones corresponding to the largest n and intermediate values of λ in the case of Table III,[5] and to $n = 2$ (and, to some extent, also to $n = 4$ and $n = 5$) in the cases of Tables II and IV.[7] The smallness of the systematic errors, however, suggests that these should be assigned to some machine or programming restrictions, rather than to the limitations of the very methods of these papers. In fact, they look as if they are simply the result of the influence of the round-off errors and/or of the presumably too early cut in the iteration procedure (to save the computer time).

The results reported so far referred to only the low-lying energy levels (up to $n = 10$, at most) but it is equally interesting to see how our method works for higher eigenvalues. To this aim we take the case $m^2 = 1$, $\lambda = \frac{1}{2}$, and $\alpha = 2$, and a representa-

TABLE I. The eigenvalues of the anharmonic-oscillator potential $v(x)=m^2x^2+2\lambda x^{2\alpha}$ of Tables III,[a] IV,[a] II,[b] and IV,[b] which have been found in error by means of the piecewise perturbation method developed in this paper.

λ	n	E_n[c]	λ	n	E_n[c]
Table III[a] ($\alpha=3, m^2=1$)			Table II[b] ($\alpha=2, m^2=1$)		
0.0005	2	2.522 24	0.1	2	3.138 624 308 493 (3)
		2.522 400 0			3.138 624 308 498 11
2.0	5	21.118 7	1.0	2	5.179 291 681 3 (12)
		21.186 913			5.179 291 687 639
3.0	5	23.352 3	10	2	10.347 055 532 (8)
		23.352 140			10.347 055 592 46
4.0	5	25.033 2	10	5	29.211 484 84 (1)
		25.032 586			29.211 484 859 7
5.0	5	26.425 4	100	2	21.906 897 97 (2)
		26.424 756			21.906 898 149 0
10.0	5	31.294 8	100	4	47.707 205 93 (3)
		31.294 638			47.707 205 885 1
20	5	37.106 7	100	5	62.281 237 93 (3)
		37.106 512			62.281 237 969 9
50	5	46.537 1			
		46.536 946	Table IV[b] ($\alpha=2, m^2=-1$)		
100	5	55.269 1	0.1	2	1.634 85 (3)
		55.268 900			1.635 188 9
100	4	40.989 3	0.1	4	3.683 582 (3)
		40.989 128			3.683 567 34
200	5	65.664 9	0.1	5	4.913 652 (3)
		65.664 627			4.913 658 66
300	5	72.640 0	1.0	2	4.253 571 28 (4)
		72.639 679			4.253 571 584 6
300	4	53.856 0	1.0	4	9.564 090 26 (3)
		53.855 778			9.564 090 201 3
400	5	78.037 4	1.0	5	12.594 620 94 (3)
		78.037 082			12.594 620 980 4
400	4	57.854 5	10	2	9.894 742 35 (2)
		57.854 304			9.894 742 494 7
500	5	82.500 5	10	3	15.522 245 (2)
		82.500 218			15.522 450 18
500	4	61.161 1	10	4	21.736 540 08 (2)
		61.160 853			21.736 540 040 6
1000	5	98.069 1	10	5	28.442 236 44 (2)
		98.068 677			28.442 236 467 2
1000	4	72.695 9	100	2	21.694 679 67 (4)
		72.695 661			21.694 679 888 0
3000	4	95.623 2	100	4	47.392 920 07 (2)
		95.622 827			47.392 920 009 0
			100	5	61.921 911 04 (2)
Table IV[a] ($\alpha=4, m^2=1$)					61.921 911 086 0
0.01	3	4.881 2			
		4.881 617			

[a] Reference 5.
[b] Reference 7.
[c] Upper entries original values, lower entries corrected values.

tive sample of eigenvalues with n ranging between zero and 10000, a case also investigated in Ref. 6. For comparison we take the method of Banerjee *et al.*[6] and the standard WKB method; both are known as very efficient and, in addition, can be programmed easily. The three methods have been used to compute the eigenvalues with seven significant exact figures and the dependences of the computation time per eigenvalue versus n are plotted on Fig. 2. One sees that for the method of Ref. 6 this increases by three orders of magnitude from $n=0$ to $n=10000$, while for our method by a factor

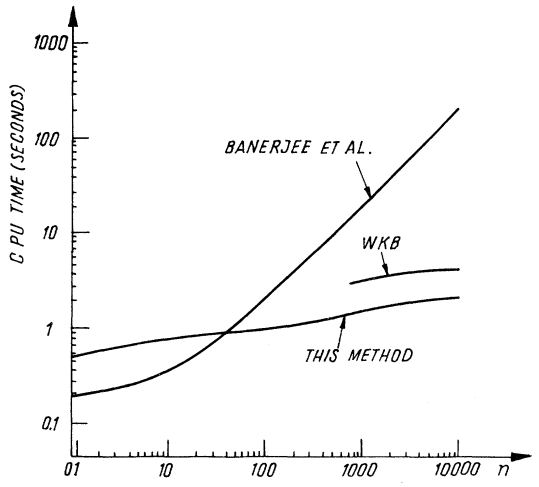

FIG. 2. Computer time per eigenvalue required by three methods (Banerjee *et al.* in Ref. 6, standard WKB, and the method of this paper) to compute the eigenvalues of the anharmonic-oscillator problem, Eq. (1.1), with seven exact significant figures. All computations have been carried out on an IBM 370/135 and the parameters used in Eq. (1.1) were $m^2=1$, $\lambda=\frac{1}{2}$, and $\alpha=2$.

of approximately 3 only. Note also the linear behavior of the curve at large values of n for the first method, in agreement with the qualitative predictions emerging from the nature of that method. Figure 2 also shows that at small n (up to 60 or so) the method of Banerjee *et al.* is faster than ours. One should, however, mention that what makes this algorithm so fast in this test is the fact that it explicitly takes advantage of the quartic shape of anharmonicity. In contrast, our algorithm remains the same for any type of anharmonicity. As for the WKB method, this is expected to yield accurate results only for large values of n. Indeed, it yields eigenvalues with seven exact figures only for $n \geq 800$. The computational effort per eigenvalue required by this method is, however, somewhat larger than for our method.

One can thus conclude that our method exhibits almost uniform efficiency for any value of n. Moreover, in each subinterval of the n range, its efficiency is approximately as high as that of the best placed one from the other methods on that subinterval.

V. CONCLUDING REMARKS

The chief point of this paper is the perturbation procedure developed in Sec. II. The difference between such a procedure and standard perturbation theory (i.e., perturbation theory as it is typically used to solve problems of quantum mechanics) consists in the domain for x on which they are applied. Indeed, the standard perturbation theory calls for the whole domain of Eq. (2.1), while our approach means essentially the application of the perturbation formalism on a *finite* (properly selected) subdomain of the equation. Because of this, the convergence of the perturbation series, which is often questionable in the case of the standard perturbation theory, becomes safe in the case of our formalism. This recommends our procedure as an appropriate tool for accurate mathematical investigation of a large class of physical phenomena, namely the ones which are described by linear second-order differential equations.

Seen in this way, the accurate numerical computation of the eigenvalues of the one-dimensional Schrödinger equation with the anharmonic-oscillator potential, which was our main concern in Secs. III and IV above, should be taken as only one of the possible applications of this piecewise perturbation procedure.

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[10]The approximate constancy of N versus the parameters of the anharmonic-oscillator problem comes from the near compensation of the opposite tendencies experienced by the density of mesh points (namely ρ), on the one hand, and by the length b of the domain $[0,b]$, on the other. For instance, in the case of fixed n, m^2, and α but variable λ, the density ρ increases with λ while the length b decreases at a rate which practically compensates the increase of ρ.