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Fixed-point perturbation theory and the potential $r^2+\lambda r^2/(1+gr^2)$: II. Construction of the solutions

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Abstract. We construct the asymptotic power-series expansions of the Green function and wavefunctions for the $\lambda r^2/(1+gr^2)$ anharmonic oscillator. As a new form of the fixed-point perturbative formalism, the method may be extended to any band-matrix Hamiltonian in principle—our results illustrate its algebraic flexibility as well as a quick numerical convergence.

1. Introduction

In the harmonic-oscillator basis $|n\rangle$, $n=0,1,\ldots$, the Schrödinger eigenvalue problem

$$H\psi = E\psi \tag{1.1}$$

with the Hamiltonian $H=H_0$ (harmonic oscillator) $+\lambda r^2/(1+gr^2)$ may be formulated as the linear three-term recurrence

$$\begin{aligned}
&b_{k-1}z_{k-1}+a_kz_k+b_kz_{k+1}=0\\
&z_k=(\varepsilon_k-E+\lambda/g)\langle k|\psi\rangle,\\
&\varepsilon_k=4k+2l+3, \qquad l=\ -1,0 \text{ or } l=0,1,\ldots\\
&a_k=\tfrac{1}{2}g\varepsilon_k+1-\lambda(\lambda+g\varepsilon_k-gE)^{-1}\\
&b_{k-1}=gk^{1/2}(k+l+\tfrac{1}{2})^{1/2}, \qquad k=0,1,\ldots
\end{aligned} \tag{1.2}$$

accompanied by the physical normalisability requirement or asymptotic boundary condition

$$z_N/z_{N-1}=1-(gN)^{-1/2}+\mathrm{O}(1/N), \qquad N\gg 1 \tag{1.3}$$

(Znojil 1983). We may also denote $z_n/z_{n-1}=b_{n-1}f_n$, i.e.,

$$z_n=z_0b_0f_1b_1f_2\ldots b_{n-1}f_n, \qquad n=1,2,\ldots \tag{1.4}$$

and interpret (1.2) as the nonlinear two-term recurrences

$$f_k^{-1}=a_k-b_k^2f_{k+1} \tag{1.5}$$

with an arbitrary initialisation f_{N+1}, $N\to\infty$, and with the physical requirement

$$f_0^{-1}=0 \tag{1.6}$$

determining the bound-state energies.

In the eigenvalue condition (1.5) and (1.6), i.e.,

$$0 = a_0 - b_0^2 \cfrac{1}{a_1 - b_1^2 \cfrac{1}{a_2 - \dots}} \tag{1.7}$$

we may accelerate the continued-fractional convergence via the asymptotic estimates $f_n \sim h_n^{(0)} \sim f_{n+1}$ and subtractions (redefinitions)

$$f_n^{(1)} = f_n - h_n^{(0)}. \tag{1.8}$$

When performed in an iterative way, this is the essence of our fixed-point perturbation theory (FPPT, Znojil 1984a) in application to our particular anharmonic oscillator (1.1) (Znojil 1984b, hereafter referred to as I).

In more detail, the eigenvalue condition

$$0 = a_0 - b_0^2 \cfrac{1}{a_1 - \dots \cfrac{1}{a_N - b_N^2 f_{N+1}^{(\mathrm{FPPT})}}} \tag{1.9}$$

with a fixed dimension parameter $N < \infty$ and FPPT series

$$f_{N+1}^{(\mathrm{FPPT})} = \sum_{m=1}^{M} h_{N+1}^{(m-1)}, \qquad M \to \infty \tag{1.10}$$

generalises the trivial $M = 0$ truncation prescription (use of the finite continued-fractional approximants). In I, the FPPT expansion (1.10) has been shown to converge in the $M \to \infty$ limit.

Our present purpose is to simplify the construction of the FPPT series and to remove its two principal shortcomings.

(1) *Ambiguity.* The separate FPPT contributions $h_{N+1}^{(m-1)}$ may be defined by the various non-equivalent recurrent algebraic prescriptions, differing possibly in the resulting rate of convergence.

(2) *Complicated structure.* The perturbation contributions are roots of quadratic equations—they may become complex for $M > M_0$ in general.

Our considerations will be inspired by an observation that from the practical point of view, many sophisticated definitions of the leading-order fixed-point approximant $h_{N+1}^{(0)}$ do not work much better than the simplest estimate (1.3) (cf, e.g., equation (3.10) in I). Thus, we may try to rearrange the infinite series (1.10) into as simple form as possible—this will be done in § 2. In § 3, a similar rearrangement of the product formula (1.4) for wavefunctions will generalise the first-order difference-equation reinterpretation of (1.3),

$$\Delta \ln \dot{z}_N = \ln z_N - \ln z_{N-1} = \ln[1 - (gN)^{-1/2} + \mathrm{O}(N^{-1})] = -(gN)^{-1/2} + \mathrm{O}(N^{-1}) \tag{1.11}$$

and its simple asymptotic solution

$$z_N \approx \exp[-2(N/g)^{1/2}], \qquad N \gg 1 \tag{1.12}$$

(cf e.g. Korn and Korn 1968). Finally, the whole formalism will be tested numerically by the evaluation of energies in § 4.

2. Rederivation of the Green function

2.1. The rearrangement of the fixed-point expansion

Let us consider the first-order FPPT prescription

$$h_N^{(0)} = (2b_N b_{N-1})^{-1}[a_N - (a_N^2 - 4b_N b_{N-1})^{1/2}] \tag{2.1}$$

(I, equation (3.12)) and expand it in the powers of N^{-1} in the $N \gg 1$ asymptotic region. Immediately, we shall find that

$$h_N^{(0)} = \text{constant } N^{-1} + \text{constant}' \, (N\sqrt{N})^{-1} + \dots \tag{2.2}$$

This is due to the leading-order cancellations taking place in the square-rooted parenthesis in (2.1). Similar cancellations do not appear in $h_N^{(1)}, h_N^{(2)}, \dots$, so that the general FPPT expansion will have the asymptotic structure

$$\text{constant } N^{-1} + \text{constant}' \, N^{-3/2} + \text{constant}'' \, N^{-2} + \text{constant}''' \, N^{-5/2} + \dots \tag{2.3}$$

and we may write, with an arbitrary shift of the indices δ,

$$f_k = \sum_{m=0}^{\infty} \varphi_m (k+\delta)^{-1-m/2} \tag{2.4}$$

2.2. A power-series solution of the nonlinear recurrences for f_n

It is not necessary to derive (2.4) from (1.10). Indeed, once we derive the structure (2.3) of f_{N+1} from its FPPT background (cf (2.1) and I), we may employ (2.4) simply as an ansatz solving the recurrences (1.5), and require that $f_k^{(1)} = 0$ in (1.8) identically.

It is a rather cumbersome algebra to find the sequence φ_n in general. Fortunately the present three-term character as well as the simple form of coefficients in (1.2) may be employed.

In the first step, we introduce the denotation

$$\begin{aligned} &\rho^2 = k+\delta, \qquad \delta = \tfrac{1}{4}(2l+3-E+\lambda g^{-1}) \\ &a_k = 2g\rho^{-2} + \beta + \gamma\rho^2, \qquad b_k^2 = g^2\rho^{-4} + \mu\rho^{-2} + \nu, \\ &\beta = 1 + \tfrac{1}{2}(gE-\lambda), \qquad \gamma = -\tfrac{1}{4}\lambda g^{-1}, \qquad \mu = g^2[1+\tfrac{1}{2}(E-\lambda g^{-1})] \\ &\nu = \tfrac{1}{4}\mu^2 g^{-2} - g^2(\tfrac{1}{2}l+\tfrac{1}{4})^2 \end{aligned} \tag{2.5}$$

which simplifies the recurrences (1.5) in the asymptotic region. Next, we recall the easily obtainable identities

$$\frac{1}{f_k} = \sum_{m=0}^{\infty} \frac{\psi_m}{(k+\delta)^{-1+m/2}}, \qquad \psi_0 = 1/\varphi_0$$

$$\psi_m = \frac{(-1)^m}{\varphi_0^{m+1}} \det \begin{pmatrix} \varphi_1 & \varphi_2 & \dots & \varphi_m \\ \varphi_0 & \varphi_1 & \dots & \varphi_{m-1} \\ 0 & \varphi_0 & \dots & \varphi_{m-2} \\ \dots & & & \\ 0 & 0 & \dots & \varphi_1 \end{pmatrix}, \qquad m = 1, 2, \dots \tag{2.6}$$

and

$$f_{k+1}=\sum_{n=0}^{\infty}\frac{\varphi_n}{(k+1+\delta)^{1+n/2}}=\sum_{m=0}^{\infty}\rho^{m+2}D_m$$

$$D_m=\sum_{t=0}^{[m/2]}\varphi_{m-2t}C^{(t,m-2t)} \tag{2.7}$$

$$C^{(m,n)}=\frac{(-1)^m}{m!}\frac{\Gamma(1+m+\frac{1}{2}n)}{\Gamma(1+\frac{1}{2}n)}$$

and insert them into (1.5). Finally, the term-by-term comparison of coefficients at the same powers of ρ generates the sequence of restrictions

$$m=0, \qquad \varphi_0^{-1}=2g-g^2\varphi_0$$

$$m>0, \qquad \frac{(-1)^m}{\varphi_0^{m+1}}\det\begin{pmatrix}\varphi_1 & \cdots & \varphi_m\\ \varphi_0 & \cdots & \varphi_{m-1}\\ \cdots & & \\ 0 & \cdots & \varphi_1\end{pmatrix}=\beta\delta_{m,2}+\gamma\delta_{m,4} \tag{2.8}$$

$$-g^2D_m-\mu D_{m-2}-\nu D_{m-4}, \qquad D_{-1}=D_{-2}=\ldots=0$$

imposed on the coefficients φ_n in (2.4).

From the first $m=0$ item, we get the degenerate quadratic equation with a unique root

$$\varphi_0=g^{-1}. \tag{2.9}$$

For $m=1$, (2.8) becomes an algebraic identity. The next $m=2$ item defines

$$\varphi_1=-g^{-3/2} \tag{2.10}$$

where the sign is not unique but it must be chosen in accord with the normalisability requirement (1.3).

Starting from $m=3$, we may observe that the $\varphi_m\times$constant components cancel and drop out of (2.8). Thus, we may eliminate

$$\varphi_2=\tfrac{1}{2}g^{-2}+\tfrac{1}{4}(1-E+\lambda g^{-1})g^{-1} \tag{2.11}$$

etc. In general, the algebraic definition (2.8) of φ_{m-1} in terms of $\varphi_{m-2}, \varphi_{m-3}, \ldots$ has the explicit and linear recurrent form

$$\varphi_{m-1}=\frac{(-1)^{m-1}}{2\varphi_1\varphi_0^{m-2}}\det\begin{pmatrix}\varphi_1 & \varphi_2 & \cdots & \varphi_{m-2} & 0 & 0\\ \varphi_0 & \varphi_1 & \cdots & \varphi_{m-3} & \varphi_{m-2} & 0\\ 0 & \varphi_0 & \cdots & \varphi_{m-4} & \varphi_{m-3} & \varphi_{m-2}\\ & \cdots & & & & \\ 0 & 0 & \cdots & 0 & \varphi_0 & \varphi_1\end{pmatrix}+\frac{\varphi_0^3}{2\varphi_1}(\beta\delta_{m,2}+\gamma\delta_{m,4})$$

$$-\frac{\varphi_0^3}{2\varphi_1}\sum_{t=1}^{[m/2]}\varphi_{m-2t}(g^2C^{(t,m-2t)}+\mu C^{(t-1,m-2t)}+\nu C^{(t-2,m-2t)}), \tag{2.12}$$

$$m=3,4,\ldots,M.$$

In this way, our construction of the modified FPPT series with the power-law dependence on the index k or $k+\delta$ is completed.

3. Resummation of the wavefunctions

We may insert expansion (2.7) into the definition (1.4) of ψ and, in the spirit of the Trotter formula for exponentials, rearrange this product also into an expansion

$$\langle n|\psi\rangle = (-1)^n c_1 (n+\delta)^{c_2} \exp\left((n+\delta)^{c_3} \sum_{m=0}^{\infty} c_{4+m}/(n+\delta)^{m/2}\right). \tag{3.1}$$

The coefficients c_i may then be determined from the consistency of (3.1) with the recurrence (1.2)—this idea has been used recently by Richardson and Blankenbecler (1979) in a somewhat different context.

In the present case, the coefficients c_i may be obtained also immediately from (1.4)—we put

$$\langle n+1|\psi\rangle/\langle n|\psi\rangle = -(n+\delta)b_n f_{n+1}/(n+1+\delta) \tag{3.2}$$

and insert (2.7) and (3.1) on the right- and left-hand sides, respectively. Then, it is sufficient to compare the expressions at the same powers of $(n+\delta)^{-1/2}$.

3.1. *Recurrences as a difference equation*

In an alternative and direct formulation, the resummation (3.1) of ψ may be based on (1.2) rewritten as an equation

$$b_{k-1}\xi[\mu(k)-1] - a_k\xi[\mu(k)] + b_k\xi[\mu(k)+1] = 0 \qquad k = 0, 1, \dots \tag{3.3}$$

for the smooth functions $\xi(\mu) = (-1)^k z_k$ of the shifted and presumably continuous variable $\mu = \mu(k) + \frac{1}{2}l + \frac{3}{4}$.

In the first step, we replace $\xi(\mu \pm 1)$ by the Taylor series

$$\xi(\mu \pm 1) = \xi(\mu) \pm \xi'(\mu) + (1/2!)\xi''(\mu) \pm \dots = \exp(\pm \mathrm{d}/\mathrm{d}\mu)\xi(\mu)$$

and decompose the coefficients in (3.3) into the odd and even functions of μ. Then, with the abbreviations

$$\mu_\pm = \mu \pm \tfrac{1}{2}, \qquad \beta_\pm = (1-\gamma/\mu_\pm^2)^{1/2}, \qquad \gamma = \tfrac{1}{4}(l+\tfrac{1}{2})^2,$$

$$\beta = \beta_+ + \beta_-, \qquad \sinh(\mathrm{d}/\mathrm{d}\mu) = \mathrm{d}/\mathrm{d}\mu + (1/3!)\,\mathrm{d}^3/\mathrm{d}\mu^3 + \dots$$

etc, we get

$$\begin{aligned}\left(\frac{1}{2\mu}\beta + \frac{2\mu}{\beta}\cdot\frac{\gamma}{\mu_+^2\mu_-^2}\right)\sinh\left(\frac{\mathrm{d}}{\mathrm{d}\mu}\right)\xi(\mu) + \left(\beta + \frac{1}{\beta}\cdot\frac{\gamma}{\mu_+^2\mu_-^2}\right)\cdot 2\sinh^2\left(\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\mu}\right)\xi(\mu) \\ = \left[\frac{1}{g\mu}\left(1 - \frac{\lambda/g}{4\mu+\lambda/g-E}\right) + \left(\frac{\mu_-^2}{1+\beta_+} + \frac{\mu_+^2}{1+\beta_-} - \frac{1}{\beta}\right)\frac{\gamma}{\mu_+^2\mu_-^2}\right]\xi(\mu)\end{aligned} \tag{3.4}$$

from (3.3).

In the next step, we put $\xi(\mu) = \exp\chi(\mu)$ and notice that $|\chi(\mu)| = \mathrm{O}(\mu^{1/2}) \ll \mu$ for $\mu \gg 1$ (cf (1.12)). Hence, the derivatives

$$\xi' = \chi'\xi, \qquad \xi'' = (\chi'^2 + \chi'')\xi, \qquad \xi''' = (\chi'^3 + 3\chi'\chi'' + \chi''')\xi, \dots$$

form a decreasing sequence for a sufficiently large μ,

$$\xi' = \mathrm{O}(\xi/\mu^{1/2}), \qquad \xi'' = \mathrm{O}(\xi/\mu^{3/2}), \dots$$

and we may treat (3.4) as a nonlinear differential equation (of an infinite order) for the functions $\chi'(\mu)$ (χ drops out). We may solve it simply by the power-law series ansatz

$$\chi'(\mu)=\sum_{m=1}^{\infty}\frac{d_m}{\mu^{m/2}}. \tag{3.5}$$

The step-by-step comparison of coefficients at the increasing powers of $\mu^{1/2}$ gives immediately the solution d_m again.

3.2. FPPT as differential equations

As an illustration of the necessary algebra, let us neglect the $O(\mu^{-5})$ components in (3.4). Such a truncation converts (3.4) (in the $\mu \gg 1$ asymptotic region) into the linear differential equation of the eighth order,

$$\left(\frac{1}{\mu}+\frac{\gamma}{2\mu^3}\right)\left(\xi^{(1)}+\frac{1}{3!}\xi^{(3)}+\frac{1}{5!}\xi^{(5)}+\frac{1}{7!}\xi^{(7)}\right)$$
$$+\left(2-\frac{\gamma}{\mu^2}\right)\left(\frac{1}{2!}\xi^{(2)}+\frac{1}{4!}\xi^{(4)}+\frac{1}{6!}\xi^{(6)}+\frac{1}{8!}\xi^{(8)}\right)$$
$$=\left[\frac{1}{g\mu}\left(1-\frac{\lambda/g}{4\mu+\lambda/g-E}\right)+\frac{\gamma}{\mu^2}+\frac{\gamma(\gamma+1)}{4\mu^4}+O\left(\frac{1}{\mu^5}\right)\right]\xi \tag{3.6}$$

or, subsequently, into a nonlinear differential equation for the derivative of χ. Finally, via (3.5), we arrive at an explicit algebraic hierarchy of definitions of the coefficients d_n for $n=1,2,\ldots,8$.

For the determination of d_1, it suffices to use the simplest non-trivial truncation of (3.4),

$$d^2\xi(\mu)/d\mu^2=[(g\mu)^{-1}+O(\mu^{-3/2})]\xi(\mu) \qquad \mu\gg 1 \tag{3.7}$$

or

$$\chi''+\chi'^2=(g\mu)^{-1}+O(\mu^{-3/2}).$$

The insertion of (3.5) gives $d_1^2=g^{-1}$ and we choose the negative sign,

$$d_1=-g^{-1/2} \tag{3.8}$$

for the normalisable solutions.

In the next asymptotic order, we have to include only the term $\xi'\mu^{-1}$ in (3.7). This implies immediately that

$$d_2=-\tfrac{1}{4}. \tag{3.9}$$

On the forthcoming level of precision, we must consider the differential equation of the fourth order

$$\tfrac{1}{12}\xi^{(4)}+\xi^{(2)}+\mu^{-1}\xi^{(1)}=[(g\mu)^{-1}+(\gamma-\lambda/4g^2)\mu^{-2}]\xi \tag{3.10}$$

and its nonlinear counterpart

$$\chi''+\chi'^2+\mu^{-1}\chi'+\tfrac{1}{12}\chi'^4=(g\mu)^{-1}+(\gamma-\lambda/4g^2)\mu^{-2} \tag{3.11}$$

with an $O(\mu^{-5/2})$ error term. We get

$$d_3=\tfrac{1}{8}g^{1/2}[(\lambda+\tfrac{1}{3})g^{-2}-l(l+1)]. \tag{3.12}$$

Finally, it is sufficient to add $\frac{1}{6}\xi^{(3)}\mu^{-1}$ to (3.10) or $\frac{1}{2}\chi'^2\chi''+\frac{1}{6}\mu^{-1}\chi'^3$ to (3.11) and the fifth-order coefficient

$$d_4=\tfrac{1}{16}g[(1-\lambda)g^{-2}+l(l+1)] \tag{3.13}$$

follows.

We shall stop our algebraic manipulations here since their general pattern becomes obvious now: in the $(2k-1)$th step, we must incorporate the $2k$th derivatives of $\xi(\mu)$. The final formula has the form

$$\xi(\mu)=\exp\left[2d_1\sqrt{\mu}+d_2\ln\mu-\sum_{m=1}^{\infty}\frac{2d_{m+2}}{m\mu^{m/2}}\right]. \tag{3.14}$$

In the old notation, the above fifth-order FPPT asymptotic expansion of our wavefunctions reads

$$\begin{aligned}\langle n|\psi\rangle &= \text{constant}\frac{(-1)^n}{\varepsilon_n^{1/4}}\cdot\frac{\exp[-(\varepsilon_n/g)^{1/2}]}{\varepsilon_n-E+\lambda/g}\\ &\quad\times\exp\{[-\tfrac{1}{2}(\lambda+\tfrac{1}{3})g^{-3/2}+\tfrac{1}{2}l(l+1)g^{1/2}]\varepsilon_n^{-1/2}\}\\ &\quad\times\exp\{[\tfrac{1}{4}(\lambda-1)g^{-1}-\tfrac{1}{4}gl(l+1)]\varepsilon_n^{-1}\}\times\exp \mathrm{O}(\varepsilon_n^{-3/2}).\end{aligned} \tag{3.15}$$

This is a quite simple formula.

Equation (3.15) may be used also in a rederivation of (2.7) up to the coefficient φ_4. From (3.2), we get the exponential formula

$$\begin{aligned}f_{n+1} &= (1-4/\varepsilon_{n+1})^{1/4}b_n^{-1}\exp\{-4/[\sqrt{g}(\sqrt{\varepsilon_n}+\sqrt{\varepsilon_{n+1}})]\}\\ &\quad\times\exp\{-4d_3/[\sqrt{\varepsilon_n}\sqrt{\varepsilon_{n+1}}(\sqrt{\varepsilon_n}+\sqrt{\varepsilon_{n+1}})]\}\\ &\quad\times\exp(-4d_4/\varepsilon_n\varepsilon_{n+1})\exp[\mathrm{O}(\varepsilon_n^{-5/2})].\end{aligned} \tag{3.16}$$

Its explicit energy-independence contrasts with (2.7) but is in full accord with the strong asymptotic suppression of E in the matrix elements a_k in (1.2) or (1.5).

4. Energies

In principle, a quickly convergent and numerically stable computational scheme for energies may be based on the FPPT secular equation (1.9) complemented by the FPPT asymptotic expansion (1.10) of the auxiliary 'effective interaction' quantity f_{N+1} as discussed in I. In practice, the recurrently specified prescriptions (2.7) and (2.12) simplify the computer coding and the other technicalities. Thus, we may employ any small computer and control the precision of energies (zeros of f_0^{-1}) in two ways—by our choice of the model-space dimension N, and by the order M of our FPPT approximation, i.e., number of terms retained in (2.7).

In table 1, a sample of results is displayed. In accord with most of the literature, we consider the one-dimensional problem (1.1) with even parity ($l=-1$) and with the following parameters:

(A) $\lambda=0.1$, $g=100$, $E_{\text{exact}}=1.000\,841\,100$ (Bessis and Bessis 1980),
(B) $\lambda=1$, $g=10$, $E_{\text{exact}}=1.059\,290$ (Mitra 1978),
(C) $\lambda=10$, $g=1$, $E_{\text{exact}}=2.782\,330$ (Mitra 1978),
(D) $\lambda=100$, $g=0.1$, $E_{\text{exact}}=9.976\,180\,088$ (Znojil 1983),

(E) $\lambda = g = 1$, $E_{\text{exact}} = 1.232\,350\,740$ (Znojil 1983),
(F) $\lambda = g = 10$, $E_{\text{exact}} = 1.580\,020$ (Mitra 1978),
(G) $\lambda = g = 100$, $E_{\text{exact}} = 1.836\,380\,500$ (Znojil 1983),
(H) $\lambda = g = 100$, $E_{\text{exact}} = 5.928$ (Mitra 1978, excited state).

These examples lead to the following observations.

(i) For $M = 0$, the zero-order FPPT approximation is defined as trivial, $f_{N+1} = 0$. It corresponds in effect to the N-dimensional truncation and standard numerical diagonalisation of the matrix. For the ground-state energy, we obtain the rigorous (variational) upper bound which converges to E_{exact} with the increasing N (see A).

(ii) With increasing FPPT order M, we may notice a 'bracketing' (majorisation/minorisation) property of the neighbouring approximants. Its geometric origin has been clarified in I. In examples B and C, it enables us also to estimate roughly the round-off error as contained in the less precise values E_{exact} of Mitra (1978).

(iii) Our FPPT energies converge with increasing M not only for $(gN)^{-1} \ll 1$, but also far beyond this 'natural' domain of convergence (cf e.g., D in the table).

Table 1. Convergence of energies—a sample of deviations $(E_{\text{computed}} - E_{\text{exact}}) \times 10^9$ in the Mth perturbative order and N-dimensional model space.

Example	M \ N				
	N	2	3	4	
A	0	37 591	29 548	24 426	
	1	−9713	−9064	−8513	
	2	−80	−32	−8	
	3	−318	−216	−157	
	N	25	50	75	
A	0	4734	1987	977	
	1	−3491	−1669	−915	
	2	10	3	1	
	3	−9	−2	−0.5	
	N	10	15	20	
B	0	475 645	200 379	96 735	
	1	−483 663	−205 025	−97 665	
	2	14 139	6182	3626	
	3	−1446	+831	+1421	
	N	10	20	30	
C	0	758 636	16 215	423	
	1	−235 861	−3255	+96	
	2	184 125	4791	+600	
	3	−78 662	+459	+505	
	N	15	20	25	30	50
D	0	−11 799	−1996	−316	−53	−0.047
	1	−11 205	−1843	−313	−49	−0.039
	2	−11 419	−1880	−307	−49	—
	3	−10 613	−1746	−282	−46	—

Table 1. (continued)

	M \ N	10	20	30	
E	−1	−31 816	−175	−13	
	0	12 223	74	−8	
	1	−14 257	−106	−12	
	2	1689	−2	−10	
	3	−347	−11	−10	
	N	30	40	50	
F	0	335 145	117 979	46 917	
	1	−313 242	−110 481	−43 476	
	2	15 361	5096	2207	
	3	−451	+339	+531	
	N	20	50	100	500
G	0	5895 986	2110 481	577 913	601
	1	−3607 723	−1813 398	−1001 019	−18 557
	2	339 924	100 691	9367	−3060
	3	−42 760	−7 871	−5056	−4932
	N	50	100	500	
H	0	78 510	22 903	2075	
	1	1279 096	−625 476	+1415	
	2	−117 765	−16 110	+2002	
	3	4004	2048	2197	

(iv) At a fixed M, say, $M = 1$, our approximants seem to form the energy bounds (lower, 'antivariational' for $M = 1$) not only at $N \gg 1$, but also in a 'non-asymptotic' domain (say, for $N = O(10)$). Thus, the lower bounds of Znojil (1983) may be interpreted as a '$M = -1$' item in table 1 (see E).

(v) The FPPT convergence deteriorates for large λ (see E–G). This may be compensated easily by our choice of a larger dimension N or order M. The precision of our $M = 3$ energies compares favourably with the other methods in a wide range of anharmonicities. For example, our $M = 3$ and $N = 4$ result A reproduces the precision of the $M = -1$ and $N = 300$ value as obtained in Znojil (1983).

(vi) The precision of energies seems to increase for the excited states (see H). This is not yet fully understood.

5. Summary

We have reformulated the algebraic constructions of I and arrived at an extremely compact form of the corresponding solution of (1.1). Due to an analytic simplicity of the new higher-order FPPT corrections, their direct use seems to be a vital improvement of the older (truncation and/or majorisation and minorisation) algorithms. Its numerical tests confirm the particular practical efficiency of the FPPT formulae, especially for the large couplings.

Complementing the more or less geometric considerations of I, our main idea was now to employ the knowledge of the asymptotic behaviour of f_{N+1} ('effective Hamiltonian') in a direct solution of recurrences via the related power-series ansatz. It has a broader methodical significance—its further applications are under current investigation at present.

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