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## Potential $V(r) = \mu r^2 + \nu r^4$ and mutual equivalence of the two recent algebraic approaches to Schrödinger equations

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**Abstract.** We consider the anharmonic oscillator Hamiltonian and solve the corresponding Schrödinger equation by means of the recently proposed fixed-point (FP) perturbation theory. The FP formalism resembles an introduction of the creation and annihilation operators, uses a vectorial generalisation of continued fractions, introduces the inverse model-space dimension as a natural and controllably small expansion parameter and is shown to define a 'smooth' (exact, effective) truncation of the Hamiltonian matrix. It also reproduces the recent  $n \gg 1$  asymptotic formulae for the wavefunctions.

### 1. Introduction

Anharmonic corrections are rarely easily tractable as a small perturbation. The traditional Rayleigh-Schrödinger perturbation series diverges (Simon 1969) and its resummations are complicated (cf, e.g., references listed in Marziani 1984). At the same time, a numerical diagonalisation of the corresponding Hamiltonian matrix

$$H = \begin{pmatrix} a_0 & b_0 & c_0 & 0 & \dots \\ \dots & & & & \\ 0 & \dots & 0 & c_{n-2} & b_{n-1} & a_n & b_n & c_n & 0 & \dots \\ \dots & & & & & & & & & \end{pmatrix} \quad (1.1)$$

$$a_n = 6\nu n^2 + (9\nu + 6\nu l + 2\mu + 2)n + O(1)$$

$$b_n = (4\nu n + 2\nu l + 5\nu + \mu - 1)\beta_n \quad c_n = \nu\beta_n\beta_{n+1}$$

$$\beta_n = (n+1)^{1/2}(n+l+\frac{3}{2})^{1/2} \quad n, l = 0, 1, \dots$$

converges quickly (Graffi and Grecchi 1975). This leads to the following rather surprising conclusion. In practice, a 'small' parameter measuring the anharmonicity might be identified with the inverse cut-off dimension in (1.1) rather than with the coupling  $\nu$  itself.

The above (rather vague) feeling finds further support in an asymptotically smooth matrix structure of  $H$ . Thus, we may try to replace (1.1) by an exact, finite-dimensional effective Hamiltonian  $H^{\text{eff}}$  by purely algebraic non-perturbative means. This has been suggested in our earlier paper (Znojil 1983, hereafter referred to as I).

Paper I starts from the numerical factorisation of the truncated Schrödinger equation  $H^{(N)}\psi = E^{(N)}\psi$ ,

$$H - E = L^T \begin{pmatrix} 1/f_0 & & & \\ & 1/f_1 & & \\ & & \dots & \\ & & & \dots \end{pmatrix} L \tag{1.2}$$

where the superscript T denotes the transposition and

$$L^T = \begin{pmatrix} 1 & g_0 f_1 & c_0 f_2 & 0 \dots \\ 0 & 1 & g_1 f_2 & c_1 f_3 & 0 \dots \\ \dots & & & & \dots \end{pmatrix}. \tag{1.3}$$

Algebraically, it is defined by the recurrences

$$f_n = (a_n - E - g_n^2 f_{n+1} - c_n^2 f_{n+2})^{-1} \tag{1.4}$$

$$g_n = b_n - c_n g_{n+1} f_{n+2} \quad n = 0, 1, \dots$$

with the initial values

$$g_{N-1}^{(N)} = f_N^{(N)} = f_{N+1}^{(N)} = 0 \quad N \gg 1. \tag{1.5}$$

Variationally, we are interested in the  $N \rightarrow \infty$  limit. Perturbatively, we shall analyse this limiting transition.

In fact, the main practical merit of factorisation (1.2) lies in the possibility of rewriting the truncated secular equation  $\det(H^{(N)} - E) = 0$  by means of the simple algebraic identity

$$\det(H^{(N)} - E) = \prod_{k=0}^N 1/f_k^{(N)}. \tag{1.6}$$

Indeed, unless the value of  $E$  coincides randomly with a zero of a submatrix of  $H^{(N)}$ , we may use the condition

$$1/f_0^{(N)} = 0 \quad N \rightarrow \infty \tag{1.7}$$

as a secular equation determining all the binding energies in principle.

In analogy with the analytic continued fractions (Wall 1948) and their matrix generalisations (e.g. Graffi and Grecchi 1975), the auxiliary triplets  $(g_n^{(N)}, f_{n+1}^{(N)}, f_{n+2}^{(N)})$  will be called here the vectorial continued fractions (vcf) in the limit  $N \rightarrow \infty$ . In paper I, their so-called fixed-point (FP) algebraic approximation concept has been developed, also in analogy with the analytic continued fractional analysis (Znojil 1984 and references therein). In § 2 below, a detailed realisation of this general FP perturbative methodical proposal will be described in application to (1.1). The whole procedure is based on a geometric analysis of the vcf convergence and leads to the introduction of a small perturbative parameter in a very natural way.

In our recent paper (Znojil *et al* 1985, hereafter referred to as II), an alternative approach to the diagonalisation of  $H$  (1.1) was based directly on a difference-equation re-interpretation (DER) of the exact Schrödinger equation. Seemingly, there is no connection between the assumptions of I and II. In the present paper, we intend to demonstrate a full equivalence between their respective geometric and analytic points of view.

With regard to the asymptotical wavefunctions (the main DER result of II), we shall see here that the FP perturbative expansions of our auxiliary VCF quantities enable us to quickly rederive the DER result. This is done in § 3. In § 4, a numerical example is used to illustrate this and show how the DER formulae and FP expansions of  $H^{\text{eff}}$  accelerate the convergence of energies.

**2. The FP perturbative VCF expansions**

The asymptotic form

$$H_{mn} \sim \binom{4}{m+2-n} \left( 1 + O\left(\frac{1}{m+n}\right) \right) \tag{2.1}$$

of elements in (1.1) implies that the VCF convergence may easily be proved. Indeed, we may denote

$$\tilde{f}_k = \nu N^2 f_{N-k} \quad \tilde{\varphi}_k = g_{N-k-1} f_{N-k}$$

and rewrite recurrences (1.4) in the leading-order approximation

$$\begin{aligned} \tilde{f}_k &= (a - \tilde{\varphi}_{k-1} / \tilde{f}_{k-1} - c^2 \tilde{f}_{k-2})^{-1} \\ \tilde{\varphi}_k &= (b - c \tilde{\varphi}_{k-1}) \tilde{f}_k \quad a = 6, b = 4, c = 1. \end{aligned} \tag{2.2}$$

With the initial values (1.5), these  $k$ -independent mappings can be solved exactly,

$$\tilde{f}_k = \frac{k(k+1)}{(k+2)(k+3)} \quad \tilde{\varphi}_k = \frac{2k}{k+2} \quad k = 0, 1, \dots \tag{2.3}$$

Due to the convergence of our VCF quantities, we may write

$$\tilde{f}_k \approx \tilde{f}_{k+1} \approx f = 1 \quad \tilde{\varphi}_k \approx \tilde{\varphi}_{k+1} \approx \varphi = 2 \quad k \gg 1 \tag{2.4}$$

where the values of  $f$  and  $\varphi$  follow from the leading-order fixed-point algebraic equations of I,

$$\begin{aligned} f + 1/f &= 6 - \varphi^2/f \\ \varphi(1+f) &= 4f. \end{aligned} \tag{2.5}$$

The solution is completely degenerate and unique, in full analogy with the matrix results of Znojil (1984).

Concerning the next FP approximations, we may notice that the formulae

$$\begin{aligned} a_N &= \nu N^2 \left( 6 + \frac{\alpha}{N} + \frac{\alpha'}{N^2} + \dots \right) \\ b_N &= \nu N^2 \left( 4 + \frac{\beta}{N} + \frac{\beta'}{N^2} + \dots \right) \\ c_N &= \nu N^2 \left( 1 + \frac{\gamma}{N} + \frac{\gamma'}{N^2} + \dots \right) \end{aligned} \tag{2.6}$$

do not lead to the same asymptotic representation of the vcf components. This would contradict, e.g., equation (3.6) of I which implies only a possibility of the weakened ansatz

$$\begin{aligned} g_N &= \nu\rho^{-8} + x\rho^{-7} + y\rho^{-6} + z\rho^{-5} + h\rho^{-4} + \dots \\ f_N &= w\rho^8 + a\rho^9 + b\rho^{10} + c\rho^{11} + d\rho^{12} + \dots \end{aligned} \tag{2.7}$$

with the ‘natural’ variable  $\rho = N^{-1/4} > 0$ .

When we switch to the scaled anharmonic coupling  $\nu = 1$  in (1.1), we may now treat  $\rho$  as a small and independent variable in the FP perturbative spirit. We obtain a coupled set of non-linear relations for the coefficients in (2.7).

From the purely technical point of view, a determination of the unknown coefficients in (2.7) is rather lengthy. The reason is twofold. First, we have to represent the changes of indices in a Taylor-series manner,

$$\begin{aligned} (N + m)^{-1/4} &= \rho - \frac{1}{4}m\rho^5 + \dots \\ \rho^8 g_{N+1} &= \nu + \dots + z\rho^3 + (h + 4)\rho^4 + \dots \end{aligned}$$

etc. The second complication stems from a biquadratic character of the second relation in (1.4). Fortunately, when we combine the first item of (1.4), namely the relation

$$\begin{aligned} v + x\rho + y\rho^2 + \dots &= 4 + \beta\rho^4 + \dots \\ -(1 + \gamma\rho^4 + \dots)(w + a\rho + b\rho^2 + \dots)(v + x\rho + \dots) \end{aligned} \tag{2.8}$$

appropriately with the second one, we obtain the equation

$$g_N g_{N-2} / c_{N-1} c_{N-2} + g_N f_N b_{N-1} / c_{N-1} + f_N f_{N+2} c_N^2 - g_N b_{N-2} / c_{N-1} c_{N-2} - f_N a_N + 1 = 0 \tag{2.9}$$

which is biquadratic in  $g$  and  $f$ .

In the light of (2.4), we have to put

$$v = 2 \quad w = 1. \tag{2.10}$$

From (2.8), we obtain

$$x = -a \quad y = -b + \frac{1}{2}a^2 \quad z = ab - c - \frac{1}{4}a^3 \dots \tag{2.11}$$

and, combining this with the definitions of the type

$$1 / c_{N-1} c_{N-2} = 1 + (6 - 2\gamma)\rho^2 + \dots$$

we arrive at the power series form

$$\sum_{k=0}^{\infty} D_k(a, b, c, \dots)\rho^k = 0$$

of the requirement (2.9). This is an equation to be satisfied term by term

$$D_k(a, b, c, \dots) = 0 \quad k = 0, 1, \dots \tag{2.12}$$

Together with the corresponding definitions, this is an implicit form of our final FP perturbative prescription.

When we analyse (2.12) in detail, we notice that the validity of (2.10) reduces the first four relations with  $k=0, 1, 2$  and  $3$  to identities. This reflects the quadruple degeneracy of the leading-order solution. From the fifth  $k=4$  item (2.12), we obtain the first non-trivial specification of parameters

$$a^4 = 16.$$

An existence of its four distinct solutions  $a = \pm 2, a = \pm 2i$  removes the above degeneracy completely. Physically (Znojil 1984), we have to choose

$$a = -2 \quad x = 2. \tag{2.13}$$

Starting from  $k=5$ , equation (2.12) simply represents a linear definition of the subsequent unknown coefficients in (2.7). For  $k=5$ , we obtain

$$b = 2 \quad y = 0 \tag{2.14}$$

etc. The algebraic manipulations are to be performed on the computer.

### 3. Wavefunctions

In the DER methodical context, the asymptotic formulae of the type

$$\langle n | \psi \rangle = (-1)^n \exp[\frac{2}{3}a(1 \pm i)n^{3/4} + O(\sqrt{n})] \tag{3.1}$$

may be derived for the wavefunction projections (II). In the present FP framework, we are able to rederive them as well. Indeed, when we put

$$\langle n | \psi \rangle = (-1)^n \chi_n = (-1)^n \xi(\rho) \quad \rho = \rho(n) = n^{-1/4} \tag{3.2}$$

and convert the Schrödinger equation  $H\psi = E\psi$  into its vcf form

$$\chi_{n-1} - 2\chi_n + \chi_{n+1} + (\chi_{n-1} - \chi_n)r_n - w_n\chi_n = 0 \tag{3.3}$$

$$r_n = c_{n-1}f_{n+1} - 1 \quad w_n = g_n f_{n+1} - 2 - r_n \quad n = 0, 1, 2, \dots$$

we may proceed in full analogy with the DER approach and interpret relations (3.3) as a difference equation. It is of second order here, but the coefficients must be represented by their FP perturbative expansions.

Of course, we shall use the variable  $\rho(n)$  rather than the index  $n$  itself. With the notation

$$\begin{aligned} \rho_{\pm} &= \rho(n \pm 1) = (n \pm 1)^{-1/4} = \rho \mp \delta_{\pm} \\ \delta_{\pm} &= \{n^{1/4}(n \pm 1)^{1/4}[n^{1/4} + (n \pm 1)^{1/4}][n^{1/2} + (n \pm 1)^{1/2}]\}^{-1} \approx \delta \\ \delta &= \frac{1}{4}\rho^5 \end{aligned} \tag{3.4}$$

the  $n \gg 1$  asymptotic domain corresponds to the right vicinity of zero in the new variable  $\rho$ . Thus, with the standard assumptions, the Taylor series

$$\xi(\rho_{\pm}) = \xi(\rho) \mp \delta_{\pm} \xi'(\rho) + \frac{1}{2} \delta_{\pm}^2 \xi''(\rho) \mp \dots \tag{3.5}$$

may be inserted in (3.3). We get the relation

$$\delta^2 \xi'' + r_n (\delta \xi' + \frac{1}{2} \delta^2 \xi'' + O(\delta^3 \xi''')) + w_n \xi + O(\delta^4 \xi'''' ) = 0 \tag{3.6}$$

*A posteriori*, we may verify that  $\delta^k \xi^{(k)} = O(\rho^k)$  and control the precision in (3.6) as well as in the more precise relations obtained in the same manner. Replacing here the coefficients  $r_n$  and  $w_n$  by their leading-order FP form, we arrive at the ordinary linear differential equation

$$\frac{1}{16}\rho^8 \xi''(\rho) + \frac{1}{4}a\rho^4 \xi'(\rho) + \frac{1}{2}a^2 \xi(\rho) = 0. \tag{3.7}$$

Its solution

$$\xi(\rho) = \exp(\lambda(\rho)\rho^{-3}) \quad \rho \ll 1 \tag{3.8}$$

where

$$\lambda(\rho) = \frac{2}{3}a(1 \pm i) + O(\rho) \tag{3.9}$$

is fully compatible with the DER result (3.1).

An inclusion of the second-order FP corrections modifies equation (3.7):

$$\frac{1}{16}\rho^8 (1 + \frac{1}{2}a\rho) \xi'' + \frac{1}{4}(a + b\rho) \xi' + [\frac{1}{2}a^2 + (ab - \frac{1}{4}a^3)\rho] \xi = 0. \tag{3.10}$$

Obviously, this modification is trivial—an overall multiplication by the factor  $1 - \rho$  implies just an improved error factor to be used in (3.1). In the same way, the higher-order corrections may also be generated.

#### 4. A test and conclusions

With an overall error estimate controlled by our choice of the model-space dimension  $N$ , our construction of the vcf quantities represents an efficient numerical eigenvalue algorithm of course. This may be illustrated on the simplest s-wave ground-state energies as displayed in table 1 for the potential  $V(r) = r^2 + r^4$ . In comparison with the variational (truncation) results, an improvement of precision is observable even on the very boundary of the asymptotic region. It may be controlled not only by an increase of the dimension  $N$ , but also via an improved FP definition of the vcf initial values.

In the light of I and II, we may interpret the present vcf initial values as an algebraic definition of the Feshbach effective Hamiltonian  $H^{\text{eff}}$  as well. In addition to the obvious coincidence

$$H_{mn}^{\text{eff}} = H_{mn} \quad m \text{ or } n < N - 1 \tag{4.1}$$

**Table 1.** Ground-state energies in the potential  $V(r) = r^2 + r^4$  as calculated from the approximate matrices  $H^{\text{eff}}$ .

Dimension $N$	Approximation	
	Zero order	Second order
9	4.650 939	4.646 486
10	4.649 440	4.648 928
11	4.648 920	4.648 825
12	4.648 824	4.648 819
$\infty$	4.648 8127	4.648 8127

we may derive the asymptotic formulae of the type

$$\frac{1}{N^2} \begin{pmatrix} H_{N-1N-1}^{\text{eff}} & H_{N-1N}^{\text{eff}} \\ H_{NN-1}^{\text{eff}} & H_{NN}^{\text{eff}} \end{pmatrix} = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix} + \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix} \rho + \begin{pmatrix} -2 & 0 \\ 0 & 2 \end{pmatrix} \rho^2 + O(\rho^3) \quad (4.2)$$

which generalise the zero-order results obtainable by the various techniques (e.g. Znojil 1984). Up to the corrections  $O(\rho^8)$ , such an asymptotic matrix  $H^{\text{eff}}$  remains energy-independent and may be still interpreted as a smoothly truncated approximation of the exact Hamiltonian which has a finite dimension. It is interesting to compare this approximation with the structure of the wavefunctions which cannot be approximated by their finite-dimensional sections with sufficient precision.

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