On the Hill-determinant method

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The difficulties encountered by various authors in connection with the application of the Hill-determinant method are investigated. The conditions of applicability of the method are deduced.

I. INTRODUCTION

Nonperturbative methods have been extensively applied to the determination of the spectrum of anharmonic oscillators.[1–3] Among them, the Hill-determinant method (HDM) has been used with success by various authors.[1,4–6] However, doubts have recently been raised as to whether the HDM can work in every case. Flessas and Anagnostatos[7] have claimed that the HDM was unable to furnish the correct spectrum of the oscillator $x^2+\lambda x^4$. We have shown that their conclusions were based on an inaccurate analysis of the problem and that the HDM effectively works in that case.[6] A more serious objection has been presented by Singh, Biswas, and Datta[8] which has been reformulated by Znojil[9] and by Chaudhuri.[10] It is the aim of this paper to try to elucidate the conditions under which the HDM works properly. For the sake of clarity we shall first concentrate on the example given by Chaudhuri, i.e., the oscillator $ax^2+bx^4+cx^6$; then we shall generalize the results.

II. THE $ax^2+bx^4+cx^6$ OSCILLATOR ($c>0$) (HILL-TAYLOR APPROACH)

A. HDM in trouble

We consider the eigenvalue equation

$$\psi''+(E-ax^2-bx^4-cx^6)\psi=0 . \quad (1)$$

It is evident that according to the values of the parameters a, b, and $c>0$, there is a finite number of negative eigenvalues (eventually zero) and an infinite number of discrete positive eigenvalues. No eigenvalue can be smaller than the least value of $ax^2+bx^4+cx^6$. Equation (1) is of order two. It possesses two independent solutions which behave quite differently at infinity along the real axis:

$$\psi_{\text{conv}}\sim \exp(-\tfrac{1}{4}c^{1/2}x^4-\tfrac{1}{4}bc^{-1/2}x^2)$$

and

$$\psi_{\text{div}}\sim \exp(\tfrac{1}{4}c^{1/2}x^4+\tfrac{1}{4}bc^{-1/2}x^2) .$$

It is inviting to make the following substitution in Eq. (1):

$$\psi=\exp(-\tfrac{1}{4}c^{1/2}x^4-\tfrac{1}{4}bc^{-1/2}x^2)\phi . \quad (2)$$

The transformed equation is written as

$$\phi''+2x(\beta-\alpha x^2)\phi'+[E+\beta+(\beta^2-a-3\alpha)x^2]\phi=0 , \quad (3)$$

where $\alpha=c^{1/2}>0$ and $\beta=-\tfrac{1}{2}bc^{-1/2}$.

Equation (3) has no singularity in the finite x plane. Therefore the function ϕ can be written as

$$\phi=\sum_{0}^{\infty} C_k x^{2k+\nu} , \quad (4)$$

where $\nu=0$ (even states) or $\nu=1$ (odd states). Here we shall concentrate on the even states only. The odd states are treated similarly. The expansion (4) is typical of a Hill-Taylor approach. The coefficients C_k obey the second-order recurrence relation

$$(2k+1)(2k+2)C_{k+1}+[E+\beta(4k+1)]C_k+[\beta^2-a-(4k-1)\alpha]C_{k-1}=0 \quad (5)$$

with $k=0,1,2,\ldots$, and $C_{-1}=0$.

The infinite Hill determinant D of the problem is written as

$$D=\begin{vmatrix} E+\beta & 1\times 2 & & & \\ \beta^2-a-3\alpha & E+5\beta & 3\times 4 & & \\ & \beta^2-a-7\alpha & E+9\beta & 5\times 6 & \\ & & \cdots & E+13\beta & \\ & & & \cdots & \ddots \end{vmatrix} .$$

The principle of the HDM is to identify the roots of D with the eigenvalues of the problem. That procedure has never been justified properly and we shall see that this can induce misleading results.

All the authors dealing with the HDM comment on Eq. (5) by saying: "The necessary and sufficient condition that nontrivial C_k exist is that the infinite determinant D vanishes." This seems a dangerous extrapolation of a theorem of linear algebra about systems of a finite number of equations. Clearly when the system is infinite, there is no need for a consistency condition since the forward calculation of the successive C_k is always possible through Eq. (5). The origin of the condition $D=0$ which effectively leads to the correct spectrum in many cases must be found elsewhere. Moreover the condition $D=0$ does not seem to include the condition of square integrability of the wave function so that the current theory of the HDM seems incomplete in many respects. Chaudhuri[10] has detailed a counterexample where precisely the HDM fails to work: he has found that when the coupling constants obey the relations

$$b<0$$

and

$$\beta^2-a-(4N-1)\alpha=0 \quad (6)$$

(where N is some given positive integer) the equation $D=0$ is unable to furnish the full spectrum of the oscillator. In fact, if Eq. (6) holds, D splits in two parts: a finite $N\times N$ determinant whose roots effectively coincide with the correct lowest (even) eigenvalues and a remaining infinite determinant whose roots are not real positive numbers when $b<0$. On the other hand, the method works if $b>0$.

Practically, the numerical calculation of the roots of D is performed by truncating D to its kth-order approximant $D^{(k)}$ and calculating the limits of the roots of $D^{(k)}$ when k tends to infinity. In the example treated, the process appears to diverge when $b=0$. That the finite $N\times N$ determinant gives the exact lowest eigenvalues is quite normal: the corresponding wave functions are square integrable since ϕ is polynomial in this case.

We have found that similar troubles occur with the HDM, even when no special relation like (6) holds, provided one has $b<0$. An example is furnished by the oscillator $x^6-2x^4+2x^2$ whose eigenvalues are positive: the HDM with the model of Eq. (2) is unable to find them.

B. Explanation of those troubles

We now proceed to establish the following.

(i) If $b>0$ the sequence $\{C_k\}$, as obtained by the HDM, leads to a function

$$\phi=\sum_0^\infty C_k x^{2k}$$

which remains bounded along the whole real axis, so that ψ behaves correctly at infinity, like ψ_{conv}.

(ii) If $b<0$ the obtained sequence $\{C_k\}$ leads to a function ϕ which behaves like

$$\exp(\tfrac{1}{2}c^{1/2}x^4+\tfrac{1}{2}bc^{-1/2}x^2)\,,$$

for $|x|$ large, so that ψ behaves like ψ_{div}. This would effectively explain why the HDM works in the first case and not in the second case.

1. The meaning of the vanishing condition $D=0$

We first prove that equating the Hill determinant D to zero amounts to searching for a nondominant solution of the associated recurrence relation which is consistent with the initialization $C_{-k}=0$ $(k=1,2,\ldots)$. The proof requires that we first remind ourselves of the general theory of linear recurrences. Let us consider a linear homogeneous recurrence of order n written as

$$A_k^{(n)}C_{k+1}+A_k^{(n-1)}C_k+\cdots+A_k^{(0)}C_{k-n+1}=0\,. \quad (7)$$

Let us consider a fundamental system or n independent solutions $C_k^{(i)}$ whose asymptotic behaviors are contrasted with the maximum. For k sufficiently large one has

$$|C_k^{(1)}|\geq|C_k^{(2)}|\geq\cdots\geq|C_k^{(n)}|\,.$$

It is well known[11] that the forward recursion is convenient for the stable numerical calculation of the dominant solution $C_k^{(1)}$ while the backward recursion stably calculates the dominated $C_k^{(n)}$. That procedure is known as Miller's algorithm.[12] The stable calculation of the intermediate solutions $C_k^{(2)}\cdots C_k^{(n-1)}$ is only possible through a generalized algorithm which has been studied by Oliver.[13] To calculate the sequence $\{C_k^{(i)}\}$ $(i\in 1,2,\ldots,n)$ one has to solve the following linear system:

$$\underbrace{\begin{vmatrix} A^{(n-i+1)}_{i-2} & \cdots & A^{(n)}_{i-2} & & & & & 0\\ \vdots & \ddots & & \ddots & & & & \\ A^{(1)}_{n-2} & \cdots & & A^{(n-i+1)}_{n-2} & \cdots & A^{(n)}_{n-2} & & \\ A^{(0)}_{n-1} & \cdots & & & A^{(n-i+1)}_{n-1} & \cdots & A^{(n)}_{n-1} & \\ & \ddots & & & & \ddots & & \ddots \\ & & & & & & & A^{(n)}_{K-1}\\ & & & & & & & \vdots \\ & 0 & & & A^{(0)}_{K+i-2} & \cdots & & A^{(n-i+1)}_{K+i-2}\end{vmatrix}}_{\text{rows: } n-i+1,\ i;\ \text{columns: } i,\ n-i+2}
\begin{vmatrix}C_0\\C_1\\ \vdots\\ \\ \vdots \\ C_K\end{vmatrix} = -\begin{vmatrix} A^{(n-i)}_{i-2}C_{-1}+\cdots+A^{(0)}_{i-2}C_{i-n-1}\\ A^{(n-i-1)}_{i-1}C_{-1}+\cdots+A^{(0)}_{i-1}C_{i-n}\\ \vdots \\ A^{(0)}_{n-2}C_{-1}\\0\\ \vdots\\0\end{vmatrix}\,.$$

The value of K must be chosen large enough to ensure the required number of significant figures in $C_1^{(i)} \cdots C_k^{(i)}$:

$$n_s \sim \log_{10} | C_K^{(i-1)} C_k^{(i)} / C_K^{(i)} C_k^{(i-1)} | \ . \qquad (8)$$

A good estimate of K is generally obtained if $C_k^{(i)}$ is replaced by its asymptotic behavior in (8).

Applying that algorithm to our problem in the case $i=2$ (since we are only interested in a nondominant solution), we obtain the linear system

$$\begin{vmatrix} E+\beta & 2 & & & & \\ \beta^2-a-3\alpha & E+5\beta & 12 & & & \\ & \beta^2-a-7\alpha & E+9\beta & 30 & & \\ & & \cdots & E+13\beta & & \\ & & & \cdots & \ddots & \\ & & & & \beta^2-a-(4K-1)\alpha & E+\beta(4K+1) \end{vmatrix} \begin{vmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \\ \\ C_K \end{vmatrix} = - \begin{vmatrix} (\beta^2-a+\alpha)C_{-1} \\ 0 \\ 0 \\ \vdots \\ \\ 0 \end{vmatrix} .$$

If we impose the initial conditions $C_{-k}=0$ ($k=1,2,\ldots$) we obtain a finite linear homogeneous system. Its nontrivial solution exists if and only if we require the vanishing of its determinant which is nothing other than the Hill determinant of the problem.

This achieves the proof.

2. *Asymptotic behavior of the wave function*

Recurrences like (5) have been studied by Birkhoff[14] and Birkhoff and Trjitzinsky[15] who showed that their solutions are asymptotic to expressions of the type

$$k^w a^k \exp(\alpha k^m + \beta k^n + \cdots)(\ln k)^r \ .$$

We have published extended tables of the coefficients $a, w, \alpha, \beta, m, n, r, \ldots$ which are useful in practical examples.[16] In the case of recurrence (5) (which is of order two) we find two asymptotes:

$$\begin{bmatrix} \alpha_k \\ \beta_k \end{bmatrix} \sim (\pm c^{1/4})^k \Gamma(k)^{-1/2} k^w \exp(\pm \tfrac{1}{2} b c^{-3/4} k^{1/2}) \ ,$$

where $w = -(\beta^2 - a + 9\alpha)/(8\alpha)$.

If $b>0$ it is apparent that α_k is dominant and that β_k is dominated; i.e., one has

$$C_k^{(1)} \sim \alpha_k \ \text{ and } \ C_k^{(2)} \sim \beta_k \ .$$

If $b=0$ we find that the asymptotes are not contrasted. If $b<0$ we observe that α_k is dominated and that β_k is dominant: i.e.,

$$C_k^{(1)} \sim \beta_k \ \text{ and } \ C_k^{(2)} \sim \alpha_k \ .$$

By another way we estimate in the Appendix the following asymptotic behaviors ($\rho > 0$):

$$\sum_0^\infty k^w \Gamma(k)^{-1/2} \exp(\lambda k^{1/2})(\rho x)^k \sim \exp(\tfrac{1}{2}\rho^2 x^2 + \lambda \rho x)$$

and

$$\left| \sum_0^\infty k^w \Gamma(k)^{-1/2} \exp(\lambda k^{1/2})(-1)^k (\rho x)^k \right| \leq M (= \text{const})$$

for x large and positive.

We conclude that

$$\phi_\alpha \sim \sum_0^\infty \alpha_k x^{2k} \sim \exp(\tfrac{1}{2} c^{1/2} x^4 + \tfrac{1}{2} b c^{-1/2} x^2) \ ,$$

hence $\psi_\alpha \sim \psi_{\text{div}}$ and that

$$|\phi_\beta| \sim \left| \sum_0^\infty \beta_k x^{2k} \right| \leq M$$

so that $\psi_\beta \sim \psi_{\text{conv}}$.

Clearly the "good" wave function is ψ_β and it is built with the aid of that sequence of C_k which behaves like β_k. Here is the clue to the problem: the asymptote β_k is dominated solely if $b>0$. Therefore in that case only the HDM is able to construct the well-behaved wave function. When $b<0$ the HDM calculates nondominant C_k which behaves like α_k and the derived wave function is not square integrable. When $b=0$ there is no contrast between dominant and nondominant asymptotes of the recurrence and in such a case the HDM is known to fail.[16]

So the origin of the troubles presented in Sec. II A is now apparent.

C. Troubles removed

It must not be thought that the HDM is unable to calculate the entire spectrum of an oscillator of the type $ax^2+bx^4+cx^6$ even in the case $b<0$. Simply, the substitution (2) is unsuitable for that purpose because it precisely corresponds to the exact asymptotic behavior of ψ. The following substitution allows the HDM to work properly in that case:

$$\psi = \exp(-\omega x^2 - \sigma x^4) \sum_0^\infty C_k x^{2k} \ \text{(even states, } \sigma > 0) \ . \qquad (9)$$

The C_k now obey the following fourth-order recurrence:

$$(2k+1)(2k+2)C_{k+1} + (E - 2\omega - 8\omega k)C_k + (4\omega^2 - a + 4\sigma - 16\sigma k)C_{k-1} + (16\omega\sigma - b)C_{k-2} + (16\sigma^2 - c)C_{k-3} = 0 \qquad (10)$$

with $k=0,1,2,\ldots$, and $C_{-1}=C_{-2}=\cdots=0$.

The Hill determinant Δ is now written as

$$\Delta=\begin{vmatrix} E-2\omega & 1\times 2 & & & & \\ 4\omega^2-a+4\sigma & E-10\omega & 3\times 4 & & & \\ 16\omega\sigma-b & 4\omega^2-a-12\sigma & E-18\omega & 5\times 6 & & \\ 16\sigma^2-c & 16\omega\sigma-b & 4\omega^2-a-28\sigma & E-26\omega & 7\times 8 & \\ & \cdots & \cdots & \cdots & E-34\beta & \\ & & & & \cdots & \ddots \end{vmatrix} .$$

The role played by the dummy parameters ω and σ is the following: though the energy levels E (eigenvalues) are independent of ω and σ it may happen that the roots of the successive kth-order approximants converge faster to E for well-selected values of ω and σ. This phenomenon is known in the literature[4] and we have indicated theoretical estimates for the optimal values of these parameters in various cases.[5]

The four asymptotes of recurrence (10) are easily calculated:[16]

$$\begin{aligned} \alpha_k &\sim (2\sigma+c^{1/2}/2)^{k/2}\Gamma(k)^{-1/2}\exp[\tfrac{1}{4}(b+4\omega c^{1/2})c^{-1/2}(2\sigma+c^{1/2}/2)^{-1/2}k^{1/2}] , \\ \beta_k &\sim (-1)^k(2\sigma+c^{1/2}/2)^{k/2}\Gamma(k)^{-1/2}\exp[-\tfrac{1}{4}(b+4\omega c^{1/2})c^{-1/2}(2\sigma+c^{1/2}/2)^{-1/2}k^{1/2}] , \\ \gamma_k &\sim (2\sigma-c^{1/2}/2)^{k/2}\Gamma(k)^{-1/2}\exp[-\tfrac{1}{4}(b-4\omega c^{1/2})c^{-1/2}(2\sigma-c^{1/2}/2)^{-1/2}k^{1/2}] , \\ \delta_k &\sim (-1)^k(2\sigma-c^{1/2}/2)^{k/2}\Gamma(k)^{-1/2}\exp[\tfrac{1}{4}(b-4\omega c^{1/2})c^{-1/2}(2\sigma-c^{1/2}/2)^{-1/2}k^{1/2}] . \end{aligned} \tag{11}$$

Less important factors of the type k^w have been omitted in each asymptote. It may be shown that in the usual domain of variation of ω and σ the dominant (the dominated) asymptote is α_k (δ_k). The intermediate solutions are asymptotic to β_k and to γ_k. In theory β_k dominates γ_k for k very large. However, for moderate values of k which are of interest for us the situation is a little more complicated. σ being fixed, there exists a critical value of ω, say $\omega_{\rm opt}$, for which one can say the following: if $\omega<\omega_{\rm opt}$ the asymptote β_k is subdominant, i.e., the order of decreasing dominance of the four asymptotes is $|\alpha_k|>|\beta_k|>|\gamma_k|>|\delta_k|$; if $\omega>\omega_{\rm opt}$ the asymptote γ_k is subdominant, i.e., the order is $|\alpha_k|>|\gamma_k|>|\beta_k|>\delta_k$. Clearly the critical value of $\omega_{\rm opt}$ is obtained when $|\beta_k|=|\gamma_k|$. We know from a previous study[5] about the HDM that the relative accuracy on the lowest eigenvalue is of the order of magnitude of $\exp(-p)\sim$ | subdominant solution | / | dominant solution |: i.e.,

$$\exp(-p)\sim|\beta_k|/|\alpha_k| \quad \text{if } \omega<\omega_{\rm opt} ,$$

$$\exp(-p)\sim|\gamma_k|/|\alpha_k| \quad \text{if } \omega>\omega_{\rm opt} ,$$

where p is the number of Napierian figures which are exact in the answer furnished by the HDM.

For example, if $\omega<\omega_{\rm opt}$ we find

$$p\sim\tfrac{1}{2}c^{-1/2}(b+4\omega c^{1/2})k^{1/2}/(2\sigma+c^{1/2}/2)^{1/2} .$$

If we fix the order k of the approximant this means that the accuracy increases linearly with ω until ω attains its optimal value $\omega_{\rm opt}$. $\omega_{\rm opt}$ is the root of the equation

$$|\beta_k|=|\gamma_k| . \tag{12}$$

When $\omega>\omega_{\rm opt}$ the precision decreases. A similar argument holds for every value of σ so that it appears that there are optimal values of σ and ω which allows us to attain the highest accuracy for a fixed value of k. The situation is illustrated by Fig. 1 in the case $k=20$ (oscillator $x^6-2x^4+2x^2$, fundamental state calculated through the HDM for various values of ω and σ); the optimal values are $\sigma_{\rm opt}\sim 0.2$, $\omega_{\rm opt}\sim 2$, and $p_{\rm opt}\sim 14.5$ (6 exact decimal figures). The accurate value is 1.241 391 715 188 58. . . .

In practical calculations it is not necessary to solve the transcendental equation (12) to get sufficient approximations of both $\sigma_{\rm opt}$ and $\omega_{\rm opt}$. It is largely sufficient to apply the generalized Miller algorithm of Sec. II B 1 for various values of σ and ω and to select values which maximize the quotient

$$\exp(p)\sim\frac{|\text{dominant solution}|}{|\text{subdominant solution}|} .$$

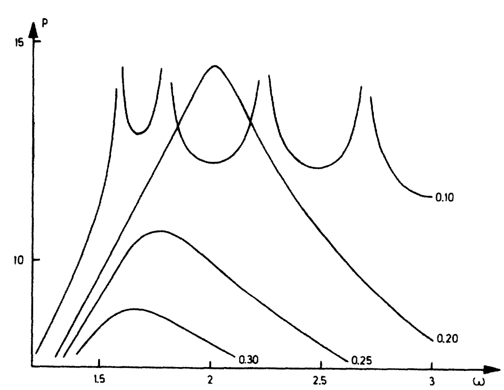

FIG. 1. Oscillator $x^6-2x^4+2x^2$, fundamental state. The lowest root of the 20th-order approximant has been calculated for various values of ω and σ. The precision p is plotted versus ω exhibiting an optimal domain (ω,σ). (Hill-Taylor approach.)

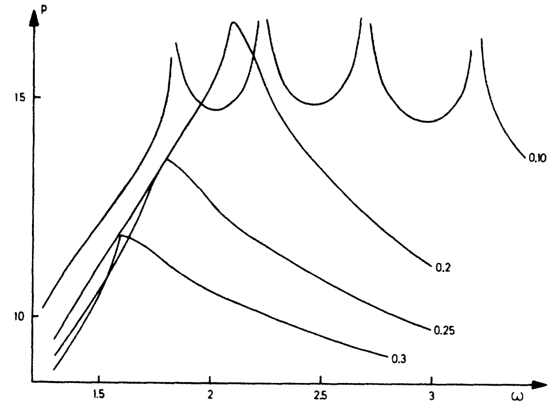

FIG. 2. Oscillator $x^6-2x^4+2x^2$, fundamental state. Theoretical prediction of the influence of ω and σ variations on the expected precision. To be compared with the experimental curve of Fig. 1.

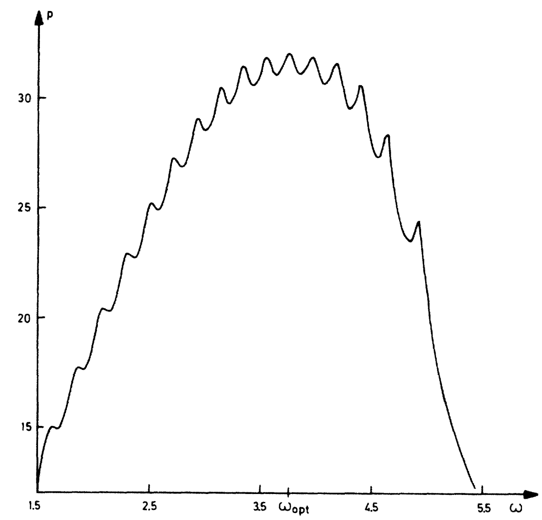

FIG. 3. Oscillator $x^6-2x^4+2x^2$, fundamental state. The lowest root of the 20th-order approximant has been calculated for various values of ω. (Hill-Weber-Hermite approach.)

In order to fix the ideas Fig. 2 shows how $p \sim \ln|C_k^{(1)}/C_k^{(2)}|$ varies as both ω and σ vary. $C_k^{(1)}$ and $C_k^{(2)}$ are deduced from the generalized Miller algorithm with the conventional choice $E=1$. That this value is not the exact one is not important since Eq. (11) shows that the asymptotes of the recurrence (10) are not sensitive to variations of E. If we compare both Figs. 1 and 2 we find that apart from a slight shift along the p axis the theoretical curves of Fig. 2 correctly predict the experimental curves of Fig. 1. In particular the theoretical optimal values of ω are rather accurate. The unpredictable shift is explained by the fact that the asymptotes are only known to a multiplicative constant factor. Finally we might verify that the resulting wave function exhibits the expected asymptote behavior ψ_{conv} by following a procedure strictly analogous to that already mentioned in Sec. II B.

III. THE $ax^2+bx^4+cx^6$ OSCILLATOR ($c>0$) (HILL-WEBER-HERMITE APPROACH)

Another approach to the same problem starts with an expansion of the wave function in terms of the scaled eigenfunctions of the harmonic oscillator, i.e., Weber-Hermite functions $D(x)$:

$$\psi=\sum_0^\infty C_k D_{2k}(\omega x)/k! \text{ (even states)} . \tag{13}$$

The odd states are treated similarly by replacing k by $k+\frac{1}{2}$ in the calculations below.

The C_k obey the sixth-order recurrence relation:

$$\begin{aligned}
&8c(2k-3)(4k^2-1)C_{k+1}+4(2k-1)(2k-3)[b\omega^2+(12k-9)c]C_k \\
&\quad+(k-\tfrac{3}{2})[240ck^2+(32b\omega^2-600c)k+420c+4a\omega^4-40b\omega^2-\omega^8]C_{k-1} \\
&\quad+\tfrac{1}{4}[640ck^3+(96b\omega^2-3360c)k^2+(16a\omega^4-336b\omega^2+6080c+4\omega^8)k+300b\omega^2-28a\omega^4-3780c-7\omega^8-4E\omega^6]C_{k-2} \\
&\quad+\tfrac{1}{4}(k-2)[240ck^2+(32b\omega^2-1080c)k+1260c+4a\omega^4-72b\omega^2-\omega^8]C_{k-3} \\
&\qquad\qquad+(k-2)(k-3)[(12k-33)c+b\omega^2]C_{k-4}+c(k-2)(k-3)(k-4)C_{k-5}=0
\end{aligned}$$

with $k=2,3,4,\ldots$ and $C_{-k}=0$ ($k=1,2,3,\ldots$).

The dummy parameter ω plays the role of a variational parameter: indeed it can be shown that the HDM in this Weber-Hermite approach is strictly equivalent to the classical Ritz variational method with ω and the C_k adjustable in the trial function (13).

The advantages of the method are the following.

(a) It is sound and efficient whatever the coefficients a, b, and $c>0$ are.

(b) It is performant as shown on Fig. 3: the 20th-order approximant leads to a precision twice as great as the corresponding approximant in the Hill-Taylor approach. The optimal value ω_{opt} may be predicted by a method similar to that described in Sec. II C.

(c) There is no need to prove that the resulting wave function is square integrable in this approach since we are sure that the minimal solution of the recurrence consistent with the initialization $C_{-k}=0$ $(k=1,2,\dots)$ generates the minimal solution of the starting Schrödinger equation. This results in a straightforward way from Parseval's theorem.

For all these reasons this approach must be preferred. Its one simple drawback is that the recurrence is more difficultly determined.

IV. GENERALIZATION

In the general case the HD is associated with the recurrence

$$A_k^{(n)}C_{k+1}+A_k^{(n-1)}C_k+\cdots+A_k^{(0)}C_{k-n+1}=0 ,$$

where $k=s,s+1,\dots$ and $C_{-k}=0$ $(k=1,2,\dots)$.

We recall that the system of contrasted asymptotes is $C_k^{(i)}$ with

$$|C_k^{(1)}|>|C_k^{(2)}|>\cdots>|C_k^{(n)}| \quad (k \text{ large}) .$$

It is written as

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

D possesses $(s+1)$ upper diagonals. In the example of Secs. II and III we had $s=0$ and $s=2$, respectively. Positive s values are encountered when sets of orthogonal functions f_k are used in the starting substitution of the type[5]

$$\psi=\sum_0^\infty C_k f_k(x) .$$

The value $s=0$ is typical of the so-called Hill-Taylor scheme for which the starting substitution is of the types (4) or (9). Generalizing the proof of Sec. II B 1 it is easy to establish that equating D to zero is equivalent to constructing an intermediate solution of the recurrence $C_k^{(s+2)}$ which obeys the initialization $C_{-k}^{(s+2)}=0$ $(k=1,2,\dots)$. In order to be sure that the HDM will work (Taylor approach) it is then necessary to verify that the corresponding function $\sum_0^\infty C_k^{(s+2)}x^k$ behaves properly at infinity like ψ_{conv}.

V. CONCLUSION

We have tried to clarify the origin of the troubles which are observed when one applies the HDM without precautions to anharmonic oscillators. The following seems to be established.

(i) The Hill condition $D=0$ is not a consistency condition for the associated infinite linear homogeneous system.

(ii) That condition simply selects a nondominant solution $C_k^{(s+2)}$ of the associated recurrence which is consistent with the initialization $C_{-k}=0$ $(k=1,2\dots)$.

(iii) The condition of square integrability is not included in the Hill-Taylor method so that the user must verify that the resulting wave function correctly behaves at infinity. In the Weber-Hermite approach the same condition is included in the method.

We have indicated in the Appendix a possible way to establish the asymptotic behaviors of the wave functions which are built through the HDM.

APPENDIX: ASYMPTOTIC BEHAVIORS OF THE WAVE FUNCTIONS

(1) We first estimate the asymptotic behavior of the following expansion $(\rho>0)$:

$$S_1=\sum_0^\infty k^w\Gamma(k)^{-1/2}\exp(\lambda k^{1/2})(\rho x)^k$$

for x large and positive. Using standard techniques we proceed to the following deductions:

$$S_1\sim\int\Gamma(z)^{-1/2}\exp(\lambda z^{1/2})(\rho x)^z dz$$

$$\sim\int\exp[-\tfrac{1}{2}\ln\Gamma(z)+\lambda z^{1/2}+z\ln(\rho x)]dz .$$

That integral is estimated through a classical saddle-point method.[17] We have, using Stirling's formula,

$$S_1\sim\int\exp[f(z)]dz\sim\exp[f(z^*)] ,$$

where $f'(z^*)=0$. We find

$$f=-\tfrac{1}{2}z\ln z+(w+\tfrac{1}{4})\ln z+\lambda z^{1/2}+z[\tfrac{1}{2}+\ln(\rho x)] ,$$

$$f'=-\tfrac{1}{2}\ln z+(w+\tfrac{1}{4})z^{-1}+\tfrac{1}{2}\lambda z^{-1/2}+\ln(ax) .$$

The saddle point z^* is easily found asymptotic to

$$z^*\sim a^2x^2 .$$

Hence

$$S_1 \sim \exp(\tfrac{1}{2}\rho^2 x^2 + \lambda\rho x) \ .$$

(2) The same technique does not apply if $\rho < 0$ because of the extreme ill conditioning of series of the type

$$\sum_0^\infty (-1)^k \Gamma(k)^{-1/2} x^k \ ;$$

when x is large and positive there exists a region of k values where the contributions of the successive terms are very large with alternated signs; the result is a dramatic cancellation which maintains the values of the series in a bounded region.

We must prove that

$$S_2 = \sum_0^\infty (-1)^k (c^{1/4})^k \Gamma(k)^{-1/2} \times \exp(-\tfrac{1}{2} bc^{-3/4} k^{1/2}) x^{2k}$$

remains bounded when $|x| \to +\infty$ along the real axis. We proceed *ad absurdum* by proving that if $S_2 = \sum C_k x^{2k}$ is not bounded then C_k cannot be asymptotically written as

$$(-1)^k c^{k/4} \Gamma(k)^{-1/2} \exp(-\tfrac{1}{2} bc^{-3/4} k^{1/2}) \ .$$

Indeed if S_2 is not bounded, it is asymptotic to

$$S_2 = \sum C_k x^{2k} \sim \exp(\tfrac{1}{2} c^{1/2} x^4 + \tfrac{1}{2} bc^{-1/2} x^2) \ .$$

But by Cauchy's theorem we have

$$C_k = \frac{1}{2i\pi} \oint x^{-(2k+1)} S_2(x) dx \ .$$

That integral may be evaluated by a classical saddle-point method:

$$C_k = \oint \exp[f(x)] dx \sim \exp[f(x^*)] \ ,$$

where the saddle point x^* is defined by $f'(x^*) = 0$.

We have, successively,

$$f(x) = \tfrac{1}{2} c^{1/2} x^4 + \tfrac{1}{2} bc^{-1/2} x^2 - (2k+1)\ln x$$

and

$$x^* \sim (kc^{-1/2})^{1/4} \ ,$$

hence

$$C_k \sim (+c^{1/4})^k \Gamma(k)^{-1/2} \ ,$$

which contradicts the starting hypothesis $C_k \sim (-c^{1/4})^k \Gamma(k)^{-1/2}$ (up to unimportant factors).

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