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Interaction $\lambda x^2/(1 + gx^2)$ Revisited

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It is shown that the refined non-perturbative Hill's method solves in a very neat way the Schrödinger equation $\psi'' + [E - x^2 - \lambda x^2/(1 + gx^2)]\psi = 0$. The refinement of the standard Hill's method consists in finding a renormalized frequency to optimize the calculation. This method appears to be preferable to the variational one recently used by A. K. Mitra in the same context.

I. INTRODUCTION

The least years have seen the development of non-perturbative methods of resolution of Schrödinger's equation (SE) in all cases where the exact solution does not exist. Such methods are necessary since the calculus of perturbation frequently provides insufficient information (low accuracy, divergent series, etc.). The best-known non-perturbative scheme is the classical variational Ritz method. More recently various authors have developed new methods [1–4]. Mitra [5] published a paper dealing with the variational calculation of the eigenstates of the potential $x^2 + \lambda x^2/(1 + gx^2)$. It contains a good illustration of the numerous problems that are encountered by the users of such a variational scheme. All these difficulties are well emphasized by the author himself throughout his paper:

(1) The $N \times N$ hamiltonian matrix contains nothing less than $N^2/2$ non-vanishing elements $H_{m,n}$.

(2) These elements are written as non-elementary integrals involving pairs of Weber–Hermite functions. They must be computed through a numerical procedure. Since the individual evaluation of each integral would be time consuming, Mitra established recurrence relations between the successive integrals and then calculated all the terms recursively.

However, recursive procedures may not be used without precautions [6] that are apparently overlooked by Mitra. Let us stress that important point. The integrals $H_{m,n}$ are defined by [5]

$$H_{m,n} = \int_{-\infty}^{+\infty} \frac{U_m U_n}{1 + gx^2}\, dx,$$

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where the U_m are the wavefunctions of the harmonic oscillator. See Ref. [5] for their explicit definitions.

Mitra has shown that the $H_{m,n}$ obey the following recurrence (two typographical errors are rectified):

$$H_{m,n} = \frac{2}{g[(n-1)(n-2)]^{1/2}}\,\delta_{m,n-2} - c_n H_{m,n-2} - d_n H_{m,n-4}, \tag{1}$$

where

$$c_n = \frac{2/g + 2n - 5}{[(n-1)(n-2)]^{1/2}} \qquad \text{and} \qquad d_n = \left[\frac{(n-3)(n-4)}{(n-1)(n-2)}\right]^{1/2};$$

$\delta_{i,j} = 0$ when $i \neq j$, $=1$ otherwise.

Equation (1) is a second-order difference equation. Therefore [6] it possesses two linearly independent solutions α_n and β_n whose asymptotic behaviours are quite different when $n \to +\infty$. More precisely, $\lim_{n\to\infty} |\beta_n/\alpha_n| = 0$; α_n is said to be dominant and β_n subdominant. As shown by Miller [11] only the dominant solution of a recurrence may be calculated through a forward calculation. If one tries to calculate the subdominant solution through the same forward algorithm, one immediately encounters a growing instability with a pollution factor which is of the order of magnitude of $|\alpha_n/\beta_n|$. The most celebrated example is the impossibility of calculating stably the successive Bessel functions $J_n(z)$ through the forward application of the well-known recurrence

$$J_{n+1} + J_{n-1} - (2n/z)\,J_n = 0.$$

That is because the associated Bessel function of the second kind Y_n is also the solution of the same recurrence with $\lim_{n\to\infty} |J_n/Y_n| = 0$ (i.e., Y_n is dominant and J_n is subdominant). Miller has developed a special algorithm in order to evaluate the subdominant solution of a three-term recurrence and Oliver [12] has extended Miller's algorithm when the recurrence contains more then three terms (see Appendix A for more details).

In the case of recurrence (1) the $H_{m,n}$ as defined by Mitra are precisely subdominant so that the simple forward calculation is strictly forbidden. Let us illustrate the situation in the special case $m = 1$. We set $f_n = H_{1,2n+3}$ so that Eq. (1) becomes

$$f_0 = \sqrt{2}/g - c_3 f_{-1}, \tag{2}$$

$$f_{n+1} + \frac{4n + 5 + 2/\sqrt{g}}{[(2n+4)(2n+3)]^{1/2}} f_n + \left[\frac{(n+1)(2n+1)}{(n+2)(2n+3)}\right]^{1/2} f_{n-1} = 0 \qquad (n = 0, 1, 2, \ldots).$$

It is possible to find two linearly independent solutions of that recurrence that are asymptotic to

$$\begin{pmatrix}\alpha_n\\ \beta_n\end{pmatrix} = (-1)^n\, n^{-1/4} \exp(\pm 2\sqrt{n/g}).$$

(The technique for obtaining them is presented in Appendix C.)

The stable forward evaluation of the subdominant solution of the recurrence is thus impossible because of the pollution factor

$$|\alpha_n/\beta_n| = \exp(4\sqrt{n/g})$$

($=10^{12}$! if $g=1$ and $n=50$, for example). Table I illustrates the situation when $g=1$: the f_n calculated through the forward recursive scheme are compared to the true values deduced from Miller's algorithm. For $n=50$ note that only four figures remain correct due to a pollution factor $\sim 10^{12} \times 10^{-16} = 10^{-4}$. The same formula also clearly indicates why the variational approach is inefficient at low g without using Miller's algorithm (the pollution factor becomes infinite).

It is to be noted that Miller's algorithm automatically furnishes the exact value of the ratio $f_0/f_{-1} = -0.2552885189$. Combining with Eq. (2) one finds ($g=1$): $f_{-1} = H_{1,1} = 0.7578721561$ as reported in Table I so that the whole discussion developed by Mitra in order to evaluate $H_{1,1}$ by numerical quadratures becomes superfluous.

(3) There is no straightforward possibility of optimization allowing one to make N minimum without altering the accuracy of the results.

(4) Moreover, no prediction is possible estimating (before the numerical investigation) the order of magnitude of N (for a given accuracy).

(5) The method is not well adapted to the calculation of the wavefunctions.

(6) A change of scale $x = \alpha z$ is made necessary when g becomes too small in order to reduce the time of the calculation.

TABLE I

$f_n = H_{1,2n+3}$ as Calculated by Mitra through the Forward Recursive Scheme Becomes Progressively Incorrect as n Increases

n	$f_n = H_{1,2n+3}$ Forward calculation	$f_n = H_{1,2n+3}$ Miller's algorithm
−1	7.57872 E − 01	7.57872 E − 01
0	−1.93476 E − 01	−1.93476 E − 01
10	−1.41839 E − 03	−1.41839 E − 03
30	−1.27277 E − 05	−1.27277 E − 05
50	−4.90085 E − 07	−4.90052 E − 07
100	−1.02924 E − 08	−1.24796 E − 09
180	−7.01608 E − 06	−1.14513 E − 12

Note. The calculations have been performed in double precision, i.e., with 16 significant figures.

In a few words such a method does not appear to be quite recommendable: it is expensive in computer time for a final result which is not most advantageous. Therefore, it should be reserved solely for the cases where no alternative method exists.

II. Refined Hill's Method

Let us reconsider the problem settled by Mitra [5]:

$$\psi'' + [E - x^2 - \lambda x^2/(1+gx^2)]\psi = 0.$$

Our aim is to show that there exists a new method which solves the problem avoiding all the drawbacks mentioned previously (and more generally that would solve in the same way SE when the potential is given by an analytic expression). It is a powerful refinement of the Hill's method recently rediscovered by Biswas *et al.* [1]. We have presented elsewhere [7] the theoretical backgrounds of the refined method and we shall systematically refer to them when necessary. Let us expand ψ in the form (even states only)

$$\psi = \sum_0^\infty C_k/k!\, D_{2k}(\omega x). \tag{3}$$

The D_{2k} are Weber–Hermite functions (see Appendix B). ω is a positive parameter whose value is not precise now. (Note that $\omega = \sqrt{2}$ would correspond to an expansion in the basis of the eigenfunctions of the harmonic oscillator.) It is easy to verify that the C_k obey the following fourth-order recurrence:

$$\begin{aligned}
&4g(\omega^4-4)(4k^2-1)\,C_{k+1}\\
&\quad+(2k-1)(-64gk+16g+2\omega^6-8\omega^2-8\lambda\omega^2+8gE\omega^2-8g\omega^4)\,C_k\\
&\quad+[-8g(12+\omega^4)\,k^2+(144g-4\omega^6-16\omega^2-16\lambda\omega^2+16gE\omega^2+12g\omega^4)k\\
&\quad+(3\omega^6+12\omega^2+12\lambda\omega^2+4E\omega^4-3g\omega^4-12gE\omega^2-60g)]\,C_{k-1}\\
&\quad+(k-1)(-32gk+40g+\omega^6-4\omega^2-4\lambda\omega^2+4gE\omega^2+4g\omega^4)\,C_{k-2}\\
&\quad+g(\omega^4-4)(k-1)(k-2)\,C_{k-3}=0, \qquad (k=1,2,3,\ldots).
\end{aligned} \tag{4}$$

The following operations are needed in order to obtain that recurrence: introduce expansion (3) in the starting SE and multiply both sides of the resulting equation by $1+gx^2$. Then by using relations (B1), (B3), and (B4) in Appendix B one obtains a relation between five successive $D_{2k}(\omega x)$ with coefficients independent of x. That relation must be identically verified for all x. Since the various $D_{2k}(\omega x)$ are independent, one deduces recurrence (4) by simply equating to zero the coefficient of $D_{2k}(\omega x)$ $(k=1,2,3,\ldots)$.

Equation (4) can be rewritten in the form of an infinite linear homogenous system with the infinity of unknowns $C_0, C_1, \ldots$. The infinite determinant D of the matrix of

the system is the Hill determinant of the problem. Its roots with respect to E are the searched eigenvalues of the problem. Practically, these eigenvalues are approximated by the roots of the kth approximant $D^{(k)}$ of D obtained by truncation of D so that only the k first lines and columns are retained. If we call E the roots of D and $E^{(k)}$ the roots of $D^{(k)}$, one defines the precision p of the approximation by

$$|E - E^{(k)}|/|E| = \exp(-p). \tag{5}$$

A clue to the whole problem results from the fact that all the ω-values are not equivalent: when k is fixed, various ω-values lead to different precisions p. So it becomes interesting to study which value of ω leads to the largest p (when k is fixed). We call this "best" value ω_{opt}. p_{opt} is the corresponding best available precision with a kth-order approximant. Figures 1–3 illustrate the experimental situation in various cases: k is fixed and (p, ω) curves are drawn corresponding to various value of λ and g. All these curves exhibit a maximum for $\omega = \omega_{opt}$.

The problem may be reversed: p is fixed (i.e., one asks for 2.3p correct significant figures in the eigenvalues) and k appears to depend on the value of ω with a minimum (k_{opt} say) when $\omega = \omega_{opt}$. Both viewpoints are strictly complementary and both will be described by Eq. (9). The interest in the determination of ω_{opt} is easily understood: if the value of ω is correctly choosen near ω_{opt}, the calculation of the eigenvalues with a given precision will need the consideration of approximants $D^{(k)}$ of minimal dimension so that the computation time will be reduced.

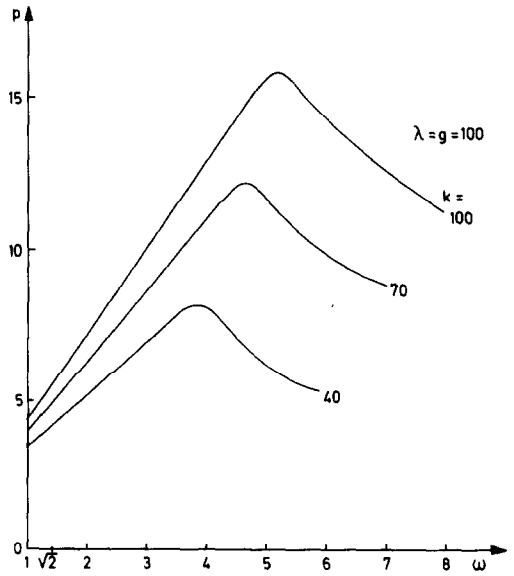


FIG. 1. Three experimental (p, ω) curves corresponding to the cases $k = 40$, 70, 100 ($\lambda = g = 100$). With λ and g fixed, note that both ω_{opt} and p_{opt} increase with k.

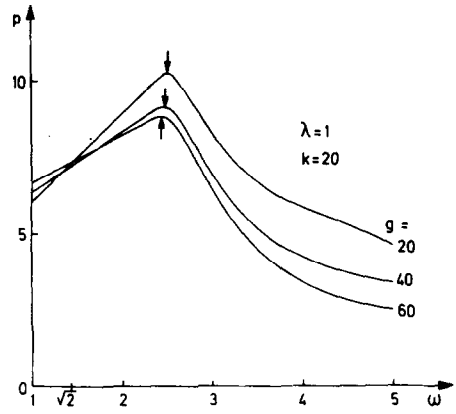


FIG. 2. Three experimental (p, ω) curves corresponding to $g = 20, 40, 60 (\lambda = 1, k = 20)$. With λ and k fixed, note that both ω_{opt} and p_{opt} increase with $1/g$.

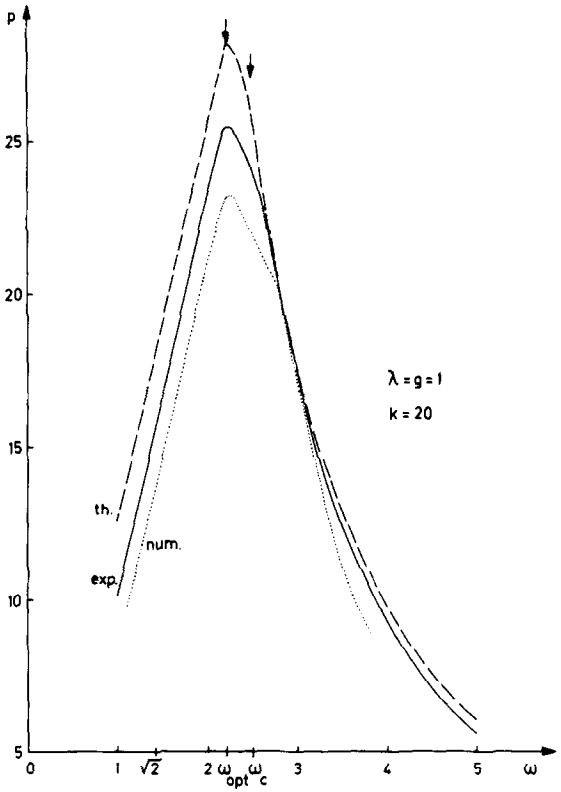


FIG. 3. The solid curve (p, ω) is experimental (corresponding to $\lambda = g = 1$, $k = 20$). The dashed curve shows results of the analytic prediction of Subsections V.1, V.2A, and V.2D. The dotted curve shows numerical results (see Subsection V.2E).

Remark. As pointed out before, the method of calculating the eigenvalues of the SE as the roots of the corresponding Hill determinant is not new. It has been recently explored by Biswas *et al.* [1]. However, these authors systematically expand the searched wavefunction in terms of the solutions of the harmonic oscillator; i.e., they would choose $\omega = \sqrt{2}$ in our case. Precisely the experimental curves of Figs. 1–3 show that the choice is not optimal since $\omega_{opt} > \sqrt{2}$. The essential role played by the parameter ω was first mentioned by Banerjee [13], who proposed empirical estimates for it. In a previous paper [7] we studied the possibility of predicting ω_{opt} in a non-empirical way in the context of anharmonic oscillators $x^2 + \lambda x^{2m}$. It must be noted that the estimates given by Banerjee do not exactly coïncide with our ω_{opt}: indeed ω_{opt} always depends on the asked precision p (or equivalently on the order of the approximant considered), while Banerjee's best ω-values do not (i.e., these estimates are not truly optimal).

III. Approximate Eigenvalues

Calling V the potential $x^2 + \lambda x^2/(1 + gx^2)$ one has the inequalities

$$x^2 < V < x^2 + \lambda/g \qquad \text{and} \qquad V < (\lambda + 1)\, x^2,$$

from which one deduces two obvious conditions on the energy:

$$2N + 1 < E_N < 2N + 1 + \lambda/g \qquad \text{and} \qquad E_N < (2N + 1)\sqrt{\lambda + 1}.$$

(a) When λ/g is small or moderate, $2N + 1$ is a good first approximation of E_N.

A closer approximation is furnished by the consideration of the first approximant $D^{(1)}$ associated with (4). When equating it to zero one obtains a surprisingly good approximation of the fundamental state eigenvalue. A similar expression is obtained for the Nth excited state by reducing D to the sole element which lies at the intersection of the $(N + 1)$th line and of the $(N + 1)$th column. That diagonal element is in fact identical to the coefficient of C_{k-1} in recurrence (4). Remembering that recurrence (4) only deals with the even states and that the recurrence for the odd states deduces by simple substitution $k \to k + 1/2$ in the coefficients of (4) [7] one finds the following equation for the approximate Nth eigenvalue E:

$$\begin{aligned} &-8g(12 + \omega^4)(N/2 + 1)^2 \\ &\quad + (144g - 4\omega^6 - 16\omega^2 - 16\lambda\omega^2 + 16gE\omega^2 + 12g\omega^4)(N/2 + 1) \\ &\quad + (3\omega^6 + 12\omega^2 + 12\lambda\omega^2 + 4E\omega^4 - 3g\omega^4 - 12gE\omega^2 - 60g) = 0, \end{aligned}$$

$N = 0, 1, 2,...$, valid for all the states odd or even. It is possible to deduce E from this relation. The value that is obtained is correct in the large g regime ($E \sim 2N+1$) provided one chooses $\omega = \sqrt{2}$ so that one gets

$$E \simeq \frac{4gN^2 + (5/2 + 2\lambda + 4gN) + 2 + \lambda + g}{2gN + g + 2} \qquad (N = 0, 1, 2,...). \tag{6}$$

For the fundamental state one has simply

$$E_0 \simeq (2 + \lambda + g)/(2 + g). \tag{7}$$

Equation (6) is equivalent to a first-order Pade approximant for E. That first approximation shows that the choice $\omega = \sqrt{2}$ is optimal when one considers low-order approximants $D^{(k)}$. However, the accuracy is of course limited. If one needs higher precision, the sole possibility is to increase k. However, Figs. 1 and 2 show that ω_{opt} increases with k in agreement with the following rules: (see also Table III for other details):

—if k is fixed and if $g \to \infty$, then $\omega_{\text{opt}} \to \sqrt{2}$ (slowly) and $p \to 0$,
—if g is fixed and if $k \to \infty$, then $\omega_{\text{opt}} \to \infty$ and $p \to \infty$.

In all cases one has $\omega_{\text{opt}} > \sqrt{2}$ except when k or p is small where $\omega_{\text{opt}} \sim \sqrt{2}$.

(b) When g is moderate or small, $(2N+1)\sqrt{\lambda+1}$ is a sufficiently accurate approximation of E_N.

(c) The sole critical case is $\lambda/g \gg 1$ and $g \gg 1$. In this case one may have recourse to Ritz principle: $E = \min_u (u, H, u)/(u, u)$ with $H = -d^2/dx^2 + V(x)$ and where the trial function u is taken as $u = (1+gx^2)\exp(-\alpha x^2)$ (α is an adjustable parameter). The result is for the fundamental state

$$E \simeq \min_{\alpha} \frac{64\alpha^4 - 32\alpha^3 g + (16 + 16\lambda + 28g^2)\alpha^2 + (24g + 12\lambda g)\alpha + 15g^2}{4\alpha(16\alpha^2 + 8\alpha g + 3g^2)}.$$

IV. Theorem about Linear nth-Order Recurrences

Before going further we need a theorem which has been established elsewhere [7]. Let us consider the general nth-order linear homogenous recurrence (where we assume its dependence on two parameters ω and E)

$$A_k^{(n)}(\omega, E)\, C_{k+1} + A_k^{(n-1)}(\omega, E)\, C_k + \cdots + A_k^{(0)}(\omega, E)\, C_{k-n+1} = 0 \tag{8}$$

with $C_k = 0$ if $k < 0$ and $k = s, s+1, \ldots$ ($s \geqslant 0$, fixed integer). The kth approximant of the associate Hill determinant is written as

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

All the elements are zero except those on the main diagonal, on the $(s+1)$ upper adjacent diagonals, and on the $(n-s-1)$ lower adjacent diagonals. As seen before, the eigenvalues of the problem are given by

$$E = \lim_{k \to \infty} E^{(k)}.$$

Recurrence (8) has n linear independent solutions that are well contrasted for large k [10]. We note them:

$$|C_k^{(1)}| \geqslant |C_k^{(2)}| \geqslant \cdots \geqslant |C_k^{(n)}| \qquad (k \text{ sufficiently large}).$$

The general method for finding the asymptotic behaviours of the $\vec{C}_k^{(i)}$ is recalled in Appendix C.

THEOREM. *The relative error committed when considering $D^{(k)}$ in place of D is of the order of magnitude of*

$$|D - D^{(k)}|/|D| \sim \rho_k = |C_k^{(s+2)}/C_k^{(s+1)}|.$$

Consequence. In the case where the roots E of D are simple we also have

$$|E - E^{(k)}|/|E| \sim \rho_k.$$

Combining the last result with Eq. (5) one finds

$$p \simeq \ln |C_k^{(s+1)}/C_k^{(s+2)}| = -\ln |\rho_k|. \tag{9}$$

That relation plays the essential role in our paper: it relates the precision p, the order k of the approximant $D^{(k)}$, and ω (by help of the $C_k^{(i)}$). It is the searched (k, ω, p) relation which must theoretically fit the experimental curves of Figs. 1–3. Section V develops the various ways of exploiting Eq. (9) in the general case of recurrence (8). The special case of recurrence (4) is also investigated and serves to clarify the situation. For that special case one has $n = 4$, $s = 1$ so that $p \simeq \ln |C_k^{(2)}/C_k^{(3)}|$.

V. Theoretical Prediction of the (k, ω, p) Curves

1. *First Method*

The $C_k^{(i)}$ are assimilated to their asymptotic behaviours. In Appendix C we calculate the asymptotes of the four solutions $C_k^{(i)}$ $(i = 1, 2,..., 4)$ of recurrence (4). They are given by

$$\alpha_k \sim k^{-1}(-1/2)^k \exp(\omega\sqrt{2k/g}),$$
$$\beta_k \sim k^{-1}(-1/2)^k \exp(-\omega\sqrt{2k/g}),$$
$$\gamma_k \sim k^{-1/4-(gE-\lambda)/(4g)}(1/2)^k(\omega^2+2)^k/(\omega^2-2)^k,$$
$$\delta_k \sim k^{-1/4+(gE-\lambda)/(4g)}(1/2)^k(\omega^2-2)^k/(\omega^2+2)^k.$$

The numbering of $\alpha_k,..., \delta_k$ in the form $C_k^{(i)}$ $(i = 1, 2, 3, \text{or } 4)$ depends on their order of dominance which itself depends on ω; when ω is fixed, one numerically calculates the four asymptotes $\alpha_k,..., \delta_k$; one excludes both dominant and subdominant solutions to retain only the two intermediates. These are introduced in the fundamental equation (9) in order to obtain the precision p: let us fix k and let ω vary:

—If $\omega < \omega_{\text{opt}}$ (ω_{opt} defined by $|\beta_k| = |\delta_k|$) one has

$$|\delta_k| < |\beta_k| < |\alpha_k| < |\gamma_k|$$

so that

$$p = -\ln|\beta_k/\alpha_k| = 2\omega\sqrt{2k/g}. \tag{10}$$

Equation (10) shows a linear increase of p with respect to ω corresponding to a straight line in the (k, ω, p) curve of Figs. 1–3. The reader may also verify that its slope is correctly given in each case by $dp/d\omega = 2\sqrt{2k/g}$.

—If $\omega_{\text{opt}} < \omega < \omega_c$ (ω_c defined by $|\alpha_k| = |\gamma_k|$) one has

$$|\beta_k| < |\delta_k| < |\alpha_k| < |\gamma_k|$$

so that

$$p = -\ln|\delta_k/\alpha_k| = -\ln|k^{3/4+(gE-\lambda)/(4g)} \exp(-\omega\sqrt{2k/g})(\omega^2-2)^k/(\omega^2+2)^k|. \tag{11}$$

—If $\omega_c < \omega$, one has

$$|\beta_k| < |\delta_k| < |\gamma_k| < |\alpha_k|$$

so that

$$p = -\ln|\delta_k/\gamma_k| = -\ln|k^{(gE-\lambda)/(2g)}(\omega^2-2)^{2k}/(\omega^2+2)^{2k}|. \tag{12}$$

These three expressions for p show that all the values of ω are not equivalent. Let us fix the dimension k of the approximant: when ω increases and approaches ω_{opt} the precision increases; for $\omega = \omega_{opt}$, p is maximum. When ω increases between ω_{opt} and ω_c the precision decreases. For $\omega > \omega_c$ the diminution of p becomes dramatic. The practical conclusion is evident: it is highly recommended that ω be chosen just next ω_{opt}. Figure 3 illustrates the situation when $\lambda = 1$, $g = 1$, $k = 20$:

The experimental curve is drawn in heavy lines. The theoretical prediction is represented by dashed lines. The slight discrepancy is due to two reasons:

—Formula (9) should be rigorously written as

$$\exp(-p) \simeq A\,|\rho_k| \text{ where } A \text{ is an unknown constant independent of } k.$$

So there is a possible shift between the experimental and theoretical curves.

—The asympotes $\alpha_k \cdots \delta_k$ are accurate only if k is very large. However, we wish to make k as small as possible so that the prediction cannot be perfect. It is, however, largely sufficient.

The theoretical prediction can also be carried out in a different way: if p is fixed relations (10) and (11) allow one to determine the best ω- and k-values. Combining (10) and (11) one finds

$$\frac{3g + gE - \lambda}{2g} \ln \frac{p^2 g}{8\omega_{opt}^2} + \frac{p^2 g}{4\omega_{opt}^2} \ln \frac{\omega_{opt}^2 - 2}{\omega_{opt}^2 + 2} + p = 0, \tag{13}$$

$$k_{opt} = \frac{p^2 g}{8\omega_{opt}^2}, \tag{14}$$

from which one deduces ω_{opt} and k_{opt} when λ and g are given.

Remarks. (1) The presence of parameter E in these equations might be judged prejudicial since we are trying to determine it precisely in an optimal way. However, the influence of E in both γ_k and δ_k is completely subdominant (indeed $E/4$ only appears as a power of k) so that a few accurate values of E are largely sufficient for the predictions that are in view. In this paper we have used the approximate E as calculated in Section III.

(2) All Equations (10)–(14) are invariant under the scale transformation $x = \alpha z$ in the starting SE. Take, for example, Eq. (10). After the change of scaling, Eq. (10) becomes $p = (2\omega/\alpha)\sqrt{2k/g_1}$, which is clearly equivalent to our $p = 2\omega\sqrt{2k/g}$ because of $\alpha^2 = g/g_1$ as established by Mitra [5].

2. *Second Method: Saddle Point Method*

In this subsection we develop another approach which can be used in a more general context. This approach is due to Magnus [14]. See also [7]. One looks for integral expressions that satisfy the fundamental recurrence relation. Further, one

tries to evaluate these integrals through a saddle point method [15]. By that method

$$\psi'' + [E - V(x)]\psi = 0 \qquad \text{with} \quad V(x) = V(-x)$$

and let us look for the even eigenstates only:

$$\psi = \sum_0^\infty C_k/k!\, D_{2k}(\omega x).$$

The C_k derive from the orthogonality property of the D_{2k} functions:

$$C_k \sim k!/(2k)! \oint_{\mathscr{C}} \psi(z)\, D_{2k}(\omega z)\, dz.$$

One can estimate C_k for k not too small in the following way:

$$\psi(z) \sim \exp\left(\pm \int_u^z \sqrt{V(x) - E}\, dx\right),$$

where u is a root of $V(u) = E$,

$$D_{2k}(\omega z) \sim \sqrt{(2k)!}\, \exp\left(\pm(4k+1)\int_1^{\omega z/\sqrt{8k+2}} (x^2-1)^{1/2}\, dx\right) \qquad \text{(see Appendix B)}$$

so that

$$C_k^{(i)} \sim k^{1/4} 2^{-k} \oint_{\mathscr{C}_i} \exp\left\{\pm\int_u^z [V(x) - E]^{1/2}\, dx \pm (4k+1)\int_1^{\omega z/\sqrt{8k+2}} (x^2-1)^{1/2}\, dx\right\} dz,$$

where the n integration contours $\mathscr{C}_i$ are chosen in the complex z-plane. The integration with respect to z is easily performed with the aid of the saddle point method [15]:

$$\oint_{\mathscr{C}} \exp[f(z)]\, dz \sim [-2\pi/f''(z^*)]^{1/2} \exp f(z^*),$$

where z^* are the saddle points of f, solutions of $f'(z) = 0$. The equation for the saddle points is in our case

$$\pm[V(z) - E]^{1/2} \pm \tfrac{1}{2}\omega[\omega^2 z^2 - (8k+2)]^{1/2} = 0,$$

i.e., $V(z) - E = \omega^4 z^2/4 - \omega^2(4k+1)/2$ with roots $z_i (i = 1, 2, \ldots, n)$. One obtains

$$C_k^{(i)} \sim k^{1/4} 2^{-k} \exp\left\{\pm\int_{u_i}^{z_i} [V(x) - E]^{1/2}\, dx \pm (4k+1)\int_1^{\omega z_i/\sqrt{8k+2}} (x^2-1)^{1/2}\, dx\right\} \qquad (15)$$

(with $u_i = \lim_{\omega \to 0} z_i$). In (15) the inessential term $[-2\pi/f''(z)]^{1/2}$ has been omitted. When $k \to \infty$ one has that the $C_k^{(i)}$ tend to the asymptotes of the recurrence as determined in Appendix C. That remark allows one to make a good choice in the signs $\pm$ that are imprecise in Eq. (15). The determination of the (k, ω, p) curve is then achieved provided the first integral $I = \int_{u_i}^{z_i} (V - E)^{1/2}\, dx$ present in (15) is evaluated. Five cases are possible:

(A) The integral can be performed analytically. In this case one immediately derives closed expressions for the $C_k^{(i)}$. A simple application of Eq. (9) furnishes the desired (k, ω, p) curve.

If $V(x) = x^2 + \lambda x^2/(1 + gx^2)$, the integral I is exactly calculable provided E is neglected so that the prediction is almost correct for the fundamental state. One successively finds:

—the equation for the saddle points $Pz^4 + Qz^2 + R = 0$ or, in greater detail,

$$g(\omega^4 - 4)\, z^4 + [\omega^4 - 4 - (8k + 2)\, \omega^2 g - 4\lambda]\, z^2 - (8k + 2)\, \omega^2 = 0;$$

—the four saddle points

$$z_i = \pm[-Q \pm (Q^2 - 4PR)^{1/2}]^{1/2}, \qquad i = 1, 2, 3, 4,$$

$$z_1 = \frac{1}{2P}\left[-Q + (Q^2 - 4PR)^{1/2}\right]^{1/2} \sim (2k/\alpha)^{1/2} \qquad \text{if} \quad k \to \infty,$$

$$z_3 = \frac{1}{2P}\,[-Q - (Q^2 - 4PR)^{1/2}]^{1/2} \sim i/\sqrt{g}\left(1 - \frac{\lambda}{4\omega^2 g k}\right) \qquad \text{if} \quad k \to \infty,$$

$$z_2 = -z_3 \qquad \text{and} \qquad z_4 = -z_1 \qquad \text{with} \quad \alpha = (\omega^4 - 4)/(4\omega^2);$$

—the four solutions $C_k^{(i)}$ $(i = 1, \ldots, 4)$:

$$C_k^{(i)} \sim k^{1/4} 2^{-k} \exp\left\{ \pm \int_{u_i}^{z_i} x[1 + \lambda/(1 + gx^2)]^{1/2}\, dx \pm (4k + 1) \int_1^{\omega z_i/\sqrt{8k+2}} (x^2 - 1)^{1/2}\, dx \right\}$$

$$\sim k^{1/4} 2^{-k} \exp\left\{ \pm \frac{1}{2g}\left[\sqrt{(1 + gz_i^2)(\lambda + 1 + gz_i^2)} - \sqrt{(1 + gu_i^2)(\lambda + 1 + gu_i^2)} \right.\right.$$

$$\left. + \lambda \ln \frac{\sqrt{1 + gz_i^2} + \sqrt{\lambda + 1 + gz_i^2}}{\sqrt{1 + gu_i^2} + \sqrt{\lambda + 1 + gu_i^2}} \right]$$

$$\pm (2k + 1/2)\left[\omega z_i \sqrt{\omega^2 z_i^2 - (8k + 2)}/(8k + 2) \right.$$

$$\left.\left. - \ln\left(\frac{\omega z}{\sqrt{8k + 2}} + \sqrt{\frac{\omega^2 z^2}{8k + 2} - 1} \right) \right] \right\}; \tag{16}$$

—the ambiguity in the $\pm$ signs is resolved as follows: when k becomes very large, the saddle points are asymptotic to $\pm(2k/\alpha)^{1/2}$ or $\pm i/\sqrt{g}$. It is then possible to simplify Eq. (16) in order to recover the asymptotes α_k, β_k, γ_k, and δ_k as calculated

in Appendix C. The coïncidence occurs if and only if one chooses the signs − and + (in that order) in Eq. (16) for $C_k^{(1)}$ and $C_k^{(2)}$, while $C_k^{(3)}$ and $C_k^{(4)}$ need the choice + and +. Now let ω vary and let us calculate the four $C_k^{(i)}$ for each value of ω. One only retains the two intermediate $|C_k^{(i)}|$. Introducing this in Eq. (9) immediately furnishes the values of the precision p. The corresponding (k, ω, p) curve coïncides with the theoretical curve determined in subsection V.1 (see dashed lines in Fig. 3 for the case $\lambda = g = 1$).

(B) The integral I is not elementary. A possibility is to evaluate it numerically. That will be easily possible only if the saddle points remain at a finite distance when ω varies. However, in the special case that interests us it is not verified since

$$\lim_{\omega \to \sqrt{2}} z_{\substack{1 \\ 4}} = \pm\infty.$$

Special refinements should be possible to allow the procedure by deforming the integration loop and avoiding the critical point $\omega = \sqrt{2}$. However, we do not explore it here, for the sake of brevity.

(C) A third possibility is the following: let us define $q_i = \ln |C_k^{(i)}|$ so that Eq. (9) becomes $p = q_{s+1} - q_{s+2}$. Let us derive the equation with respect to ω:

$$\frac{dp}{d\omega} = \frac{dq_{s+1}}{d\omega} - \frac{dq_{s+2}}{d\omega}, \tag{17}$$

where

$$\frac{dq_i}{d\omega} = \text{Real}\left\{ \pm \frac{dz_i}{d\omega} [V(z_i) - E]^{1/2} \pm \frac{1}{2}\left(z_i + \omega \frac{dz_i}{d\omega} \right) [\omega^2 z_i^2 - (8k+2)]^{1/2} \right\}. \tag{18}$$

Equation (18) is more advantageous than Eq. (15) since all the functions are now elementary. However, Eq. (18) presents a small drawback: the (k, ω, p) curve is now replaced by a $(k, \omega, dp/d\omega)$ curve. Fortunately a simple numerical integration allows to construct the curve by knowing its slope provided the curve is known at one point. Precisely when $\omega = 0$, Eq. (15) gives the $C_k^{(i)}$ under the calculable form:

$$|C_k^{(i)}| = \exp q_i = k^{1/4} 2^{-k} \exp\left(\text{Real}\left(\pm(4k+1) \int_1^{\alpha_i} (x^2 - 1)^{1/2}\, dx \right) \right)$$

with

$$\alpha_i = \lim_{\omega \to 0} [\omega z_i / \sqrt{8k+2}].$$

However, the method fails if one or several $C_k^{(i)}$ are not continuous in the ω-domain between 0 and ω_{opt}. This is due to the fact that the numerical integration becomes inefficient in that case. Precisely, in the case of potential $V(x) = x^2 + \lambda x^2/(1+gx^2)$ one has that γ_k is discontinuous in $\omega = \sqrt{2}$ (see its asymptotic expression in Appendix C). Since $\omega_{\text{opt}} > \sqrt{2}$, we must look for another approach.

(D) Fourth method: when the method exposed in case C is impossible one calculates the four solutions $C_k^{(i)}$ for a value of ω say ω' so that the $C_k^{(i)}$ remain continuous in the whole domain between ω' and ω_{opt}. In order to evaluate the $C_k^{(i)}$ for $\omega = \omega'$ two possibilities exist:

—to use the asymptotic expressions for $\omega = \omega'$ as determined in Appendix C or

—to determine the $C_k^{(i)}$ for $\omega = \omega'$ through the extended Miller algorithm as presented in Appendix A.

The procedure is efficient for the specific potential $V = x^2 + \lambda x^2/(1 + gx^2)$ provided one chooses $\omega' > \sqrt{2}$. It leads to a (k, ω, p) curve which is practically identical to the curve previously obtained with the aid of Eq. (15). Therefore it has not been reproduced in Figure 3. This fact confirms the subdominant influence of the energy parameter in our asymptotic estimations.

(E) A fifth method exists which is purely a numerical one. It suffices to determine numerically the solutions $C_k^{(s+1)}$ and $C_k^{(s+2)}$ through the extended Miller algorithm in the whole range of values of ω. Then applying (9) furnishes a numerical (k, ω, p) curve (see dashed line in Fig. 3 for the case $\lambda = g = 1$).

VI. Numerical Applications

We have used the techniques described above in order to predetermine the values of ω_{opt} in the whole range of λ- and g-values. The precision p has been chosen equal to 13.8 (six significant figures in the eigenvalues since $\exp(-13.8) = 10^{-6}$).

In fact the prediction of ω_{opt} is not useful when $\lambda, g < 1$ because very low values of k furnish the searched eigenvalues. When g (or λ) increases the prediction becomes useful and progressively necessary. It is interesting to point out that high g-values require consideration of large-order approximants $D^{(k)}$ (for a given precision). That remark also held in Mitra's approach. What we have performed is simply the selection of the best ω in order to minimize k. In other words Hill's method has been optimized with respect to ω. We may also note that the potential $x^2 + \lambda x^2/(1 + gx^2)$ exhibits two singularities in $x = \pm i/\sqrt{g}$ that approach the real axis when g increases.

Tables II and III show the spectrum of the eigenvalues for the potential $x^2 + \lambda x^2/(1 + gx^2)$ with the corresponding values of ω_{opt} and k_{opt}. Our tables are consistent with the results published by Mitra [5] except for minor discrepancies: for example, when $\lambda = g = 100$ Mitra finds 1.8364 while the correct value is 1.83634 (the same is true for $\lambda = 0{,}1$, $g = 1$). It must also be noted that Table II for the eigenvalues covers a larger range of (λ, g)-values than Mitra's paper, especially in the low g-regime where the variational method (as used by Mitra) becomes inefficient.

TABLE II

Eigenstates of the Potential $x^2 + \lambda x^2/(1+gx^2)$ for Various λ- and g-Regimes

g \ λ	10^{-3}	10^{-2}	10^{-1}	1	10	10^2	10^3
10^{-3}	1.000499	1.00498	1.04874	1.41384	3.31594	10.0491	31.6378
10^{-2}	1.000493	1.00492	1.04814	1.41051	3.30983	10.0425	31.6311
10^{-1}	1.000439	1.00438	1.04317	1.38053	3.25026	9.97618	31.5638
1	1.000242	1.00242	1.02411	1.23235	2.78233	9.35942	30.9066
10	1.0000594	1.000594	1.00594	1.05930	1.58002	5.79394	25.5488
10^2	1.0000084	1.000084	1.00084	1.00841	1.08406	1.83634	8.92080
10^3	1.00000096	1.0000096	1.000096	1.00096	1.00946	1.09458	1.94512

Note. The precision is everywhere equal to or greater than $p = 13.8$ (six significant figures). These values have been calculated by taking into account the corresponding values of ω_{opt} as determined in Section V (see also Table III).

TABLE III

Values of ω_{opt} for various λ- and g-Regimes as Determined through the Numerical Method of Subsection V.2E.

g \ λ	1	,10	100	1000
1	2 (10)			
10	3 (30)	3.3 (30)	4.2 (25)	
100		5.5 (100)	5.8 (95)	6.5 (70)
1000				10 (200)

Note. The corresponding values of k_{opt} are given in parentheses. The blanks correspond to the cases where the prediction is not useful since very low k-values furnish the correct eigenvalue in the whole range of ω-values.

VII. Conclusion

The new method appears valuable in many respects:

—The $N \times N$ determinant whose roots are to be calculated is a five-band determinant containing only $(5N-6)$ non-vanishing elements (to be compared with the $N^2/2$ elements of the variational method).

—All the elements are given by simple algebraic expressions: no integral is needed, no recursive calculation.

—Both prediction and optimization are possible. They make it possible to estimate the time of the numerical computations and the precision of the results.

—No change of scale is needed at low g because the optimization automatically selects the best value of ω present in (3). Strictly speaking, ω plays in Eq. (3) the role of an arbitrary scaling parameter so that ω_{opt} appears to be the best scaling possible.

—The wavefunctions are easily deduced through the recursive calculation of the C_k. However, one must be careful that the C_k that are interesting for our purpose form the subdominant solution of the recurrence. The forward calculation of the successive C_k is therefore strictly forbidden because of the probable instability that will occur. The calculation must be performed backwards in accordance with the Miller algorithm [11] or with the extended Miller algorithm [12] (see Appendix A).

We have performed various numerical tests on the obtained eigenfunctions. For example the orthogonality property of the various excited states has been verified:

$$\int_{-\infty}^{+\infty} \psi\psi' \, dx = \sum_{0}^{\infty} (\sqrt{2\pi}/\omega)(2k)! \, C_k C'_k/(k!)^2 \leqslant \exp(-p),$$

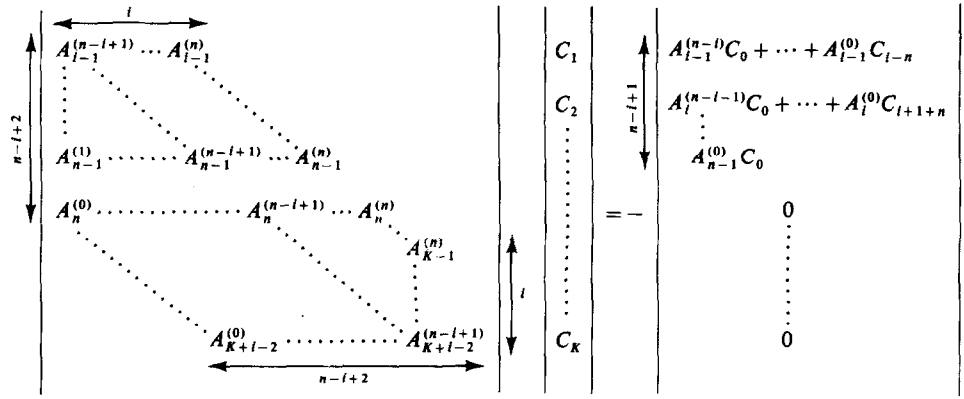
i.e., the overlap integral is always less than the asked precision. In the same way we have verified that $H\psi/\psi = E$ at various space points even in the non-classical region.

APPENDIX A: EXTENDED MILLER'S ALGORITHM

An nth-order linear homogenous recurrence like (8) has n independent solutions that are asymptotically well contrasted [6, 10]. They are written

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

$C_k^{(1)}$ is said to be dominant and $C_k^{(n)}$ is subdominant. The others are intermediate. Each linear combination of the type $\lambda_1 C_k^{(1)} + \cdots + \lambda_n C_k^{(n)}$ is dominant if $\lambda_1 \neq 0$ and non-dominant otherwise. The forward recursive evaluation of the C_k is stable if and only if C_k is dominant. In the other cases one needs a special algorithm which has been discovered by Miller when $n = 2$ and by Oliver when $n > 2$. Miller's simple algorithm determines the subdominant C_k through a backward recursive scheme. The procedure is justified by the fact that working backwards interchanges the dominant and subdominant character of the solutions of the recurrence. However it fails when the searched solution is intermediate. If one wishes to compute the intermediate solutions, one must refer to the extended Miller algorithm due to Oliver [12]. Since this extended algorithm calculates the n solutions in a stable way, we shall present it in greater details. Suppose one wishes to calculate $C_k^{(l)}$. One starts with recurrence (8) rewritten under the form of a linear infinite system (with $k = i, i+1, \ldots$ successively). Then one truncates the infinite system by only retaining the K first equations and by setting $C_k = 0$ when $k > K$. The truncated system is written as (in matrix notation)



The coefficients C_0, $C_{-1}, \ldots, C_{l-n}$ which appear in the second member are the initial conditions that can be chosen arbitrarily (however, not simultaneously zero). The

numerical resolution of that system furnishes stable approximations of the successive $C_k^{(i)}$. The precision on $C_k^{(i)}$ is given by [10, 12]

$$\text{precision on } C_k^{(i)} \sim |C_K^{(i)} C_k^{(i-1)} / C_K^{(i-1)} C_k^{(i)}| \qquad (i = 2, 3, \ldots, n). \tag{A1}$$

So the accuracy of the algorithm decreases when k approaches K. Equation (A1) is interesting since it allows one to choose K correctly in order to obtain the searched $C_k^{(i)}$ with the desired precision. In formula (A1) the expressions $C_k^{(i)}$ may be assimilated to their asymptotes as determined in Appendix C.

Note. If $i = 1$, formula (A1) is inapplicable. However, that does not matter since the extended Miller algorithm calculates the dominant solution $C_k^{(1)}$ in a totally stable way even if k approaches K. Therefore the precision on $C_k^{(1)}$ is equal to the precision of the calculator.

APPENDIX B: The Weber–Hermite Functions $D_k(u)$ [8].

The functions $D_k(u)$ obey the following relations:

$$D_k''(u) = (u^2/4 - k - 1/2)\, D_k(u), \tag{B1}$$

$$uD_k(u) = D_{k+1}(u) + kD_{k-1}(u). \tag{B2}$$

Successive applications of (B2) lead to

$$u^2 D_k = D_{k+2} + (2k+1)\, D_k + k(k-1)\, D_{k-2}, \tag{B3}$$

$$u^4 D_k = D_{k+4} + (4k+6)\, D_{k+2} + (6k^2 + 6k + 3)\, D_k + k(k-1)(4k-2)\, D_{k-2} + k(k-1)(k-2)(k-3)\, D_{k-4}. \tag{B4}$$

The $D_k(u)$ are orthogonal according to the formula

$$\int_{-\infty}^{+\infty} D_m(u)\, D_n(u)\, du = 0 \qquad \text{if} \quad m \neq n$$

$$= \sqrt{2\pi} n! \qquad \text{if} \quad m = n.$$

A classical WKB calculation allows one to derive from (B1) the asymptotic behaviour of $D_k(u)$ (valid when $k \gg |u|$); one finds

$$D_k(u) \sim \sqrt{k}!\, \exp\left(\pm(2k+1) \int_1^{u/\sqrt{4k+2}} \sqrt{x^2 - 1}\, dx \right). \tag{B5}$$

Remark. Equation (B5) should be rigorously written as

$$D_k(u) \sim \sqrt{k}!\, \exp\left\{ \pm(2k+1) \int_1^{u/\sqrt{4k+2}} \sqrt{x^2 - 1}\, dx - \frac{1}{4} \ln[u^2/4 - (k + 1/2)] \right\}.$$

However, the logarithmic term is largely inessential beside the other term present in the exponential.

APPENDIX C: DETERMINATION OF THE ASYMPTOTES OF THE SOLUTIONS OF A LINEAR HOMOGENOUS nth-ORDER RECURRENCE

Let us consider the general recurrence (8)

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

with

$$A_k^{(j)} = \sum_{p=0}^{\infty} a_{j,p}k^{-p/r} \qquad (r \text{ is a fixed integer}).$$

The recurrence is said to be regular of type r in the sense of Poincaré if and only if $a_{0,0} \neq 0$ and $a_{n,0} \neq 0$. Its characteristic equation is written as

$$a_{n,0}z^n + a_{n-1,0}z^{n-1} + \cdots + a_{0,0} = 0$$

with n roots distinct or not. Successive studies carried on by Norlund [16], Birkhoff [17], Culmer [18], and Turrittin [19] have shown that the n expressions to which the $C_k^{(i)}$ $(i = 1, 2, \ldots, n)$ are asymptotic are of the following type:

$$\text{asymptotes} \sim z^k k^w \exp[\alpha k^{(m-1)/m} + \beta k^{(m-2)/m} + \cdots + \eta k^{1/m}](\ln k)^g, \qquad \text{(C1)}$$

where m is an integer such that $m \leqslant r\mu$ (where μ is the multiplicity of the root z as a solution of the characteristic equation). Coefficients w, α, $\beta, \ldots, \eta$, and g are to be determined. Denef and Piessens [9] have indicated a possible way to attain them: they introduce the whole expression (C1) in the recurrence and then expand the resulting expression in successive powers of $k^{-1/m}$. Then by equating to zero the coefficients of the highest powers in k they obtain the relations that allow one to determine those coefficients. We have used the same method in another paper [10] in order to extend the results to the largest possible number of cases. Tables have been published that immediately furnish the asymptotic expressions when the recurrence is given. If one applies that method to recurrence (4), one finds the four asymptotes in the following way: the recurrence is regular of type 1 $(r = 1)$ in the sense of Poincaré. Its characteristic equation is written as

$$16g(\omega^4 - 4)z^4 - 128gz^3 - 8g(12 + \omega^4)z^2 - 32gz + g(\omega^4 - 4) = 0.$$

The four roots are:

$$\frac{1}{2} \text{ (double root)}, \qquad \frac{1}{2}\frac{\omega^2+2}{\omega^2-2} \text{ (simple root)}, \qquad \frac{1}{2}\frac{\omega^2-2}{\omega^2+2} \text{ (simple root)}.$$

The two asymptotes associated to the double root are according to Eq. (C1) of the type:

$$(-1/2)^k k^w \exp(\alpha\sqrt{k})(\ln k)^g,$$

while the simple roots give rise to asymptotes of the type

$$(1/2)^k[(\omega^2 \pm 2)/(\omega^2 \mp 2)]^k k^{w'}(\ln k)^{g'}.$$

The tables that are included in Refs. [9, 10] allow one to calculate the values of coefficients α, w, w', g, and g' precisely. Finally one finds

$$\begin{matrix}\alpha_k \\ \beta_k\end{matrix} \sim k^{-1}(-1/2)^k \exp(\pm\omega\sqrt{2k/g}),$$

$$\begin{matrix}\gamma_k \\ \delta_k\end{matrix} \sim k^{-1/4\mp(gE-\lambda)/(4g)}(1/2)^k\left(\frac{\omega^2 \pm 2}{\omega^2 \mp 2}\right)^k.$$

APPENDIX D. NUMERICAL EVALUATION OF HILL'S APPROXIMANTS

If we need m correct significant figures in the results, we know from Eq. (5) that we must choose $p = 2.3m$. With p so fixed, a careful application of the technique described in Section V leads to the best value of ω to be used (called ω_{opt}) and also to the corresponding best dimension k_{opt} of the Hill approximant $D^{(k_{\text{opt}})}$. In order to obtain the searched root of this approximant the simplest methods is to detect the change of sign of $D^{(k_{\text{opt}})}$ in the neighbourhood of the approximate E_0 deduced from Section III. To check the obtained result it is possible to increase the dimension of $D^{(k_{\text{opt}})}$ by 10 units (say) in order to verify that the root remains stable with m figures. Working in that way allows to deal with the sole $D^{(k_{\text{opt}})}$: no recursive calculation of the successive $D^{(k)}(k = 1, 2, ..., k_{\text{opt}})$ is needed. In fact it must be recalled that when $s > 1$ (see Eq. (8) for the definitions of s) no linear recurrence does exist between the successive $D^{(k)}$. However, their recursive calculation would be possible through non-linear schemes [7] (together with the extended Miller's algorithm to avoid loss of significant figures).

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