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

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The sole restriction on \( \varphi_k \) 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:
\[
\sum_0^\infty \sum c_k [\varphi_{2k} (\omega, x) + (E - x^2) \varphi_{2k} (\omega, x)] = 0
\]

If it is possible to express \( \varphi_{2k} \) and \( x^2 \varphi_{2k} \) by means of a finite number of consecutive \( \varphi_{2j} \) 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:
\[
A_k^{(n)} (\omega, E) c_k + 1 + A_k^{(n-1)} (\omega, E) c_k
+ \cdots + A_k^{(0)} (\omega, E) c_k = 0
\]
with \( c_k = 0 \) if \( k < 0 \) and \( k = s, s + 1, \ldots \) (\( s > 0 \), 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 \( c_k \).

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:

\[
D = \begin{vmatrix}
A_s^{(n-s-1)} (\omega, E) & A_s^{(n-s)} (\omega, E) & \cdots & A_s^{(n)} (\omega, E) \\
A_s^{(n-s-2)} (\omega, E) & A_s^{(n-s-1)} (\omega, E) & \cdots & A_s^{(n-1)} (\omega, E) & 0 \\
A_s^{(n-s)} (\omega, E) & A_s^{(n-s-1)} (\omega, E) & \cdots & A_s^{(n-1)} (\omega, E) & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
A_s^{(n-s)} (\omega, E) & \cdots & A_s^{(n-s+1)} (\omega, E) & \cdots & A_s^{(n-1)} (\omega, E) \\
0 & \cdots & \cdots & \cdots & \cdots \\
A_s^{(n)} (\omega, E) & \cdots & \cdots & \cdots & \cdots \\
\end{vmatrix}
\]

All the elements are zero except those on the main diagonal, on the \((s + 1)\) upper adjacent diagonals and on the \((n - s)\) 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 \( \omega \). 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:

\[ D(k) = \lim_{k \to \infty} D(k) \] 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:

\[ |E_N - E_N^{(k)}| = e^{-\delta} \quad \text{(absolute error)} \quad (5) \]

\[ |E_N - E_N^{(k)}| / |E_N| = e^{-p} \quad \text{(relative error = precision)} \quad (6) \]

We further have:

\[ \delta = p - \ln |E_N| \quad (7) \]

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 \( \omega \). That dependence will be called the \((k, \omega, p)\) relation or equivalently because of (7) the \((k, \omega, \delta)\) relation. The interest for this relation is easily understood: if the value of \( \omega \) 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 \( \varphi_k \) 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 \( D_k \) 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:
\[ u^{1/2} D_n (u) = a_{1/2} D_{n-1} + a_{-1/2} D_{n-1} + \ldots + a_{1/2} D_{n+1} \]
\[ (l = 1, 2, \ldots) \]

where the \( a_j \) are given by hypergeometric expressions
\[ (j = -1/2, -1/2 + 1, \ldots, 1/2) : \]
\[ a_j = \frac{(n+1)!}{(n+1-j)!} \frac{(1/j)! (1/2-j)!}{(2j)!} \]
\[ 1/2; j! + 1; 2) \]

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. \( s = m - 1 \):
\[ [E \omega^2 m - \omega^2 m + 2 (k + 5/4 - m)] c_m + \omega^2 m + 2/4 (k - m + 1) c_{m+1} + \omega^2 m + 2/2 (2k - 2m + 3) c_{m-2} \]
\[ - \frac{m}{
\sum_{j=m}^{m} (2k-2j-2m+2)! (2m)! (2j)! (2j)!(k-j)! (k-j+1)!} F(-2k-j+1) j! (1/2-j)!(1/2)! \]
\[ F(-2k-j+1) j! (1/2-j)!(1/2)! c_{k-j-1} \]

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 \( c_{k+1}, c_{k+1}, \ldots, c_{k+2m+1} \).
The coefficients are polynomials in \( k \) of degree \( m \).
When \( m > 3 \) equ. (8) is rather complicated so that this approach becomes intractable. We have performed various numerical tests in the case \( m = 2 \) in order to estimate the \( (k, \omega, \delta) \) relation. Figure 1 exhibits the \((k, \omega)\) behaviour for the first three 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 \( \omega \) increases and the limiting \( k_{opt} \sim 12 \). In practice it is therefore evident that a sufficiently large \( \omega \)-value must be chosen in order that \( k \) be next \( k_{opt} \). For example \( \omega \approx 2.5 \) should be convenient. A too large \( \omega \)-value is not only unnecessary but also prejudicial since in the recurrence (8) \( \omega \) 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.

Remark: it might be tempting to expand \( \Psi \) 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
\[ \phi_k (\omega, x) = \exp \left[ -x^2 \omega^2 / (2q + 1) \right] D_k (\omega, x) / \Gamma(k+2+1) \]

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):
\[ E \omega^2 q - \omega^2 q^2 - (k + 1/4 - q) c_{k-q} + \omega^2 q^2 + 2/(4-k-1) c_{k-q} - \]
\[ + \omega^2 q^2 / (2k-2q+1) c_{k-q} + \]
\[ \sum_{j=0}^{q-1} (2k-2j-q-1)! (2j+1)! (q-j)! (j)! (j)! F(-2k-j+1) j! (1/2-j)! (1/2)! c_{k-j} = 0 \]

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-
The results are collected in figure 2 which exhibits the main features of the \((k, \omega, \delta)\) 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:

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

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 \((k, \omega, \delta)\) 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 \(\omega\) in the neighbour of \(\omega_{opt}\) if one wishes to optimize the efficiency of the method. That feature of the \((k, \omega)\) curves is characteristic of that approach for the \(x^{2m}\) potential. We have reported in table 1 the experimental values of \(k_{opt}\) and \(\omega_{opt}\) 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 \(\omega_{opt}\); they also increase with \(\delta\). All the \((k, \omega)\)

curves fit in to each other. All the minima approximatively lie on a same curve independent of \( E \) and of \( \delta \). We shall reexamine this point later. We have used the values of \( \omega_{\text{opt}} \) contained in table 1 in order to calculate the first 30 states (even and odd) for the oscillators \( x^4 \) to \( x^{1.4} \). 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 \( k_{\text{opt}} \) and \( \omega_{\text{opt}} \) (p = 28)**

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

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

Remark: when \( m = 2 \) one has \( \omega_{\text{opt}} = 2.4 \) if \( \delta = 28 \) (fundamental state). It is interesting to point out the work of Biwas et alii [3] on the same oscillators: they systematically change \( \omega = 0.5 \) without suspecting the role played by the factor \( \omega \). The result was that they had to deal with approximants of large order \( k = 140 \) about six times \( k_{\text{opt}} \). The phenomenon was increased when \( m = 3, 4, ... \) since in these cases \( \omega_{\text{opt}} \) 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 \((k, \omega, \delta)\) Relation

Section 3 has shown several possible \((k, \omega)\) behaviours which are to be interpreted. The interest of the theory is evident since it would allow to predict the values of \( k_{\text{opt}} \) and \( \omega_{\text{opt}} \) 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

\[
N_j^{(k)} (j = 1, ..., s + 1) \text{ satisfying the recurrence (3) with the following initialization (} k < s): 
N_j^{(k)} = \delta_{k, j - 1} (-1 \text{ if } k = j - 1, \text{ otherwise } 0)
\]

One has the following identity:

\[
D^{(k)} = \begin{bmatrix}
A^{(n-s-1)}_0 & \cdots & A^{(n)}_0 \\
\vdots & \ddots & \vdots \\
A^{(n-s-1)}_0 & \cdots & A^{(n-s-1)}_0 \\
\end{bmatrix}
\]

\[
N_j^{(k)} = \begin{bmatrix}
N_j^{(s+1)}_0 & \cdots & N_j^{(s+1)}_k \\
\vdots & \ddots & \vdots \\
N_j^{(s+1)}_0 & \cdots & N_j^{(s+1)}_k \\
\end{bmatrix}
\]

Wherever large be \( k \), the \( k \times k \) determinant \( D^{(k)} \) is equal to a \((s+1) \times (s+1)\) determinant which order is fixed. Its \((s+1)^2\) elements can be calculated recursively through (3). Recurrence (3) (without the conditions \( c_k = 0 \iff k < 0 \)) 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.:

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

We call subdominant solution any linear combination of \( c_k^{(s+1)}, ..., c_k^{(n-1)} \), and dominant solution any non subdominant linear combination of \( c_k^{(0)}, ..., c_k^{(n-1)} \).

The subdominant solutions of the recurrence have been numerically studied by Gautachi [4] (in the case \( n = 2 \), \( s = 0 \) and Oliver [5]. We shall see that the coefficients \( c_k^{(l)} \) present in equ. (2) precisely correspond to a subdominant solution of (3). Let us note \( \rho_k \) the ratio of that form which tends the least fast to zero: \( \rho_k \) 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 \( \rho_k \) : to see it we first express the \( N_j^{(k)} \) in function of the \( c_k^{(l)} \):

\[
N_j^{(k)} = \sum_{i=0}^{n-1} a_{ij} c_k^{(l)} \quad j = 1, ..., s + 1
\]
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 \(\rho_k\). Introducing these simplified expressions in equ. (11) we get:

\[
\begin{pmatrix}
N_k^{(1)} & \cdots & N_k^{s+1} \\
\vdots & \ddots & \vdots \\
N_{k+s}^{(1)} & \cdots & N_{k+s}^{s+1}
\end{pmatrix}
\begin{pmatrix}
c_k^{(1)} \\
\vdots \\
c_{k+s}^{(1)}
\end{pmatrix}
\approx
\begin{pmatrix}
a_{1,1} & \cdots & a_{1,s+1} \\
\vdots & \ddots & \vdots \\
a_{s+1,1} & \cdots & a_{s+1,s+1}
\end{pmatrix}
\begin{pmatrix}
(1) \\
\vdots \\
(1)
\end{pmatrix}
\]

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

\[
\lim_{k \to \infty} D(k) = (-1)^{k(s+1)} A_s^{(n)} \cdots A_{s+k-1}^{(n)} 
\begin{pmatrix}
c_k^{(1)} & \cdots & c_k^{(s+1)} \\
\vdots & \ddots & \vdots \\
c_{k+s}^{(1)} & \cdots & c_{k+s}^{(s+1)}
\end{pmatrix}
\]

The roots \(E_N\) of \(D\) thus coincide with the roots of

\[
\begin{pmatrix}
a_{1,1} & \cdots & a_{1,s+1} \\
\vdots & \ddots & \vdots \\
a_{s+1,1} & \cdots & a_{s+1,s+1}
\end{pmatrix}
\]

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 \(c_k = \gamma_1 N_k^{(1)} + \cdots + \gamma_{s+1} N_k^{s+1}\) 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,

\[
\Psi(x) = \sum_{k=0}^{\infty} c_k D_{2k}(\omega x)(k!) \text{ is square integrable if...}
\]

and only if

\[
f = \int_0^{\infty} |\Psi(x)|^2 \, dx = \sum_{k=0}^{\infty} (\sqrt{2\pi/\omega})(2k)! |c_k|^2 / (k!)^2 < \infty.
\]

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

\[
|x|^{-m/2} \exp[-|x|^{m+1}/(m+1)]\text{ when }x\text{ is a large real (positive or negative) number, whereas any dominant solution of (10) gives birth to a function behaving like }|x|^{-m/2} \exp[|x|^{m+1}/(m+1)]\text{ in the same conditions.}
\]

If we note \(E_N^{(k)}\) the roots of the approximant \(D_N^{(k)}\) we have

\[
|E_N^{(k)} - E_N| = 0(\rho_k) \quad \text{if } E_N \text{ is of multiplicity one.}
\]

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:

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

\[
p = -\ln|\rho_k| + \ln |E_N|
\]

Equ. (12) is precisely the \((k, \omega, \delta)\) relation that we look for since \(\rho_k\) depends on \(\omega\) 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 \(k_{\text{opt}}\) and \(\omega_{\text{opt}}\). 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 \(c_k^{(1)}, \ldots, c_k^{(n-1)}\). One verifies that \((s+1)\) solutions dominate the \((n-s-1)\) others. One writes \(\rho_k\) as the ratio of the largest subdominant solution to the smallest dominant one. Equ. (12) furnishes the desired \((k, \omega, \delta)\) 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 \((k, \omega, \delta)\) relation in the case where \(\Psi\) 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:

\[(16k^2 - 4)c_k^{+1} + [32k^2 - (24 + 6\omega)k + (4 + 6\omega/2)]c_k + [24k^2 + (\omega^2 - 36)k + (15 - 3\omega^2/4 - Ec^2)]c_k^{-1} + [8k^2 - (18 + \omega/4)k + (10 + \omega/4)]c_k^{-2} + (k^2 - 3k + 2)c_k^{-3} = 0 \quad \text{(14)}
\]

\[c_k \sim a_k k^w \exp(\alpha_k^{3/4} + \beta_k^{2/4} + \gamma_k^{1/4} + \ldots)\]

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 \(k^{-1/2}\). 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 \(a, w, \alpha, \beta, \gamma, \ldots\). The result is \((l = 0, 1, 2, 3)\):

\[c_k^{(l)} = (-1/2)^l k^w \exp(-3\omega/2 \pi(2l+1)/4 (2k)^{3/4} - 2k^{9/2}/24 \pi(2l+1)/4 (2k)^{1/4} + \ldots) \quad \text{k}^{-3/8}\]

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 sub-dominant solutions only verify the condition

\[\sum_0^\infty |c_k(k)|^2 (2k)!(k)!^2 < \infty \text{ and thus alone correspond to a square integrable eigenfunction of the SE(1) provided there exists a non trivial linear combination of these that vanishes when } k < 0. \]

It is easy to calculate:

\[|\rho_k| = |c_k^{(1)}/c_k^{(0)}| \approx \exp \left[-\sqrt{2} \frac{2}{3} \omega^{3/2} (2k)^{3/4}\right] + \frac{\sqrt{2}}{24} \omega^{9/2} (2k)^{1/4}\]

from which we deduce the theoretical \((k, \omega, \delta)\) relation:

\[\delta \approx \sqrt{2} \frac{2}{3} \omega^{3/2} (2k)^{3/4} \quad \text{or} \quad \omega \approx \sqrt{2} \frac{9/2}{24} (2k)^{1/4}\]

When \(\delta = 28\) the corresponding \((k, \omega)\) curve is represented with dashed lines on figure 1. When \(\omega\) increases \(k\) decreases, passes through a minimum \(k^{opt} = \sqrt{6}/\delta/64\), \(\omega^{opt} = (48/\sqrt{6})^{1/6}\) 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 \(c_k^{(1)}\).

4.2. Theoretical study of the \((k, \omega, \delta)\) relation in the case where \(\Psi\) 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:

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

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

\[d_k^{(l)} = \left[\frac{2\pi l}{(m+1)}(2k)^{2l}/(m+1)\right]^{1/2} \exp\left[\omega 2\pi l/(m+1)/(2k)^{2l/2}\right] - \frac{2\omega^2}{m+1} e^{-4\pi l/(m+1)} (2k)^{(3-m)/(m+1)} + \ldots\]

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

\[|\rho_k| = |c_k^{(1)}/c_k^{(0)}| \approx \exp\left[\frac{\omega(\cos 2\pi m + 1)}{m+1} - \frac{2\omega^2}{m+1} \cos 4\pi - 1)/(2k)^{(3-m)/(m+1)}\right]\]

We deduce the \((k, \omega, \delta)\) relation:

\[\delta = 2\omega \sin 2\frac{\pi}{m+1} (2k)^{2l}/(m+1) - \frac{4\omega^2}{m+1} \sin 2\frac{\pi}{m+1} (2k)^{(3-m)/(m+1)}\]

The corresponding \((k, \omega)\) 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).
\[ \omega_{opt} = \delta \csc^2 \frac{\pi}{m+1} [(m+1) \tan^2 \frac{\pi}{m+1} / (165)]^{2(m+1)} \]

\[ k_{opt} = 8 \delta \cot^2 \frac{\pi}{m+1} / (m+1) \]

When \( \delta = 28 \) the numerical values of \( k_{opt} \) and \( \omega_{opt} \) 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 Eq. (1):

\[ \Psi = \sum_{k} c_k e^{-\omega x^2 / x^2} \Psi(x)^{-2k-1} \text{ dx} \]  

(18)

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

\[ c_k = \frac{2\pi}{\Phi_k} e^{\omega x^2 / x^2} \Psi(x)^{-2k-1} \text{ dx} \]

On another side the independent solutions

\[ c_k^{(1)} \]

of (3) (without the restrictions

\[ c_k = 0 \text{ if } k < 0 \]  

are given by such integrals calculated on distinct contours \( \gamma_0, \gamma_1, \ldots, \gamma_m \).

Let us suppose that \( \gamma_1 \) does not approach too much the origin; it is then possible to replace \( \Psi \) by its asymptotic behaviour for large \( x \):

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

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

\[ \frac{\delta}{\Phi(x)^{m+1}} \exp \left[-x^{m+1} / (m+1)\right] \text{ when } x \to \infty \]

One has: \( f(x) = \omega x^2 / x^2 + m + 1 / (m+1) - (2k + 1 + m/2) \ln x \)

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

\[ c_k^{(1)} = \exp \left[\omega x^2 / x^2 + m + 1 / (m+1) - (2k + 1 + m/2) \ln x \right] \]

(19)

where \( x_1 \) are the saddle points of \( f \) i.e. the roots of:

\[ 2\omega x_1^2 + x_1^m - (2k + 1 + m/2) / x_1 = 0 \]

(20)

It is assumed that only \( x_1 \) and \(-x_1 \) lie on \( \gamma_1 \) [recall that \( \Psi(x) \) is odd or even so that \( x_1 \) and \(-x_1 \) contribute for the same quantity in (19)].

Equ. (20) implies that:

\[ x_1^{2m+2} - (2k + 1 + m/2 - 2\omega x_1^2)^2 = 0 \]

where \( x_1 \) is the root located in the sector \( \pi 2^{1-1} / 2m + 2 < \arg x_1 < \pi 2^{1+1} / 2m + 2 \) (\( l = 0, 1, \ldots, m \)).

This assumption is justified by the fact that for \( \omega \) not too large one has \( \lim \arg x_1 = \pi / m + 1 \) and that \( x_1 \approx m + 1 - 2k > 0 \) because of (20).

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

\[ |x|^{-m/2} \exp \left(-x^{m+1} / (m+1)\right) \]

(18) behave like a subdominant solution of the recurrence (3) that means that \( x_0 \) and \(-x_0 \) are not saddle points of \( e^{\omega x^2 / x^2} \Psi(x)x^{-2k-1} \).

The conclusion is that

\[ |\Psi(x)| \approx \frac{x}{m+1} \exp \left(-x^{m+1} / (m+1)\right) \text{ when } x \to \infty \]

\( \Psi \) is a square integrable solution of the SE(1).

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

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

\[ \delta = \omega \frac{m+1}{m+1} R \left( x_0^2 - x_1^2 \right) + (2k + 1 + m/2) \ln |x_1/x_0| \]

(21)

Let us expand \( x_0 \) and \( x_1 \) in terms of powers of \( \omega \) by starting with Eq. (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

\[ \delta = R \left[ f(x_0^2) - f(x_1^2) \right] \]

with the conditions

\[ f'(x_0^2) = f'(x_1^2) = 0 \]

When \( \omega \) varies \( k \) passes through a minimum if

\[ \frac{dk}{d\omega} = 0 \text{ i.e. if} \]

\[ R \left[ \frac{\partial f(x_0^2)}{\partial \omega} - \frac{\partial f(x_1^2)}{\partial \omega} \right] = 0 \]

which leads to \( R 2^{-1} = R x_1^2 \).

The root \( x_0 \) is real > 0 but \( x_1 \) is complex. We put:

\[ x_1^2 = x_0^2 (1 + i \gamma) \]

If we introduce these expressions in Eq. (20) with

\[ \pm x_0^m = x_0^m \text{ and } \pm x_1^m = x_1^m \]

one obtains:

\[ x_0^m = R \frac{x_1^m}{x_1^m} \]

Hence the equation for \( \gamma \):

\[ \frac{m^2}{m+1} \gamma = x_0^m - x_1^m \]

(22)
Combining with (20) and (21) one finds:
\[ k_{\text{opt}} = -\delta / \ln \cos \sigma - m/4 - 1/2 \]  
(23)
\[ x_0^{m+1} = (2k_{\text{opt}} + m/2 + 1)(1 - \cot \sigma \tan \frac{m+1}{2} \sigma)^{-1} \]
\[ \omega_{\text{opt}} (2k_{\text{opt}} + m/2 + 1)(1-m)/(m+1) \]
\[ \sigma = - \frac{1}{2} \cot \sigma \tan \frac{m+1}{2} \sigma (1 - \cot \sigma \tan \frac{m+1}{2} \sigma)^{(1-m)/(m+1)} \]  
(24)
\sigma easily deduces through (22) and \( k_{\text{opt}} \) and \( \omega_{\text{opt}} \) follows with (23) and (24). We have calculated the values of \( k_{\text{opt}} \) and \( \omega_{\text{opt}} \) 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 \((k, \sigma)\) 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 \( \omega_{\text{opt}} \) in that case one finds that \( \omega_{\text{opt}} \) varies very slowly with \( \lambda \) so that it is possible to perform the numerical calculations by adopting the values of \( \omega_{\text{opt}} \) 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 \( \lambda \) 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 \( \omega \) which enters in the expansion tried for \( \Psi \):
\[ \Psi = \sum_0 c_k \varphi_k (\omega, x) \]
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 \( \Psi \) in the form
\[ \Psi = e^{-\omega x^2} \sum_0 c_k x^k \]
it is important to assign to \( \omega \) a numerical value next \( \omega_{\text{opt}} \) otherwise \( k \) will be needlessly large. The theory of section 4 has learned us how to predict the \((k, \omega, \delta)\) 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 eq. (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 \([-2\pi \int e^{-x^2}|x|]^{-1/2} \) beside the exponential.

c) In the same integral \( \Psi \) 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 \( k_{\text{opt}} \) and \( \omega_{\text{opt}} \) are only present in the combination
\[ \omega_{\text{opt}} (2k_{\text{opt}} + m/2 + 1)(1-m)/(m+1) \]  
(24)
\( \omega \) and \( \delta \) are. The fact is visible in eq. (24).

In the special case \( m = 2 \) eq. (24) is written as:
\[ \omega_{\text{opt}} = 0.780507 \]

The corresponding \((k, \omega)\) 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 \((k, \omega)\) curves when \( E \) and \( \delta \) vary. However the coincidence may not be perfect because eq. (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 \( \omega_{\text{opt}} \) and \( k_{\text{opt}} \) become present under various forms incompatible with (24). One could hope to improve the pre-
Table 2. 30 first eigenvalues of $x^{2n}$ oscillators.

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

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Table 4. Eigenvalues of the $x^2 + \lambda x^{12}$ oscillator.
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 asymptotically 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 $(k, \omega, \delta)$ 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 $\Psi$ which is more accurate than the one we have considered (which was independent of $E$).

REFERENCES


