Calculation of the eigenvalues of Schrödinger equations by an extension of Hill's method

André Hautot (*) and Alphonse Magnus (**)

ABSTRACT

The eigenfunctions of the one dimensional Schrödinger equation $\Psi'' + [E - V(x)]\Psi = 0$, where $V(x)$ is a polynomial, are represented by expansions of the form $\sum_{k=0}^{\infty} c_k \varphi_k(\omega, x)$. The functions $\varphi_k(\omega, x)$ are chosen in such a way that recurrence relations hold for the coefficients c_k : examples treated are $D_k(\omega x)$ (Weber-Hermite functions), $\exp(-\omega x^2)\, x^k$, $\exp(-cx^q)\, D_k(\omega x)$. From these recurrence relations, one considers an infinite bandmatrix whose finite square sections permit to solve approximately the original eigenproblem. It is then shown how a good choice of the parameter ω may reduce dramatically the complexity of the computations, by a theoretical study of the relation holding between the error on an eigenvalue, the order of the matrix, and the value of ω. The paper contains tables with 10 significant figures of the 30 first eigenvalues corresponding to $V(x) = x^{2m}$, $m = 2(1)7$, and the 6 first eigenvalues corresponding to $V(x) = x^2 + \lambda x^{10}$ and $x^2 + \lambda x^{12}$, $\lambda = .01(.01).1(.1)1(1)10(10)100$.

1. INTRODUCTION

We first recall the form of the one-dimensional Schrödinger equation (SE) : $\Psi'' + [E - V(x)]\ \Psi = 0$ with the limiting condition for the eigenstates : $\int |\Psi|^2\, dx < \infty$. The aim of this paper is the calculation of the eigenvalues (ev) E_N ($N = 0, 1, \ldots$) of the energy parameter when the potential function $V(x)$ is of the type :

$$V(x) = x^{2m} + \lambda x^{2n} + \mu x^{2p} + \ldots \qquad (1 \leqslant m < n < p < \ldots \text{ integers})$$

Our method will be based on the use of the Hill determinant as presented in a previous paper [1]. However our principal goal here will be the optimalization of the method. We shall try to solve the problem in a simple and neat way. It is known that when λ is small the potential $x^{2m} + \lambda x^{2n}$ can be treated as a x^{2m} potential sligthly perturbed by the x^{2n} term. When λ is large the same potential can be assimilated to a x^{2n} potential sligthly perturbed by the x^{2m} term. That is the reason why we shall first study the potential $V(x) = x^{2m}$. We shall see later that more complex potentials of the type $x^{2m} + \lambda x^{2n} + \ldots$ can be treated in a similar way.

2. THE HILL DETERMINANT METHOD AND THE (k, ω, δ) RELATION

The starting equation can be written as :

$$\Psi'' + (E - x^{2m})\ \Psi = 0 \qquad (1)$$

We look for a solution of the type

$$\Psi = \sum_{0}^{\infty} c_k \varphi_k(\omega, x)$$

where the parameter ω is a priori arbitrary. Its essential role will be precised later. Since $V(x) = x^{2m}$ is an even function of the variable x it is eventually possible to deal separately with the odd and even eigenstates by setting :

$$\Psi = \sum_{0}^{\infty} c_k \varphi_{2k}(\omega, x) \quad \text{for the even states} \qquad (2)$$

$$\Psi = \sum_{0}^{\infty} c_k \varphi_{2k+1}(\omega, x) \quad \text{for the odd states}$$

(*) A. Hautot, University of Liège, Institute of Physics, Sart Tilman 4000, Liège 1, Belgium.

(**) A. Magnus, U.C.L., Institute of Pure and Applied Mathematics, Chemin du Cyclotron 2, 1348 Louvain la Neuve, Belgium.

The sole restriction on φ_k is : $\varphi_k(-x) = (-1)^k \varphi_k(x)$.
Since the distinction between even and odd states brings non negligible simplifications in the calculations we shall use it as far as possible. Note that the generality of the theory is not affected by that distinction.
Let us introduce the expansion (2) in equ. (1); one finds :

$$\sum_0^\infty c_k [\varphi''_{2k}(\omega, x) + (E - x^{2m}) \varphi_{2k}(\omega, x)] = 0$$

If it is possible to express φ''_{2k} and $x^{2m} \varphi_{2k}$ by means of a finite number of consecutive φ_{2j} functions then by collecting the corresponding terms and by identifying the whole expressions to zero one gets a finite recurrence between the c_k. It is always possible to rewrite that recurrence under the following canonical form :

$$A_k^{(n)}(\omega, E)\, c_{k+1} + A_k^{(n-1)}(\omega, E)\, c_k + \ldots + A_k^{(0)}(\omega, E)\, c_{k-n+1} = 0 \qquad (3)$$

with $c_k = 0$ if $k < 0$ and $k = s, s+1, \ldots$ ($s \geqslant 0$, fixed integer).
In the cases where the recurrence (3) only regards the even states, the other recurrence which corresponds to the odd states can be deduced from it by simply replacing k by $k + 1/2$ in the coefficients of $c_{k+1}, c_k \ldots$
It is possible to rewrite the set of recurrent relations (3) under the form of an infinite linear homogeneous system with the infinity of unknowns $c_0, c_1, \ldots$ The determinant D of the infinite matrix of the system is called the Hill determinant of the recurrence :

$$D = \begin{vmatrix} A_s^{(n-s-1)}(\omega,E) & A_s^{(n-s)}(\omega,E) & \ldots & A_s^{(n)}(\omega,E) & & \\ A_{s+1}^{(n-s-2)}(\omega,E) & A_{s+1}^{(n-s-1)}(\omega,E) & \ldots & A_{s+1}^{(n-1)}(\omega,E) & A_{s+1}^{(n)}(\omega,E) & 0 \\ \vdots & & & & & \\ A_{n-1}^{(0)}(\omega,E) & \ldots & & & & A_{n-1}^{(n)}(\omega,E) \\ 0 & & & & & \end{vmatrix} \qquad (4)$$

All the elements are zero except those on the main diagonal, on the $(s+1)$ upper adjacent diagonals and on the $(n-s-1)$ lower adjacent diagonals. The ev E_N ($N = 0, 1, 2, \ldots$) of equ. (1) are precisely the roots of D. These ev may of course not depend on the value given to ω. Practically it is not necessary to consider all the elements of D. Let us truncate D by only considering its k first lines and columns : the $k \times k$ resulting determinant $D^{(k)}$ is the k^{th} approximant of D. With the restriction that the procedure will converge we have : $D = \lim_{k \to \infty} D^{(k)}$ and in the same way the roots $E^{(k)}$ of $D^{(k)}$ tend to those of D : $E_N = \lim_{k \to \infty} E_N^{(k)}$.
More generally even when the sequence $D^{(k)}$ diverges we shall show in section 4 that the roots of $D^{(k)}$ effectively tend to the eigenvalues of equ. (1).
Finally we shall adopt the following technique for the calculations : we intend to compute an ev E_N of equ. (1) with a precision at least equal to e^{-p}. We shall compute the corresponding root $E_N^{(k)}$ of the smallest approximant $D^{(k)}$ so that the consideration of a larger approximant would not affect the value just found in the limits of the given precision. Let us precise the notations; we shall write :

$$\left| E_N - E_N^{(k)} \right| = e^{-\delta} \qquad \text{(absolute error)} \qquad (5)$$

$$\left| E_N - E_N^{(k)} \right| / \left| E_N \right| = e^{-p} \qquad \text{(relative error = precision)} \qquad (6)$$

We further have : $\delta = p - \ln \left| E_N \right|$ (7)

When one tries to calculate numerically the roots $E_N^{(k)}$ with the aid of a given algorithm one remarks that the order k of the approximant which leads to the ev looked for with the precision e^{-p} strongly depends on the value of the parameter ω. That dependence will be called the (k, ω, p) relation or equivalently because of (7) the (k, ω, δ) relation. The interest for this relation is easily understood : if the value of ω is correctly chosen the calculation of the ev E_N with a given precision will need the consideration of approximants $D^{(k)}$ of minimal dimension and the computation time will be reduced.

3. CALCULATION OF THE ev OF EQUATION (1)

We shall successively adopt three types of φ_k functions. Each procedure will exhibit its own advantages.

3.1. First approach : $\varphi_k(\omega,x) = D_k(\omega,x)/\Gamma(k/2+1)$

The D_n are the classical Weber-Hermite functions [2]. They satisfy the following relations :

$$D_n''(u) = (u^2/4 - n - 1/2)\, D_n(u)$$

$$u\, D_n(u) = D_{n+1}(u) + n\, D_{n-1}(u)$$

The last equation can be generalized as follows :

$$u^l D_n(u) = a_{-l/2} D_{n-l} + a_{-l/2+1} D_{n-l+1} + \ldots + a_{l/2} D_{n+l}$$

$$(l = 1, 2, \ldots)$$

where the a_j are given by hypergeometric expressions $(j = -l/2, -l/2 + 1, \ldots, l/2)$:

$$a_j = \frac{\Gamma(n+1)\, l!\, 2^{|j|-l/2}}{\Gamma(n+1+j-|j|)(l/2-|j|)!\,|2j|!}\, F(-n+|j|-j, |j| - l/2; 2|j|+1; 2)$$

These relations allow to find the recurrence satisfied by the c_k of equ. (2). After a little calculation one finds $(k = m-1, m, \ldots$ i.e. $s = m-1)$:

$$[E\omega^{2m} - \omega^{2m+2}(k + 5/4 - m)]\, c_{k-n+1}$$

$$+ \omega^{2m+2}/4\,(k - m + 1)\, c_{k-m}$$

$$+ \omega^{2m+2}/2\,(2k - 2m + 3)\, c_{k-m+2}$$

$$- \sum_{j=-m}^{m} \frac{(2k-2j-2m+2)!\,(2m)!\,2^{|j|-m}\,(k-m+1)!}{(2k-j-|j|-2m+2)!\,(m-|j|)!\,|2j|!\,(k-j-m+1)!}$$

$$F(-2k + j + |j| + 2m - 2, |j| - m; 2|j| + 1; 2)\, c_{k-j-m+1} = 0 \qquad (8)$$

Recurrence (8) holds for even states only. The recurrence for odd states can be deduced by simply replacing k by $k + 1/2$ in the coefficients of (8). Recurrence (8) contains $(2m+1)$ terms connecting $c_{k+1}, c_k, \ldots, c_{k-2m+1}$. The coefficients are polynomials in k of degree m. When $m > 3$ equ. (8) is rather complicated so that this approach becomes untractable. We have performed various numerical tests in the case $m = 2$ in order to estimate the (k, ω, δ) relation. Figure 1 exhibits the (k, ω) behaviour for the four first even states $(N = 0, 2, 4, 6)$ in the case $p = 28$ (about 12 correct figures for the ev). We remark the decrease of k when ω increases and the limiting $k_{opt} \sim 12$. In practice it is therefore evident that a sufficiently large ω-value must be chosen in order that k be next k_{opt}. For example $\omega = 2.5$ should be convenient. A too large ω-value is not only unnecessary but also prejudicial since in the recurrence (8) ω appears at the power $2m + 2 = 6$; it is evident that large coefficients in the recurrence could induce loss of significant figures in the numerical calculations.

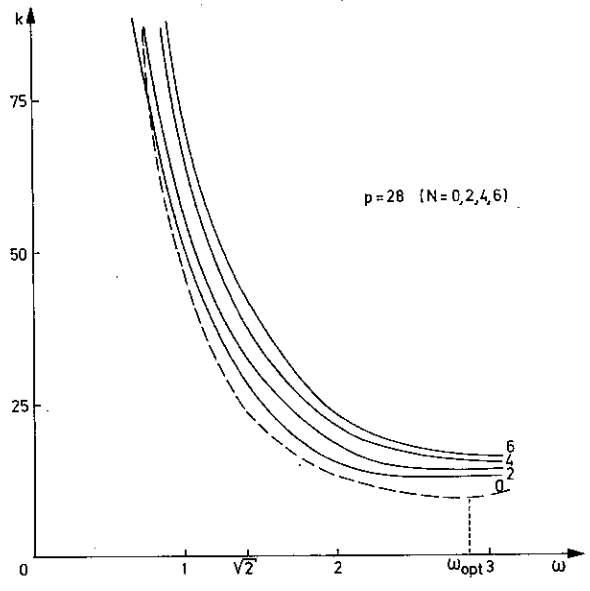

Fig. 1.

Remark : it might be tempting to expand Ψ in series of the eigenfunctions of the harmonic oscillator x^2 i.e. for the even states :

$$\Psi = \sum_0^\infty c_k\, D_{2k}\,(x\sqrt{2})/k!$$

That expansion corresponds to the choice $\omega = \sqrt{2}$. Figure (1) shows that this choice is not the best since the corresponding value of k is about three times k_{opt}.

3.2. Second approach

$$\varphi_k(\omega, x) = \exp[-x^{2q+2}/(2q+2)]\, D_k(\omega, x)/\Gamma(k/2+1)$$

This approach is interesting only if $m = 2q+1$ $(q = 1, 2, \ldots)$ corresponding to the oscillators $x^6, x^{10}, \ldots$ Proceeding as in section 3.1 one gets the following recurrence between the c_k (even states) : $k = q, q+1, \ldots$

$$[E\omega^{2q} - \omega^{2q+2}(k + 1/4 - q)]\, c_{k-q} + \omega^{2q+2}/4(k-q)\, c_{k-q-1}$$

$$+ \omega^{2q+2}/2(2k - 2q + 1)\, c_{k-q+1}$$

$$+ \sum_{-q-1}^{q+1} \frac{(2k-2j-2q)!\,(2q+1)!\,2^{|j|-q}\,(k-q)!\,j}{(2k-2q-j-|j|)!\,(q-|j|+1)!\,|2j|!\,(k-q-j)!}\, F(-2k + 2q + j + |j|, |j| - q - 1; 2|j| + 1; 2)\, c_{k-q-j} = 0 \qquad (9)$$

Recurrence (9) contains $(2q + 3)$ terms and its coefficients are polynomials in k of degree $q + 1$. Let us recall that in the first approach the number of terms was $(4q + 3)$ and the degree of the coefficients was $2q + 1$. It is seen that this approach is simpler but it does not allow to deal with all the values of m. The sole values of q which are practically tractable by this method are the values $q = 1$ or 2. When $q > 2$ the recurrence (9) is too complicated. We have performed several numerical investigations in the case $q = 1$ (po-

tential x^6). The results are collected in figure 2 which exhibits the main features of the (k, ω, δ) relation for the four first even states. One observes a behaviour quite similar to that of the first approach. Of course, the value of k_{opt} is modified.

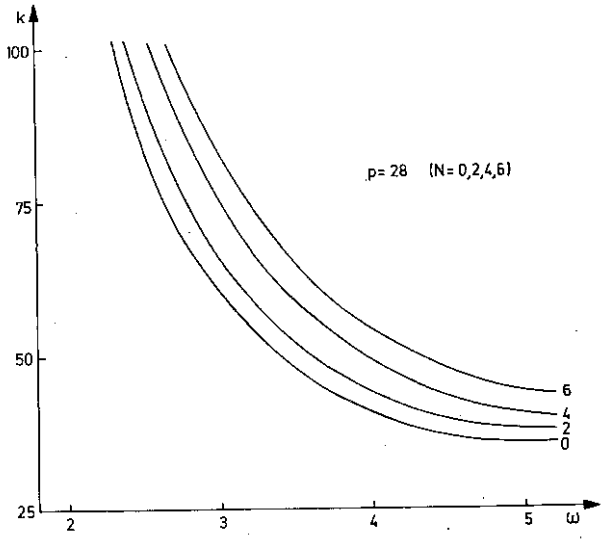

Fig. 2.

3.3. Third approach

$$\varphi_k(\omega, x) = \exp(-\omega x^2)\, x^k$$

In this approach the recurrence between the c_k is easily deduced in the form :

$$(2k+1)(2k+2)c_{k+1} + (E-2\omega-8\omega k)\, c_k + 4\omega^2 c_{k-1} - c_{k-m} = 0 \qquad k = 0,1,2,\ldots \text{ (even states)} \tag{10}$$

For the odd states let us recall that k must be replaced by $k + 1/2$. That recurrence is of order $(m + 1)$ though only four terms are different from zero. The structure of the coefficients is quite simple which facilitates the numerical calculations. We have studied numerically the (k, ω, δ) relation in the case $m = 2$. Figure 3 represents with solid lines the essential of the results for eight even states ($N = 0, 4, 8, \ldots, 28$) calculated at the precision e^{-28}. Figure 4 does the same for the sole fundamental state at various precisions. One remarks that the bearing of the curves is essentially different : k presents a minimum, k_{opt}, when $\omega = \omega_{opt}$. Therefore numerical investigations must be carried on with a value of ω in the neighbour of ω_{opt} if one wishes to optimalize the efficiency of the method. That feature of the (k, ω) curves is characteristic of that approach for the x^{2m} potential. We have reported in table 1 the experimental values of k_{opt} and ω_{opt} for the fundamental state of the potentials x^4 to x^{20} determined at the precision $e^{-28} \sim 10^{-12}$. If one considers the excited states one remarks an increase in the values of k_{opt} and ω_{opt}; they also increase with δ. All the (k, ω)

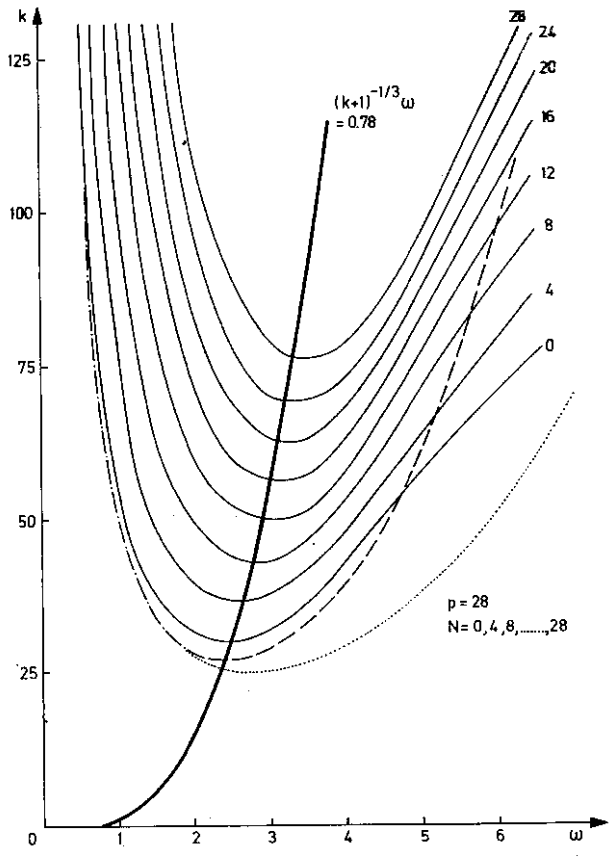

Fig. 3.

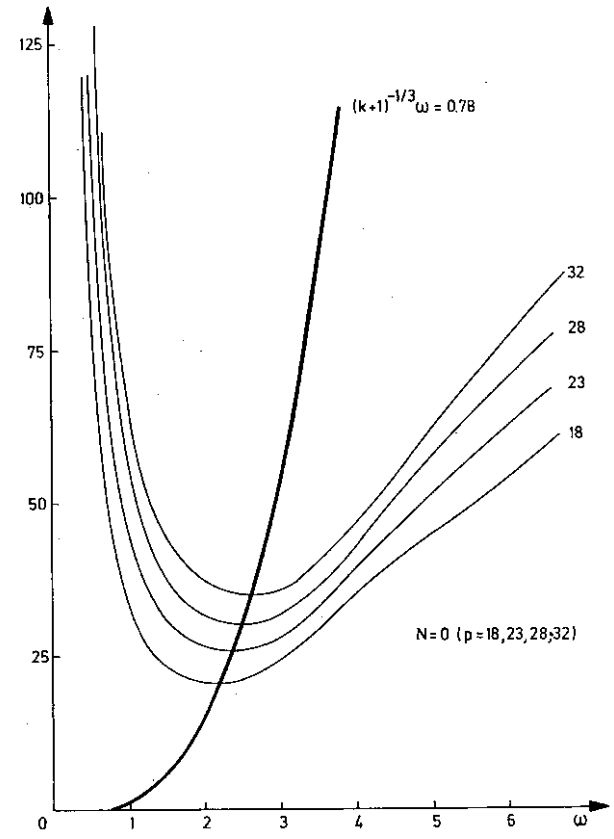

Fig. 4.

curves fit in to each other. All the minima approximatively lie on a same curve independent of E and of δ. We shall reexamine this point later. We have used the values of ω_{opt} contained in table 1 in order to calculate the first 30 states (even and odd) for the oscillators x^4 to x^{14}. They are reported in table 2. Let us recall that the ev spectra are given by simple formulas in two extreme cases :

Table 1. Experimental and theoretical values of k_{opt} and ω_{opt} (p = 28)

m	k_{opt} (exp.)	ω_{opt} (exp.)	k_{opt} (simpl. proc.)	ω_{opt} (simpl. proc.)	k_{opt} (refined proc.)	ω_{opt} (refined proc.)
2	30	2.4	25	2.76	27	2.37
3	53	6.0	56	5.29	50	5.83
4	79	11.2	85	10.4	77	11.3
5	109	19	112	18.4	108	19.0
6	143	29.5	138	29.9	143	29.1
7	179	42	163	45.0	182	41.8
8	219	57	188	64.1	226	57.0
9	262	74.5	212	87.4	273	75.0
10	310	95	236	115	324	95.7

if m = 1 then $E_N = 2N + 1$ and if m = ∞ then $E_N = \pi^2 (N + 1)^2/4$.

Remark : when m = 2 one has $\omega_{opt} = 2.4$ if $\delta = 28$ (fundamental state). It is interesting to point out the work of Biswas et alii [3] on the same oscillators : they systematically choose $\omega = 0.5$ without suspecting the role played by the factor ω. The result was that they had to deal with approximants of large order $k \approx 140$ about six times k_{opt}. The phenomenon was increased when m = 3, 4, ... since in these cases ω_{opt} is very different from 0.5. The numerical results they obtained were fragmentary and it is not surprising they renounced to complete them because the time of calculation was excessive.

4. THEORETICAL STUDY OF THE (k, ω, δ) RELATION

Section 3 has shown several possible (k, ω) behaviours which are to be interpreted. The interest of the theory is evident since it would allow to predict the values of k_{opt} and ω_{opt} in practical cases. In order to attain this aim it is necessary to estimate the error committed when truncating the infinite determinant D to the value $D^{(k)}$ of its k^{th} approximant. A theorem has been presented elsewhere [1] which allow to calculate recursively the various approximants $D^{(k)}$. Let us recall its statement : if one constructs (s + 1) sequences $N_k^{(j)}$ (j = 1, ..., s + 1) satisfying the recurrence (3) with the following initialization ($k \leqslant s$) :

$$N_k^{(j)} = \delta_{k,\,j-1} \quad (=1 \text{ if } k = j-1, \text{ otherwise } = 0)$$

One has the following identity :

$$D^{(k)} = \begin{vmatrix} A_s^{(n-s-1)} & \cdots & A_s^{(n)} & & 0 \\ \vdots & & & \ddots & \\ A_{n-1}^{(0)} & & & & A_{k-2}^{(n)} \\ & \ddots & & & \vdots \\ 0 & & A_{k+s-1}^{(0)} & \cdots & A_{k+s-1}^{(n-s-1)} \end{vmatrix}$$

$$= (-1)^{k(s+1)} A_s^{(n)} A_{s+1}^{(n)} \cdots A_{k+s-1}^{(n)} \begin{vmatrix} N_k^{(1)} & \cdots & N_k^{(s+1)} \\ \vdots & & \vdots \\ N_{k+s}^{(1)} & \cdots & N_{k+s}^{(s+1)} \end{vmatrix} \qquad (11)$$

Whatever large be k, the k×k determinant $D^{(k)}$ is equal to a (s+1) × (s+1) determinant which order is fixed. Its $(s+1)^2$ elements can be calculated recursively through (3). Recurrence (3) (without the conditions $c_k = 0$ if $k < 0$) has n independent solutions which are noted $c_k^{(l)}$ (l = 0, 1, ..., n - 1). Let us make the assumption (always verified in the practical cases that are in view) that it is possible to order these n solutions so that the (s + 1) first dominate the (n - s - 1) others i.e. :

$$\lim_{k \to \infty} c_k^{(l')} / c_k^{(l)} = 0 \quad \text{with} \quad 0 \leqslant l \leqslant s < l' \leqslant n-1$$

We call *subdominant solution* any linear combination of $c_k^{(s+1)}, \ldots, c_k^{(n-1)}$, and *dominant solution* any *non subdominant* linear combination of $c_k^{(0)}, \ldots, c_k^{(n-1)}$. The subdominant solutions of the recurrence have been numerically studied by Gautschi [4] (in the case n = 2, s = 0) and Oliver [5]. We shall see that the coefficients c_k present in equ. (2) precisely correspond to a subdominant solution of (3). Let us note ρ_k the ratio of that form which tends the least fast to zero : ρ_k appears as the quotient of the largest subdominant solution to the smallest dominant solution. It is easy to prove that the errors resulting of the replacement of D by its approximant $D^{(k)}$ behave like ρ_k : to see it we first express the $N_k^{(j)}$ in function of the $c_k^{(l)}$:

$$N_k^{(j)} = \sum_{i=0}^{n-1} a_{i,j}\, c_k^{(i)} \qquad j = 1, \ldots, s+1$$

If we ignore the $(n-s-1)$ last terms in the summation we neglect the subdominant solutions and the error is of the order of ρ_k. Introducing these simplified expressions in equ. (11) we get :

$$\begin{vmatrix} N_k^{(1)} & \cdots & N_k^{(s+1)} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ N_{k+s}^{(1)} & \cdots & N_{k+s}^{(s+1)} \end{vmatrix}$$

$$= \begin{vmatrix} c_k^{(1)} & \cdots & c_k^{(s+1)} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ c_{k+s}^{(1)} & \cdots & c_{k+s}^{(s+1)} \end{vmatrix} \begin{vmatrix} a_{1,1} & \cdots & a_{1,s+1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{s+1,1} & \cdots & a_{s+1,s+1} \end{vmatrix} (1 + 0(\rho_k))$$

where $0(\rho_k)$ means "tends to zero in the same way as ρ_k when $k \to \infty$". One has :

$$\begin{vmatrix} a_{1,1} & \cdots & a_{1,s+1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{s+1,1} & \cdots & a_{s+1,s+1} \end{vmatrix}$$

$$= \lim_{k \to \infty} \frac{D^{(k)}}{(-1)^{k(s+1)} A_s^{(n)} \ldots A_{s+k-1}^{(n)} \begin{vmatrix} c_k^{(1)} & \cdots & c_k^{(s+1)} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ c_{k+s}^{(1)} & \cdots & c_{k+s}^{(s+1)} \end{vmatrix}}$$

The roots E_N of D thus coincide with the roots of

$$\begin{vmatrix} a_{1,1} & \cdots & a_{1,s+1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{s+1,1} & \cdots & a_{s+1,s+1} \end{vmatrix}$$

This determinant is generally an analytic function of E, and has therefore isolated zeros in the complex plane. If E is such a zero, and only then, a linear combination $c_k = \gamma_1 N_k^{(1)} + \ldots + \gamma_{s+1} N_k^{(s+1)}$ exists which is a subdominant solution of (3). Consequently, for these values of E only, the Schrödinger equation has a solution whose expansion (2) is built with a subdominant solution of (3). In order to be sure that the original eigenvalue problem has been solved, one must show that these expansions only correspond to square integrable functions. The way to achieve this depends on the choice of the functions $\varphi_k(\omega, x)$. For instance, from the orthogonality relations of the Weber-Hermite functions,

$\Psi(x) = \sum_{k=0}^{\infty} c_k D_{2k}(\omega x)/(k!)$ is square integrable if and only if

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = \sum_{k=0}^{\infty} (\sqrt{2\pi}/\omega)(2k)! \, |c_k|^2/(k!)^2 < \infty .$$

As another example, it will be shown in section 4.3 that, if c_k is a subdominant solution of (10), $\Psi(x) = \sum_{k=0}^{\infty} c_k x^{2k} \exp(-\omega x^2)$ behaves like $|x|^{-m/2} \exp[-|x|^{m+1}/(m+1)]$ when x is a large real (positive or negative) number, whereas any dominant solution of (10) gives birth to a function behaving like $|x|^{-m/2} \exp[|x|^{m+1}/(m+1)]$ in the same conditions.

If we note $E_N^{(k)}$ the roots of the approximant $D^{(k)}$ we have $|E_N^{(k)} - E_N| = 0(\rho_k)$ if E_N is of multiplicity one. On account of equ. (5) it is possible to rewrite this relation in the following way :

$$|E_N^{(k)} - E_N| = |g(E_N)| \, |\rho_k| = e^{-\delta}$$

The function g(E) is unknown and in fact it seems rather impossible to specify its form through theoretical deductions. In practice we can only hope that $g(E) = 0(1)$ so that we should have with a good approximation :

$$\delta = -\ln|\rho_k| \quad \text{or equivalently on account of equ. (7)} \quad (12)$$

$$p = -\ln|\rho_k| + \ln|E_N| \qquad (13)$$

Equ. (12) is precisely the (k, ω, δ) relation that we look for since ρ_k depends on ω and k. It plays an essential role since it allows to predict the order k of the smallest approximant to be considered if one wishes to calculate the ev to a given accuracy. It also allows to predict approximately the values of k_{opt} and ω_{opt}. The procedure can be summarized as follows : one starts with the recurrence brought into the form (3). One calculates the asymptotic behaviour of the n independent solutions $c_k^{(0)}, \ldots, c_k^{(n-1)}$. One verifies that $(s+1)$ solutions dominate the $(n-s-1)$ others. One writes ρ_k as the ratio of the largest subdominant solution to the smallest dominant one. Equ. (12) furnishes the desired (k, ω, δ) relation. In order to determine the asymptotic behaviour of the solutions one has the choice between two different methods which we shall successively use in order to be able of comparing their respective advantages.

4.1. Theoretical study of the (k, ω, δ) relation in the case where Ψ is expanded in terms of Weber-Hermite functions

Here we try to recover theoretically the numerical results of section 3.1. The recurrence is given by (8). For the sake of simplicity we only deal with the case m = 2. One has :

$$(16k^2-4)c_{k+1}+[32k^2-(24+\omega^6)k+(4+\omega^6/2)]c_k$$

$$+[24k^2+(\omega^6-36)k+(15-3\omega^6/4-E\omega^4)]c_{k-1}$$

$$+[8k^2-(18+\omega^6/4)k+(10+\omega^6/4)]c_{k-2}$$

$$+(k^2-3k+2)c_{k-3}=0 \qquad (14)$$

$(k = 1, 2, \ldots,$ i. e. $s = 1)$.

Here we shall use the technique of Denef and Piessens [6]. The recurrence is of order 4; let us make the hypothesis that when k is large c_k is of the type :

$$c_k \sim a^k\, k^w \exp(\alpha k^{3/4} + \beta k^{2/4} + \gamma k^{1/4} + \ldots)$$

In order to be sure that the assumption is valid we introduce that expression in the recurrence (14) previously divided by c_k. We then obtain expressions that can be developed in powers of $k^{-1/4}$. Collecting the corresponding terms and equating to zero the coefficients of the highest powers of k we obtain the relation that fixes the values of a, w, α, β, γ, ... The result is $(l = 0, 1, 2, 3)$:

$$c_k^{(l)} \approx (-1/2)^k \exp\left[-\frac{2}{3}\omega^{3/2} e^{i\pi(2l+1)/4}(2k)^{3/4}\right.$$

$$\left.-\frac{\omega^{9/2}}{24}e^{-i\pi(2l+1)/4}(2k)^{1/4}+\ldots\right]k^{-3/8}$$

It is immediately seen that solutions $c_k^{(0)}$ and $c_k^{(3)}$ dominate $c_k^{(1)}$ and $c_k^{(2)}$. On the other side the subdominant solutions only verify the condition $\sum_0^\infty |c_k|^2 (2k)!/k!^2 < \infty$ and thus alone correspond to a square integrable eigenfunction of the SE(1) provided there exists a non trivial linear combination of these that vanishes when $k < 0$. It is easy to calculate :

$$|\rho_k| = |c_k^{(1)}/c_k^{(0)}| \approx \exp\left[-\sqrt{2}\,\frac{2}{3}\omega^{3/2}(2k)^{3/4}\right.$$

$$\left.+\frac{\sqrt{2}}{24}\omega^{9/2}(2k)^{1/4}\right]$$

from which we deduce the theoretical (k, ω, δ) relation :

$$\delta \approx \sqrt{2}\,\frac{2}{3}\omega^{3/2}(2k)^{3/4} - \frac{\sqrt{2}}{24}\omega^{9/2}(2k)^{1/4}$$

When $\delta = 28$ the corresponding (k, ω) curve is represented with dashed lines on figure 1. When ω increases k decreases, passes through a minimum $k_{opt} = 9\sqrt{6}\,\delta/64$, $\omega_{opt} = (48\delta/\sqrt{6})^{1/6}$ and increases in accordance with the numerical data. However a discrepancy arises when k becomes too small due to the fact that at low k it is impossible to ensure the validity of the asymptotic expressions for $c_k^{(l)}$.

4.2. Theoretical study of the (k, ω, δ) relation in the case where Ψ is expanded as a Taylor series.

Here we try to explain the numerical results related in section 3.3. We shall deal with the general case of the oscillator x^{2m}. We start with recurrence (10) (even states). We look for the asymptotic behaviour of the c_k by two different ways.

4.2.1. Simplified procedure

We use again the technique of Denef and Piessens. Let us first put :

$$c_k = d_k/\Gamma[1 + 2k/(m+1)]$$

The recurrence for the d_k can be written as :

$$(m+1)(2k+1)d_{k+1} + (E-2\omega-8\omega k)\left(\frac{2k}{m+1}\right)^{(1-m)/(m+1)}$$

$$\ldots\left[1+\frac{1-m}{1+m}(2k)^{-1}+\ldots\right]d_k$$

$$+4\omega^2\left(\frac{2k}{m+1}\right)^{(3-m)/(m+1)}\left[1+0k^{-1}+\ldots\right]d_{k-1}$$

$$-(2k-m+1)/(m+1)\,d_{k-m}=0 \qquad (15)$$

Where use has been made of the well-known identity :

$$z^{b-a}\Gamma(z+a)/\Gamma(z+b) \sim 1+(a-b)(a+b-1)/(2z)+\ldots$$

Proceeding as in section 4.1 it is easy to establish that $(l = 0, 1, 2, \ldots, m)$:

$$d_k^{(l)} = \left[\frac{e^{2i\pi l/(m+1)}}{(m+1)^{2/(m+1)}}\right]^k k^{\frac{-m}{2m+2}} \exp\left[\omega e^{-2i\pi l/(m+1)}(2k)^{2/}\right.$$

$$\left.-\frac{2\omega^2}{m+1}e^{-4i\pi l/(m+1)}(2k)^{(3-m)/(m+1)}+\ldots\right] \qquad (16)$$

It is easily seen that $c_k^{(0)}$ dominates the other solutions. We have :

$$|\rho_k| = |c_k^{(1)}/c_k^{(0)}| \approx \exp\left[\omega(\cos\frac{2\pi}{m+1}-1)(2k)^{2/(m+1)}\right.$$

$$\left.-\frac{2\omega^2}{m+1}(\cos\frac{4\pi}{m+1}-1)(2k)^{(3-m)/(m+1)}\right]$$

We deduce the (k, ω, δ) relation :

$$\delta = 2\omega\sin^2\frac{\pi}{m+1}(2k)^{2/(m+1)}$$

$$-\frac{4\omega^2}{m+1}\sin^2\frac{2\pi}{m+1}(2k)^{(3-m)/(m+1)} \qquad (17)$$

The corresponding (k, ω) curve has been plotted in dotted lines on figure 3 in the case $(m = 2, \delta = 28)$. The coordinates of the minimum are easily deduced from (17) :

$$\omega_{opt} = \delta \operatorname{cosec}^2 \frac{\pi}{m+1} [(m+1) \operatorname{tg}^2 \frac{\pi}{m+1} / (16\delta)]^{2/(m+1)}$$

$$k_{opt} = 8\delta \operatorname{cotg}^2 \frac{\pi}{m+1} / (m+1)$$

When $\delta = 28$ the numerical values of k_{opt} and ω_{opt} are reported in table 1 in the column "simplified procedure". The agreement with the experimental values is good especially when m is small.

4.2.2. Refined procedure

We now turn to another more subtle approach. Let us first recall the expansion guessed for the solution of equ. (1) :

$$\Psi = \sum_0^\infty c_k e^{-\omega x^2} x^{2k} \quad \text{(even states)}$$

The c_k may be evaluated in the complex plane via Cauchy's theorem :

$$c_k = \frac{1}{2i\pi} \oint_\ell e^{\omega x^2} \Psi(x) x^{-2k-1} dx \qquad (18)$$

On another side the independent solutions $c_k^{(0)}, \ldots, c_k^{(m)}$ of (3) (without the restrictions $c_k = 0$ if $k < 0$) are given by such integrals calculated on distincts contours $\ell_0, \ldots, \ell_m$ [7, 8].

Let us suppose that ℓ_l does not approach too much the origin; it is then possible to replace Ψ by its asymptotic behaviour for large x :

$$\Psi \approx x^{-m/2} \exp [\pm x^{m+1}/(m+1)]$$

If we introduce that Ψ in equ. (18) we can evaluate the integral with the aid of the saddle point method [9].

$$\oint \exp [f(x)] dx \approx \sqrt{-\frac{2\pi}{f''(x^*)}} \exp f(x^*)$$

with $f'(x^*) = 0$

One has : $f(x) \approx \omega x^2 \pm x^{m+1}/(m+1) - (2k+1+m/2) \ln x$

Hence neglecting the factor $[-2\pi/f''(x^*)]^{1/2}$ one easily finds :

$$c_k^{(l)} \approx \exp [\omega x_l^2 \pm x_l^{m+1}/(m+1) - (2k+1+m/2) \ln x_l]$$

$$(l = 0, 1, \ldots, m) \qquad (19)$$

where x_l are the saddle points of f i.e. the roots of :

$$2\omega x_l \pm x_l^m - (2k+1+m/2)/x_l = 0 \qquad (20)$$

It is assumed that only x_l and $-x_l$ lie on ℓ_l [recall that $\Psi(x)$ is odd or even so that x_l and $-x_l$ contribute for the same quantity in (19)].

Equ. (20) implies that :

$$x_l^{2m+2} - (2k+1+m/2 - 2\omega x_l^2)^2 = 0$$

where x_l is the root located in the sector

$$\pi \frac{2l-1}{2m+2} < \arg x_l < \pi \frac{2l+1}{2m+2} \quad (l = 0, 1, \ldots, m).$$

This assumption is justified by the fact that for ω not too large one has $\lim_{\omega \to 0} \arg x_l = \frac{\pi l}{m+1}$ and that $\pm x_l^{m+1} \sim 2k > 0$ because of (20).

From another side following Sibuya [10] each solution of the SE(1) behaves like

$$|x|^{-m/2} \exp(-\frac{|x|^{m+1}}{m+1}) \text{ or like } |x|^{-m/2} \exp(\frac{|x|^{m+1}}{m+1})$$

when $x \to \infty$ in the direction $\arg x = \pi l/(m+1)$: however the second behaviour only corresponds to (19). Now if the coefficients c_k given by (18) behave like a subdominant solution of the recurrence (3) that means that x_0 and $-x_0$ are not saddle points of $e^{\omega x^2} \Psi(x) x^{-2k-1}$.

The conclusion is that

$|\Psi(x)| \approx |x|^{-m/2} \exp(-\frac{|x|^{m+1}}{m+1})$ when $x \to \pm \infty$ i.e. Ψ is a square integrable solution of the SE(1).

The ratio $|\rho_k|$ is easily calculated as equal to $|c_k^{(1)}/c_k^{(0)}|$.

Combining with equ. (12), (19) and (20) one finds :

$$\delta = \omega \frac{m-1}{m+1} R (x_0^2 - x_1^2) + (2k + 1 + m/2) \ln |x_1/x_0| \qquad (21)$$

Let us expand x_0 and x_1 in terms of powers of ω by starting with equ. (20); the two leading terms of the expansions introduced in (21) restitute result (17). However it is possible to determine exactly k_{opt} provided (19) is valid in the region $k \sim k_{opt}$. The calculation is performed as follows : one has

$\delta = R [f(x_0) - f(x_1)]$ with the conditions

$f'(x_0) = f'(x_1) = 0$

When ω varies k passes through a minimum if $dk/d\omega = 0$ i.e. if

$$R \left[\frac{\partial f(x_0)}{\partial \omega} - \frac{\partial f(x_1)}{\partial \omega} \right] = 0 \text{ which leads to } R x_0^2 = R x_1^2.$$

The root x_0 is real > 0 but x_1 is complex. We put : $x_1^2 = x_0^2 (1 + i \operatorname{tg} \sigma)$. If we introduce these expressions in equ. (20) with $\pm x_0^m = x_0^m$ and $\pm x_1^m = -x_1^m$ one obtains

$$-x_0^{m+1} = R x_1^{m+1}$$

Hence the equation for σ :

$$\cos \frac{m+1}{2} \sigma = -\cos^{\frac{m+1}{2}} \sigma, \quad \frac{\pi}{m+1} < \sigma < \frac{2\pi}{m+1} \qquad (22)$$

Combining with (20) and (21) one finds :

$$k_{opt} = -\delta/\ln\cos\sigma - m/4 - 1/2 \qquad (23)$$

$$x_0^{m+1} = (2k_{opt} + m/2 + 1)(1 - \mathrm{cotg}\,\sigma\,\mathrm{tg}\,\frac{m+1}{2}\sigma)^{-1}$$

$$\omega_{opt}(2k_{opt} + m/2 + 1)^{(1-m)/(m+1)}$$

$$= -\frac{1}{2}\mathrm{cotg}\sigma\,\mathrm{tg}\,\frac{m+1}{2}\sigma\,(1-\mathrm{cotg}\sigma\,\mathrm{tg}\,\frac{m+1}{2}\sigma)^{(1-m)/(m+1)} \qquad (24)$$

σ easily deduces through (22) and k_{opt} and ω_{opt} follows with (23) and (24). We have calculated the values of k_{opt} and ω_{opt} and we have reported them in table 1 in the column "refined procedure". One notes the remarkable agreement with the experimental numerical data. On another side the (k, ω) curve corresponding to the fundamental state with $\delta = 28$ has been plotted in dashed lines on figure 3. One sees that the theoretical curve behaves like the experimental one provided $\omega < 5$.

5. APPLICATION TO THE $x^2 + \lambda x^{2m}$ OSCILLATORS

It is possible to deal with the anharmonic oscillators $x^2 + \lambda x^{2m}$ exactly in the same way. If one calculates ω_{opt} in that case one finds that ω_{opt} varies very slowly with λ so that it is possible to perform the numerical calculations by adopting the values of ω_{opt} which are deduced from (22), (23) and (24). Tables 3 and 4 give the six first states (even and odd) of the oscillators $x^2 + \lambda x^{10}$ and $x^2 + \lambda x^{12}$ for λ varying between 0.01 and 100. To the best of our knowledge these quantities are calculated for the first time. That is also the first time that a method is presented that makes the access to the ev of an equation like (1) rather simple.

6. CONCLUSIONS

We now summarize the results. Wishing to calculate the ev of the SE(1) we have exhibited the central role played by the factor ω which enters in the expansion tried for Ψ :

$$\Psi = \sum_0^\infty c_k\,\varphi_k(\omega, x)$$

We have successively used an expansion in terms of Weber-Hermite functions and a Taylor expansion. At first sight the first choice seems preferable because of the orthogonality of W-H functions with the following consequences :

- the evaluation of the norm, of matrix elements,... is simplified
- if the oscillator $x^2 + \lambda x^{2m}$ is treated in a perturbative way the present method allows to calculate all the terms of the perturbative series with all the desired precision. Let us recall indeed that the functions $D_k(x\sqrt{2})$ are the eigenfunctions of the harmonic x^2 oscillator.

That approach is also interesting since it needs the calculation of approximants of peculiarly low order k. Unfortunately the recurrence (8) is rather complicated and for $m > 3$ it is hardly usable.

On the other side the calculation of the coefficients c_k of the eigenfunction is simpler in the approach with Taylor expansions. Let us now turn to that approach which finally appears as the most advantageous. When one expands Ψ in the form

$$\Psi = e^{-\omega x^2} \sum_0^\infty c_k\,x^k$$

it is important to assign to ω a numerical value next ω_{opt} otherwise k will be needlessly large. The theory of section 4 has learned us how to predict the (k,ω, δ) curves. If the agreement is not perfect that is of course due to the fact that the method is approximative in various aspects :

a) In equ. (12) $\ln|g(E)|$ is neglected beside $\ln|\rho_k|$.

b) In the calculation of the integral giving $c_k^{(1)}$ by the saddle point method we neglect the factor $[-2\pi/f''(x^*)]^{-1/2}$ beside the exponential.

c) In the same integral Ψ is replaced by its asymptotic behaviour.

Approximations a) and b) have for consequence that the theory predicts k systematically displaced with respect to the real value. The fact is visible on figure 3. Approximation a) also has for consequence that the prediction is mostly valuable at low E. When E increases (excited states) the discrepancy grows. Approximation a) is interesting to be discussed because it entails that in the calculations k_{opt} and ω_{opt} are only present in the combination

$$\omega_{opt}(2k_{opt} + m/2 + 1)^{(1-m)/(m+1)}$$ whatever E and δ are. The fact is visible in equ. (24).

In the special case $m = 2$ equ. (24) is written as :

$$(k_{opt} + 1)^{-1/3}\,\omega_{opt} = 0.780507$$

The corresponding (k, ω) curve has been plotted in heavy lines on figures 3 and 4. We note that it sensibly coincides with the locus of the minima of the (k,ω) curves when E and δ vary. However the coincidence may not be perfect because equ. (24) is not rigorous : that can be seen by pursuing the calculations to higher orders in the frame of the simplified procedure of section 4.2.1. It is found at the third order that ω_{opt} and k_{opt} become present under various forms incompatible with (24). One could hope to improve the pre-

Table 2. 30 first eigenvalues of x^{2m} oscillators.

N	m = 2	m = 3	m = 4	m = 5	m = 6	m = 7
0	1.060362090	1.144802454	1.225820114	1.298843701	1.363761485	1.421438884
1	3.799673030	4.338598712	4.755674414	5.097376529	5.386941566	5.636185031
2	7.455697938	9.073084581	10.24494698	11.15431820	11.89300911	12.51210199
3	11.64474551	14.93516963	17.34308797	19.18880956	20.66163758	21.87477520
4	16.26182602	21.71416542	25.80900675	28.97146721	31.48947138	33.54989074
5	21.23837292	29.29964594	35.49789881	40.34261544	44.21805376	47.38927498
6	26.52847118	37.61308656	46.31277050	53.19230577	58.73115625	63.27679623
7	32.09859771	46.59521145	58.17964995	67.43821316	74.94121674	81.12250701
8	37.92300103	56.19930085	71.03925768	83.01428708	92.77847260	100.8546172
9	43.98115810	66.38728171	84.84262459	99.86555654	112.1848896	122.4135996
10	50.25625452	77.12734146	99.54835286	117.9451916	133.1108601	145.7486045
11	56.73421406	88.39237577	115.1208011	137.2125943	155.5131898	170.8152866
12	63.40304869	100.1589279	131.5288311	157.6320740	179.3537422	197.5743945
13	70.25239463	112.4064358	148.7449100	179.1718918	204.5984667	225.9907866
14	77.27320048	125.1186807	166.7444474	201.8035511	231.2166779	256.0327095
15	84.45746628	138.2783727	185.5052932	225.5012574	259.1805036	287.6712482
16	91.79806681	151.8618318	205.0073490	250.2414935	288.4644561	320.8798978
17	99.28860666	165.8687392	225.2322620	276.0027124	319.0450905	355.6342237
18	106.9233074	180.2819389	246.1631799	302.7650201	350.9007303	391.9115861
19	114.6969174	195.0902772	267.7845515	330.5100082	384.0112429	429.6909157
20	122.6046390	210.2834723	290.0819640	359.2205492	418.3578541	468.9525272
21	130.6420687	225.8520061	313.0420062	388.8806922	453.9229926	509.6779636
22	138.8051479	241.7870341	336.6521555	419.4753366	490.6901596	551.8498643
23	147.0901213	258.0803093	360.9006807	450.9905258	528.6438175	595.4518535
24	155.4935023	274.7241181	385.7765605	483.4129554	567.7692944	640.4684432
25	164.0120436	291.7112248	411.2694125	516.7300945	608.0527020	686.8849505
26	172.6427120	309.0348244	437.3694321	550.9300780	649.4808639	734.6874251
27	181.3826662	326.6885012	464.0673398	586.0016462	692.0412533	783.8625859
28	190.2292387	344.6661934	491.3543345	621.9340933	735.7219380	834.3977651
29	199.1799188	362.9621614	519.2220527	658.7172213	780.5115319	886.2808594

Table 3. Eigenvalues of the $x^2 + \lambda x^{10}$ oscillator.

$\lambda \backslash N$	0	1	2	3	4	5
0.01	1.07688396	3.50093097	5.59222370	10.48429623	15.15429423	20.54576845
0.02	1.11126835	3.68360376	7.07747895	11.40444788	16.61545091	22.64065097
0.03	1.13610273	3.80993858	7.40335501	12.01203115	17.57153489	24.00424966
0.04	1.15605409	3.90893928	7.65454334	12.47609441	18.29824809	25.03782923
0.05	1.17294402	3.99133121	7.86126370	12.85569004	18.89079344	25.87904246
0.06	1.18770153	4.06240650	8.03811122	13.17898778	19.39426640	26.59287679
0.07	1.20087332	4.12520643	8.19334718	13.46179595	19.83392594	27.21554249
0.08	1.21281176	4.18165583	8.33213950	13.71393945	20.22533409	27.76942365
0.09	1.22375888	4.23305741	8.45795324	13.94197170	20.57888295	28.26938762
0.10	1.23388897	4.28033769	8.57323365	14.15049764	20.90185687	28.72584481
0.20	1.30888218	4.62332974	9.39881047	15.63414121	23.19210402	31.95639924
0.30	1.35990215	4.85115413	9.93889204	16.59740457	24.67330733	34.04107028
0.40	1.39953087	5.02577086	10.34937584	17.32654508	25.79217390	35.61389094
0.50	1.43231862	5.16895166	10.68406560	17.91944883	26.70073546	36.89006429
0.60	1.46048203	5.29112184	10.96845228	18.42224475	27.47044235	37.97057169
0.70	1.48528376	5.39814840	11.21677410	18.86060312	28.14098104	38.91144160
0.80	1.50751761	5.49368575	11.43784912	19.25037754	28.73682643	39.74719889
0.90	1.52771805	5.58017598	11.63754296	19.60208998	29.27420397	40.50071666
1.00	1.54626351	5.65933772	11.81996788	19.92310357	29.76445746	41.18797768
2.00	1.67996278	6.22425713	13.11359426	22.19291669	33.22584805	46.03618913
3.00	1.76813237	6.59236273	13.95027378	23.65601615	35.45321630	49.15285910
4.00	1.83544885	6.87156537	14.58230135	24.75922862	37.13115849	51.49947717
5.00	1.89050496	7.09891287	15.09554333	25.65401580	38.49126163	53.40091545
6.00	1.93739386	7.29190633	15.53035504	26.41139505	39.64198423	55.00921630
7.00	1.97841068	7.46030174	15.90915186	27.07074879	40.64342219	56.40858490
8.00	2.01498114	7.61013233	16.24575771	27.65633482	41.53256886	57.65083685
9.00	2.04805590	7.74540663	16.54933719	28.18421908	42.33391273	58.77026266
10.00	2.07830279	7.86893228	16.82629768	28.66562483	43.06455387	59.79080128
20.00	2.29355957	8.74373534	18.78181828	32.06022544	48.21322186	66.97953796
30.00	2.43337437	9.30868507	20.04022807	34.24137107	51.51885995	71.59288965
40.00	2.53923875	9.73511172	20.98824819	35.88317379	54.00605600	75.06317274
50.00	2.62534252	10.08121574	21.75670527	37.21327339	56.02048716	77.87336821
60.00	2.69837383	10.37432081	22.40687062	38.33817095	57.72379269	80.24924908
70.00	2.76205518	10.62959274	22.97269481	39.31683582	59.20543875	82.31575212
80.00	2.81868588	10.85637941	23.47507715	40.18554826	60.52045302	84.14970923
90.00	2.86979219	11.06087530	23.92785258	40.96831439	61.70523836	85.80194091
100.00	2.91644227	11.24740973	24.34068195	41.68189145	62.78520075	87.30791151

Table 4. Eigenvalues of the $x^2 + \lambda x^{12}$ oscillator.

$\lambda \backslash N$	0	1	2	3	4	5
0.01	1.12387348	3.76427647	7.33525661	11.98353987	17.67491522	24.34105579
0.02	1.16516425	3.97168762	7.86737165	12.97643604	19.24348517	26.58697993
0.03	1.19347679	4.10946405	8.21366340	13.61558751	20.24757611	28.02342879
0.04	1.21556182	4.21500379	8.47587489	14.09665564	21.00101745	29.09795127
0.05	1.23388502	4.30148236	8.68903653	14.48615989	21.60980761	29.96518091
0.06	1.24965491	4.37521696	8.86971282	14.81532085	22.12350699	30.69633121
0.07	1.26356295	4.43976527	9.02714075	15.10145715	22.56953432	31.33074163
0.08	1.27604533	4.49734433	9.16703264	15.35523617	22.96474304	31.89256669
0.09	1.28739655	4.54943607	9.29318328	15.58372163	23.32027798	32.39776052
0.10	1.29782560	4.59708359	9.40824996	15.79184673	23.64390792	32.85744185
0.20	1.37317062	4.93617723	10.21950397	17.25254941	25.91011400	36.07221231
0.30	1.42294463	5.15616980	10.73990880	18.18452566	27.35213284	38.11469308
0.40	1.46096018	5.32248897	11.13086529	18.88260264	28.43064797	39.64102294
0.50	1.49204918	5.45756355	11.44701490	19.44598195	29.30019233	40.87091924
0.60	1.51851898	5.57197396	11.71394135	19.92094308	30.03272870	41.90659593
0.70	1.54166541	5.67161079	11.94581258	20.33304990	30.66795748	42.80440205
0.80	1.56229427	5.76011264	12.15134422	20.69799787	31.23023001	43.59888193
0.90	1.58094331	5.83989448	12.33630178	21.02615348	31.73561729	44.31282361
1.00	1.59799050	5.91264618	12.50470841	21.32474112	32.19531193	44.96289193
2.00	1.71905884	6.42512257	13.68505327	23.41279878	35.40640780	49.49451535
3.00	1.79741446	6.75355698	14.43695139	24.73935019	37.44370182	52.36793741
4.00	1.85657577	7.00017969	14.99965504	25.73063867	38.96498218	54.51266257
5.00	1.90458142	7.19955450	15.45351784	26.52936844	40.19017326	56.23946529
6.00	1.94521709	7.36785295	15.83598502	27.20199216	41.22149066	57.69271291
7.00	1.98058799	7.51402637	16.16772853	27.78505059	42.11524756	58.95191283
8.00	2.01199333	7.64357941	16.46142822	28.30100094	42.90594907	60.06576884
9.00	2.04029481	7.76015247	16.72545801	28.76464421	43.61634821	61.06636968
10.00	2.06609502	7.86628529	16.96565073	29.18628460	44.26228015	61.97611766
20.00	2.24766462	8.60997055	18.64425846	32.12960732	48.76875613	68.32096478
30.00	2.36389879	9.08357908	19.70986336	33.99553090	51.62371032	72.33900833
40.00	2.45112644	9.43796890	20.50581813	35.38823621	53.75382017	75.33626674
50.00	2.52161435	9.72378664	21.14699120	36.50954595	55.46840391	77.74849220
60.00	2.58109751	9.96462963	21.68579056	37.45321347	56.91108617	79.77796440
70.00	2.63274870	10.17352095	22.15464782	38.27067080	58.16093940	81.53602526
80.00	2.67851823	10.35845100	22.56860043	38.99414581	59.26638876	83.09086369
90.00	2.71969545	10.52469444	22.94054442	39.64388952	60.25935285	84.48740524
100.00	2.75717980	10.67592552	23.27875005	40.23401061	61.16203793	85.75691171

diction for the excited states by taking into account the contributions of the third, fourth, ... order which are influenced by E. The calculation is perfectly possible but unfortunately the series for $c_k^{(1)}$ is found to be divergent though it is of course asymptoticaly convergent. As shown in section 4.2.1 it happens that the series limited to its two first terms gives the essential of the results attainable through that procedure.
If one wishes to refine the prediction of the (k,ω, δ) relation for the excited states it is necessary to return to the refined procedure of section 4.2.2 and to introduce the energy parameter E in the calculations. To attain that goal it is necessary to start with an asymptotic expansion for Ψ which is more accurate than the one we have considered (which was independent of E).

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