Partial sums and optimal shifts in
shifted large-\(\ell\) perturbation expansions
for quasi-exact potentials

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Abstract

For the \(N\)-plets of bound states in a quasi-exactly solvable (QES) toy model (sextic oscillator), the spectrum is known to be given as eigenvalues of an \(N\) by \(N\) matrix. Its determination becomes purely numerical for all the larger \(N > N_0 = 9\). We propose a new perturbative alternative to this construction. It is based on the fact that at any \(N\), the problem turns solvable in the limit of very large angular momenta \(\ell \to \infty\). For all the finite \(\ell\) we are then able to define the QES spectrum by convergent perturbation series. These series admit a very specific rational resummation, having an analytic or branched continued-fraction form at the smallest \(N = 4\) and 5 or \(N = 6\) and 7, respectively. It is remarkable that among all the asymptotically equivalent small expansion parameters \(\mu \sim 1/(\ell + \beta)\), one must choose an optimal one, with unique shift \(\beta = \beta(N)\).

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1 Introduction

The $D$–dimensional and central Schrödinger bound-state problem

$$[-\Delta + V(|\vec{r}|)] \Psi(\vec{r}) = \mathcal{E} \Psi(\vec{r})$$

finds its applications as an approximate model in nuclear physics [1] as well as in quantum chemistry [2] and atomic physics [3]. Last but not least, it is encountered as a popular exercise in textbooks on quantum mechanics [4]. In all these cases, the main mathematical merit of the model (1) lies in its separability, i.e., reducibility to the set of the ordinary (so called radial) differential equations

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} + V(r)\right] \psi(r) = \mathcal{E} \psi(r), \quad \ell = (D - 3)/2 + m, \quad m = 0, 1, \ldots \, .$$

They are all easily solvable by any standard numerical technique [5].

Whenever we need a non-numerical solution, we must restrict the class of our potentials $V(|\vec{r}|)$ to a subset which is exactly solvable (ES, say, harmonic-oscillator) or at least quasi-exactly solvable (QES, see, e.g., the monograph [6] for a thorough review). Of course, the real appeal of any ES or QES potential derives from an agreement of its shape or spectrum with some “more realistic” numerical model $V[\text{phys}](|\vec{r}|)$. In this sense, many practical applications of the ES subset are marred by its comparatively small size and, hence, by a very narrow variability of the available shapes of $V[\text{ES}](|\vec{r}|)$ (cf., e.g., ref. [7] for their representative list). In parallel, the wealth of the forms of the multi-parametric wells $V[\text{QES}](|\vec{r}|)$ may happen to be more than compensated by the much more complicated tractability of their perturbations [8]. Moreover, even the very zero-order QES constructions may become quite complicated, whenever the size $N$ of the required QES multiplet leaves the domain of $N \leq N_0$ where the practical determination of the spectrum remains non-numerical [9]. Although the latter remark sounds like a paradox, one must keep in mind that even in the simplest QES models, the explicit construction of the larger QES multiplets with $N > N_0$ requires the more or less purely numerical diagonalization of asymmetric $N$ by $N$ matrices (see below). In purely pragmatic terms, many closed
QES constructions [10, 11] are in fact more difficult than an immediate numerical solution of the differential Schrödinger eq. (1) itself.

In what follows we shall argue that it is possible to avoid the latter brute-force methods even in the QES domain where $N > N_0$. We shall recommend the use of the so called large-$\ell$ (or large-$D$ [12]) expansion philosophy [13] in its new implementation which takes into account several specific features of QES models. We shall reduce all the inessential technicalities to a necessary minimum and restrict our attention just to one of the most elementary illustrative QES examples

$$V^{[\text{QES}]}(|\vec{r}|) = a |\vec{r}|^2 + c |\vec{r}|^6, \quad c = \gamma^2 > 0$$

which is known to possess an elementary $N$-plet of QES solutions at any $N$ [14]. On the background of this example we shall start our considerations in section 2 by showing that due to the absence of the quartic term in eq. (2), the QES solvability conditions are transparent and instructive (cf. subsection 2.1). In subsection 2.2 we show how these conditions simplify even the standard large-$\ell$ perturbation expansions of the spectrum where one uses just an asymptotic, $\ell \gg 1$ simplification of the differential Schrödinger equation (1). In section 2.3 we add that in the more specific, QES-related setting, the algebraic construction of the solutions might be preferrable, at least due to its amazingly transparent form.

The latter expectations are more than confirmed in the subsequent section 3. After a step-by-step analysis of the QES secular equations for the energies in dependence on the growing dimension $N$, we are able to reveal their general polynomial structure and perturbation form. The first subsection 3.1 shows that the models with $N \leq 3$ are all fully solvable via an elementary re-scaling of the matrix secular equation. Formally, our presently conjectured “optimally shifted” large-$\ell$ series remain trivial in this case. The zero-order result is exact and its secular polynomial does not contain any perturbation. All the higher-order corrections simply vanish. Still, the structure of the $N = 3$ secular equation is already rich enough to illustrate, why the “optimal” value of the shift of $\ell \gg 1$ is so exceptional, and how a return to its “non-optimal” values would re-introduce non-vanishing perturbation corrections.
In subsection 3.2, some of these observations are re-confirmed at $N = 4$. Elementary analysis offers the explanation why our “optimally shifted” large-$\ell$ power series are convergent. The determination of the explicit value of the radius of convergence $\mu_{\text{max}}$ reveals that the circle of convergence covers the whole domain of physical interest, i.e., formally, all the positive spatial dimensions $D > 0$.

Subsection 3.3 uses the slightly modified $N = 5$ example and shows that a Padé-like re-summation of our power series exists. The “re-summed” energies $E$ (as well as their squares $\Omega = E^2$) acquire an analytic continued-fraction form.

In subsection 3.4, the “first nontrivial” example is shown to emerge at $N = 6$. We sample there the energies in their “generalized” or “branched” continued-fraction form as well as in their more standard power-series representation. A few questions concerning their convergence are clarified.

In subsection 3.5, an extrapolation of all the preceding constructions to any size $N$ of the QES multiplets is described and discussed. For quadruplets of $N = 4K, 4K + 1, 4K + 2$ and $4K + 3$, our main result is formulated as an iterative $K$–term formula for the systematic construction of the energies in a generalized continued-fraction form. Simultaneously, the Taylor-expansion technique is shown to generate the standard power series with the “optimally shifted” large-$\ell$ perturbation structure. The last illustrations are added showing the smoothness of transition from the “last solvable” $N \leq N_0 = 9$ to “the first unsolvable” $N = 10$.

In section 4 a thorough re-interpretation of our optimally shifted large-$\ell$ perturbation series is given in the more standard language of the textbook Rayleigh-Schrödinger perturbation theory. Once more we summarize our approach in the last section 5, as a source of new types of perturbation expansions tailored for the computation of the QES spectra at any multiplet size $N$. 
2 Conditions of quasi-exact solvability

2.1 Toy model: sextic oscillator

Sextic oscillator (2) may support elementary bound states

$$\psi(r) = \sum_{n=0}^{N-1} h_n r^{2n+\ell+1} \exp\left(-\frac{1}{4}\gamma r^4\right)$$

provided only that we choose one of the couplings in consistent manner [14],

$$a = a(N) = -\gamma (4N + 2\ell + 1).$$

The latter condition increases a phenomenological appeal of our example by assigning to potential (2) the manifestly non-perturbative double-well shape. Many computational difficulties of “realistic” calculations may be mimicked, even within such a framework, whenever one chooses a larger degree \(N\) in wave function (3). Integer \(N\) measures the “dimension” of our problem since, under the constraint (4) and after the insertion of (3), our differential Schrödinger equation (1) is transformed into equivalent matrix problem

$$\begin{pmatrix}
0 & C_0 \\
A_1 & 0 & C_1 \\
& \ddots & \ddots \\
& & \ddots & \ddots \\
& & & A_{N-2} & 0 & C_{N-2} \\
&&& & A_{N-1} & 0
\end{pmatrix}\begin{pmatrix}
h_0 \\
h_1 \\
\vdots \\
h_{N-2} \\
h_{N-1}
\end{pmatrix} = \mathcal{E}\begin{pmatrix}
h_0 \\
h_1 \\
\vdots \\
h_{N-2} \\
h_{N-1}
\end{pmatrix}.$$  \hspace{1cm} (5)

The matrix of this system is asymmetric,

$$A_n = -4\gamma (N-n), \quad C_n = -2(n+1)(2n+2\ell+3), \quad n = 0, 1, \ldots$$

so that up to the first few lowest dimensions \(N\), equation (5) need not be easy to solve at all. The advantages gained by the polynomiality of \(\psi\) may be quickly lost with the growth of their degree \(N\). The merits of the “exceptional” QES levels seem to disappear in the domain of the larger \(N \gg 1\). However, these states may
“remember” and share some features of the completely solvable harmonic oscillator.
In this sense, our oversimplified toy example may serve as a guide towards a future better understanding of the partially solvable Schrödinger equations with more free parameters [11].

2.2 Large-\(\ell\) domain in coordinate representation

For our particular QES model of section 2.1, the radial Schrödinger eq. (1),

\[
\left[ -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} - \gamma (4N + 2\ell + 1) r^2 + \gamma^2 r^6 \right] \psi(r) = E \psi(r),
\]

may be treated by the so called \(1/N\) (i.e., in the present notation, \(1/\ell\)) expansions along the lines recommended in the recent review [15]. This approach visualizes the Hamiltonian in eq. (7) as composed of an “effective” kinetic energy in one dimension and of an “effective” one-dimensional potential well \(V_{\text{eff}}(r)\) with a steep and repulsive peak near the origin and also with a confining growth at large \(r\). Its minimum is unique and may be localized at the point

\[
r = R(\ell) = \left( \frac{4N + 2\ell + 1 + \Delta(\ell)}{6\gamma} \right)^{1/4},
\]

\[
\Delta(\ell) = \sqrt{16N^2 + 16N\ell + 8N + 16\ell^2 + 16\ell + 1}.
\]

At an illustrative strength \(\gamma = 1\) and for the simplest \(N = 0\) we have

\[
V_{\text{eff}}(r) = \left( \frac{\ell^2}{r^2} - 2\ell r^2 + r^6 \right) [1 + \mathcal{O}(1/\ell)] = 16\ell [r - R(\ell)]^2 + 16\ell^{3/4} [r - R(\ell)]^3 + \ldots.
\]

As long as the position of the minimum grows with \(\ell\) (or \(D\)) to its asymptotically leading-order value \(R(\ell) = (\ell/\gamma)^{1/4}(1 + \mathcal{O}(1/\ell))\) (note that we switched to \(\gamma = 1\) temporarily), we may abbreviate \(r - R(\ell) = \xi/(2\ell^{1/4})\) and replace our Schrödinger equation (7) by its \(\ell \gg 1\) asymptotically equivalent anharmonic-oscillator form

\[
\left[ -\frac{d^2}{d\xi^2} + \xi^2 + \frac{1}{2\sqrt{\ell}} \xi^3 + \frac{5}{16\ell} \xi^4 + \mathcal{O}\left( \frac{\xi^5}{\ell^{3/2}} \right) \right] \phi(\xi) = \frac{E}{4\sqrt{\ell}} \phi(\xi)
\]
In terms of perturbation theory, the leading-order energies coincide with a re-scaled equidistant spectrum of harmonic oscillator,

$$\mathcal{E} = 4 \sqrt{\ell} (2n + 1) \left[1 + \mathcal{O}(1/\sqrt{\ell})\right], \quad n = 0, 1, \ldots \quad (10)$$

All the higher-order corrections may be computed in systematic manner, leading to an asymptotic, divergent [15] power series in $\lambda = \mathcal{O}(1/\sqrt{\ell})$. In our present paper, we are going to replace them by convergent series in the powers of $\lambda^4$.

### 2.3 Large–$\ell$ Domain in Matrix Representation

Partially, our present paper has been motivated by all the realistic models (1) where the dimension $D$ is large enough [like, e.g., in ref. [1] where $D = \mathcal{O}(10^3)$]. In the preceding subsection we also saw that there might exist correlations between the changes of $D$ (or $\ell$) and of the conditions of (quasi-) exact solvability. Let us now pay more attention to this phenomenon which appeared as a source of inspiration in several studies of QES problems [16] where it has been noticed that, at a fixed matrix dimension $N$, the solutions are getting simpler whenever the spatial dimension $D$ grows to infinity.

In an introductory step we imagine that the QES constraint (4) merely replaces the definition (6) of the lower diagonal in eqs. (5) by the shorter formula $A_n = 4 \gamma (n - N)$. An uncomfortable asymmetry of our linear algebraic problem $Q(\mathcal{E})\vec{h} = 0$ (5) is still there but it may be weakened by the shift of the large integer $2\ell = D + 2m - 3$ (in the $m$–th partial wave) to another (and also large) auxiliary integer $G = D + 2m + N - 2$. This shift represents $Q(\mathcal{E})$ as a slightly more balanced matrix.
dominated by its upper diagonal,
\[
\begin{pmatrix}
\mathcal{E} & 2(G + 2 - N) \\
4(N - 1)\gamma & \mathcal{E} & 4(G + 4 - N) \\
& \ddots & \ddots & \ddots \\
& & 8\gamma & \mathcal{E} & 2(N - 1)(G - 2 + N) \\
& & & 4\gamma & \mathcal{E}
\end{pmatrix}.
\]

We re-scale it by its pre-multiplication by the diagonal matrix \( \hat{\rho} \) with elements \( \rho^j \) where \( \rho = \sqrt{G/(2\gamma)} \). The parallel renormalization of the Taylor coefficients \( h_j \to p_j = [G/(2\gamma)]^{j/2}h_j \) enables us to re-scale the energy,
\[
\mathcal{E} = 2\sqrt{2\gamma G} E,
\]
re-expressing QES spectrum in terms of eigenvalues of asymmetric two-diagonal matrix
\[
H(\mu) = \begin{pmatrix}
0 & f_1(\mu) \\
f_{(N-1)}(0) & 0 & f_2(\mu) \\
& \ddots & \ddots & \ddots \\
f_2(0) & 0 & f_{(N-1)}(\mu) \\
f_1(0) & 0
\end{pmatrix}
\]
where we abbreviated
\[
f_n(\mu) = n - (N - 2n) \mu n, \quad \mu = \frac{1}{G} = \frac{1}{2m + N + D - 2}.
\]

This matrix will now be understood as our QES "Hamiltonian" which is to be diagonalized perturbatively. In a way guided by a few experiments made at the first few lowest dimensions \( N \), we shall reveal and describe a new and efficient recipe for such a construction in the next section.
3 Perturbation expansions in $\mu^2$

3.1 Optimal shift: matrix dimension $N = 3$

In our notation where the spatial dimension $D$ and all the angular momenta $\ell = (D - 3)/2 + m$ with $m = 0, 1, \ldots$ are “very” large, $D \gg 1$, the integer $N$ denotes just the matrix dimension in eq. (5) and its numerical value may be arbitrary. Thus, our perturbation expansions will use the smallness of $\mu = 1/G$ or, in a more general setting, of $\mu' = 1/[D + 2m + \delta(N)]$ where we have a full freedom in the choice of an $N$–dependent shift $\delta = \delta(N)$.

Let us select $\delta(N) = 1 + \varepsilon$ at $N = 3$, and reduce the diagonalization of our “Hamiltonian” (12) to the elementary secular equation

$$\det \begin{bmatrix} E & 1 - \mu (1 + \varepsilon) & 0 \\ 2 & E & 2 + 2\mu (1 - \varepsilon) \\ 0 & 1 & E \end{bmatrix} = 0.$$ 

Although its explicit polynomial form $E^3 - 4E + 4E\mu\varepsilon = 0$ is virtually trivial, it may be still simplified and made perturbation independent, provided only that we choose the above shift $\delta$ with the special and unique $\varepsilon = 0$. After this “optimal” choice, all the three zero-order energy roots $E_j \in \{-2, 0, 2\}$ remain safely real and become manifestly independent of the spatial dimension $D$. As a consequence, all the higher-order corrections vanish at $\varepsilon = 0$, and the only $D$–dependence of the energies $\mathcal{E}$ remains encoded in the above-mentioned scaling rule (11).


3.2 Continued fractions: matrix dimension $N = 4$

In the next case at $N = 4$ one reveals that with another “optimal” $\delta(N) = 2$, an explicit linear $\mu$-dependence disappears again from the secular equation

$$\det \begin{bmatrix} E & 1 - 2\mu & 0 & 0 \\ 3 & E & 2 & 0 \\ 0 & 2 & E & 3(1 + 2\mu) \\ 0 & 0 & 1 & E \end{bmatrix} = 0$$

Only the quadratic term persists in the secular polynomial $E^4 - 10E^2 + 9 - 36\mu^2$. Thus, the choice of $N = 4$ should be understood as “the first nontrivial” model. Not nontrivial enough of course: the quadruplet of the secular roots keeps its closed form, $E_j \in \{\pm\sqrt{5} \pm 2\sqrt{4 + 9\mu^2}\}$. Circumventing the standard and tedious perturbation recipes, all these four roots may be Taylor-expanded giving directly all the four perturbation expansions in the powers of $\mu^2$,

$$E_1 = -E_4 = 3 + \frac{3}{4}\mu^2 - \frac{33}{64}\mu^4 + \frac{309}{512}\mu^6 - \frac{14133}{16384}\mu^8 + \frac{179643}{31072}\mu^{10} + O(\mu^{12}) , \quad (14)$$

$$E_2 = -E_3 = 1 - \frac{9}{4}\mu^2 - \frac{81}{64}\mu^4 - \frac{2187}{512}\mu^6 - \frac{137781}{16384}\mu^8 - \frac{3601989}{31072}\mu^{10} + O(\mu^{12}) . \quad (15)$$

Due to the analyticity of these expressions in the complexified variable $\mu$, all of these four series have, obviously, the same and non-vanishing circle of convergence with the radius $\mu_{\max} = 1/2$ determined by the nearest branch point in the complex plane of $\mu$. Once we recollect that for any $m \geq 0$ and $D > 0$ we always have $1/\mu > \delta(4) = 2$, we may conclude that for all our four shifted-large-$\ell$ perturbation series at $N = 4$, the circle of convergence is amply sufficient to cover the whole domain of physical interest.

The overall square-root form of the “energies” $E$ might have been taken into account in this context. At least, one may expect a simplification of the formulae when the squares of the energies $\Omega = E^2$ are taken into consideration. For example, in place of the latter two series (15), the “unified” power-series formula reads

$$\Omega(\mu^2) = E_{2,3}^2 = 1 - \frac{9}{2}\mu^2 + \frac{81}{32}\mu^4 - \frac{729}{256}\mu^6 + O(\mu^8) . \quad (16)$$
Its use improves the rate of convergence because we removed one of the branch points, arriving at the new value $\mu_{\text{improved}}^{[\text{max}]} = 2/3$ for the radius of convergence. In a broader context, it is therefore not surprizing that the underlying idea of expanding a suitable function of $E$ (in our case, a square) rather than this observable quantity itself did find non-trivial applications elsewhere [17].

The transition from $E$ to its square $\Omega$ inspires also a slightly counterintuitive re-arrangement of our secular polynomial in an incompletely factorized form where the small corrections are manifestly separated,

$$(\Omega - 9) (\Omega - 1) = 36 \mu^2.$$ 

This defines an explicit analytic continued-fraction re-arrangement of the complete, “perturbed” $\Omega(\mu) = \Omega(0) + \mu^2 \omega(\mu)$. For example, once we select $\Omega(0) = E_{1,4}^2 = 9$, we arrive at the easily verified identity

$$\Omega(\mu^2) = 5 + 2 \sqrt{4 + 9 \mu^2} = 9 + \frac{36 \mu^2}{8 + \frac{36 \mu^2}{8 + \ldots}}.$$ 

(17)

The backward conversion of the analytic continued fraction on the right-hand side to the plain perturbative power series in $\mu^2$ is routine [18] and almost as trivial as its above-mentioned Taylor-series derivation from the left-hand-side square root.

3.3 Convergence of iterations: matrix dimension $N = 5$

Our experience gained from the preceding, completely and easily solvable examples applies to all of the higher $N$’s in a more or less straightforward manner. Firstly, by extrapolation we conjecture (and subsequently verify) that the “optimally shifted” small parameter $\mu$ is always defined by eq. (13). Secondly, we pick up the next
$N = 5$ and re-write the secular equation

$$\det \begin{bmatrix} E & 1 - 3 \mu & 0 & 0 & 0 \\ 4 & E & 2(1 - \mu) & 0 & 0 \\ 0 & 3 & E & 3(1 + \mu) & 0 \\ 0 & 0 & 2 & E & 4(1 + 3 \mu) \\ 0 & 0 & 0 & 1 & E \end{bmatrix} = 0$$

in the polynomial form $E^5 - 20 E^3 + 64 E - 288 E \mu^2 = 0$ showing that we may factor the zero root $E = E_3 = 0$ out. Later on we shall see that such a root exists (and will be dropped) at all the odd $N$. The fact that one of our roots is identically vanishing and may be factored out, strengthens the parallels between $N = 4$ and $N = 5$. In the latter case we get a quadruplet of the nontrivial roots,

$$E_1 = -E_5 = \sqrt{10 + 6 \sqrt{1 + 8 \mu^2}} = 4 + 3 \mu^2 - \frac{57}{8} \mu^4 + \frac{939}{32} \mu^6 - \frac{75957}{512} \mu^8 + O(\mu^{10}) \,,$$

$$E_2 = -E_4 = \sqrt{10 - 6 \sqrt{1 + 8 \mu^2}} = 2 - 6 \mu^2 + 3 \mu^4 - 39 \mu^6 + \frac{483}{4} \mu^8 - \frac{3693}{4} \mu^{10} + O(\mu^{12}) \,.$$

In full parallel with $N = 4$ it is easy to show that $\mu_{\text{max}} = 1/(2 \sqrt{2})$. This time, the domain of the perturbative convergence covers more than we really need. On its boundary we set $m = 0$ and $D = 1$ and get $\mu = \mu_{\text{max phys}} = 1/4 < 1/(2 \sqrt{2}) = \mu_{\text{max math}}$. In comparison with $N = 4$ a tendency is observed towards and improvement of the overall rate of convergence, which are good news in the light of our intention to move towards any $N$ in principle.

Let us once more recollect the existence of the $N = 4$ continued fractions for $\Omega$'s. It is related to the partial factorization of the secular equation which may be easily transferred to $N = 5$,

$$(\Omega - 16) (\Omega - 4) = 288 \mu^2 \,.$$  \hspace{1cm} (18)

Re-scaling the measure of perturbation $\mu^2 = \lambda/72$ and picking up the zero-order root $\tilde{\Omega}^{[0]} = 4$ for definiteness, the corrections in $\Omega(\mu^2) = 4 (1 - Z)$ may be defined
by iterations of eq. (18), \( Z_{[\text{new}]} = \lambda/(3 + Z_{[\text{old}]}), \) and they coincide again with an analytic continued fraction,
\[
Z = \frac{\lambda}{3 + \frac{1}{3 + \ldots}}.
\]  
(19)

The proof of its convergence is easy when performed in the spirit of the fixed-point method of ref. [19]. Indeed, the mapping \( Z_{[\text{old}]} \to Z_{[\text{new}]} \) has just two fixed points, the values of which are known and given by the quadratic equation \( Z^{(\pm)}_{[FP]} = Z_{[\text{old}]} = Z_{[\text{new}]} \). In the next step one imagines that in the vicinity of these two points, the obvious sufficient condition for the convergence/divergence of interactions of our mapping (i.e., of our continued fraction with constant coefficients) is that the derivative \( Y(z) = Z'_{[\text{new}]} \) (of the dependent variable \( Z = Z_{[\text{new}]} \) with respect to the independent variable \( z = Z_{[\text{old}]} \)) is smaller/bigger than one in its absolute value, respectively [19, 20]. We have all the necessary quantities at our disposal so that the criterion is verified by trivial insertions. In perturbative regime of the smallest \( \lambda \ll 1 \) it is sufficient to specify the leading-order estimates for the small positive \( Z^{(\pm)}_{[FP]} = \lambda/12 + \ldots \) and for the much larger and negative \( Z^{(-)}_{[FP]} = -3 - \lambda/3 + \ldots \). We may conclude that the large fixed point is unstable since \( Y^{(-)} = -9/\lambda + \ldots \ll -1 \) while the small fixed point is stable since \( Y^{(+)} = -\lambda/9 + \ldots \in (-1, 1) \).

We described this proof of convergence of continued fractions in full detail because its idea is easily transferred to all the higher dimensions \( N \). In the language of fixed points (or accumulation points), one can also better understand the transition to the power-series perturbation expansions of our squared energies \( \Omega(\mu^2) \). They may be re-constructed directly from the recurrences [20], without any recourse to the closed square-root formulae.

### 3.4 \( N = 6 \) and the branching continued fractions

At \( N = 6 \) the extraction of the roots from the secular equation
\[
-225 + 259 E^2 - 35 E^4 + E^6 + 3600 \mu^2 - 1296 \mu^2 E^2 = 0
\]  
(20)
ceases to be easy. Fortunately, the $D \to \infty$ asymptotic analysis of this equation
reveals that there still exists an elementary partial factorization of this equation,

$$(E + 5) (E + 3) (E + 1) (E - 1) (E - 3) (E - 5) = 144 q m^2 (3 E - 5) (3 E + 5). \quad (21)$$

Both the existence and the simplicity of this relation opens to us new horizons. We realize that we may succeed in an algebraic
determination of the perturbation representations of the roots in an almost as closed form as above. What is now vital is that the
construction does not still require any explicit knowledge of the roots and might remain feasible at the higher $N$’s.

Once we return to eqs. (17) and (19) for guidance, we find that a specific generalization of the continued fractions exists at
$N = 6$ since Firstly, perturbation anzatz

$$\Omega(\mu^2) = 1 + \mu^2 \omega(\mu^2)$$

converts equation (21) into iterative recipe

$$\omega^{(k)}_{[\text{new}]} = -\frac{144 (25 - 9 \Omega)}{(9 - \Omega)(25 - \Omega)} \Omega = 1 + \mu^2 \omega^{(k)}_{[\text{old}]}, \quad k = 0, 1, \ldots . \quad (22)$$

In comparison with the continued-fraction predecessors of this nonlinear two-term recurrence, just a “branching” of the continued fraction occurs,

$$\omega^{(k)}_{[\text{new}]} = 72 \left( \frac{7}{8 - \mu^2 \omega^{(k)}_{[\text{old}]}} - \frac{25}{24 - \mu^2 \omega^{(k)}_{[\text{old}]}} \right), \quad k = 0, 1, \ldots . \quad (23)$$

These formulae generate the sequence of the values $\omega^{(k+1)}_{[\text{odd}]} = \omega^{(k)}_{[\text{new}]}$ with $k = 0, 1, \ldots$ starting from the initial $\omega^{(0)}_{[\text{odd}]} = 0$ and giving

$$\omega^{(0)}_{[\text{new}]} = -12, \quad \omega^{(1)}_{[\text{new}]} = -\frac{12 (4 + 27 \mu^2)}{(2 + 3 \mu^2)(2 + \mu^2)}, \quad \ldots . \quad (24)$$

In the limit $k \to \infty$ (whenever it exists), one gets the function $\omega^{(\infty)}_{[\text{odd}]} = \omega^{(\infty)}_{[\text{new}]}$ of $\mu^2$ whose form is a generalization of the standard analytic continued fraction. Its dependence on $\mu^2 \geq 0$ is smooth. From the negative value $\omega(0) = -12$ in the origin this function decreases to a minimum $\omega(0.400186) = -24.94120$ and then it very slowly grows again.

Whenever necessary, one can establish a number of parallels between iterations (23) and the current theory of continued fractions [18]. In particular, the fixed-point
pattern of the proofs of convergence of ref. [19] applies to functions \( \Omega(\mu^2) \) at both \( N = 4 \) or 5 and \( N = 6 \) (and, as we shall see below, 7). Thus, for the “first nontrivial” \( N = 6 \) mapping \( \omega^{(k)}_{[\text{old}]} \rightarrow \omega^{(k)}_{[\text{new}]} \), we may skip the details (like, e.g., all the small–\( \lambda \) analysis) and emphasize only that the proof of the convergence of our branched continued fraction consists of three steps now. Firstly, one demonstrates that there is just one fixed-point root which is compatible with the perturbation smallness of corrections. Secondly, one confirms that this “only acceptable” fixed point is stable (by showing that the derivative of the mapping at this point is sufficiently small, \( |Y(z)| < 1 \)). Finally, one shows that the stable point is unique, which follows from the observation that \( |Y(z)| > 1 \) at the other two fixed points.

For giving to the reader a rough estimate of the rate of convergence of the iterations, let us pick up a sample value of the parameter \( \lambda = \mu^2 = 1/10 \), giving the fairly small \( Y(z) \approx 0.25949 \) at the accumulation point \( z \approx -2.30666 \), while the quick divergence of the iterations at the other two fixed points results from the large magnitude of the derivatives \( Y(5.26698) \approx 3.0556 \) and \( Y(37.03969) \approx -5.5675 \) there.

For many practical purposes, it is desirable to convert our branched continued fractions \( \omega^{(\infty)}_{[\text{old}]} = \omega^{(\infty)}_{[\text{new}]} \) in example (22) into the more common Rayleigh-Schrödinger-type power series. We performed such a conversion giving, for the squared energy, the following perturbation series in \( \mu^2 \),

\[
\Omega = 1 - 12 \mu^2 - 57 \mu^4 - \frac{591}{4} \mu^6 + \frac{4215}{16} \mu^8 + \frac{286293}{64} \mu^{10} + \frac{3702951}{256} \mu^{12} - \frac{63786951}{1024} \mu^{14} - \frac{3242255193}{4096} \mu^{16} - \frac{32707656915}{16384} \mu^{18} + \frac{1182033909831}{65536} \mu^{20} + \mathcal{O}(\mu^{22}).
\]

(25)

Up to the order \( \mathcal{O}(\mu^{26}) \) we verified the validity of an empirical rule that the signs are changing after every third order. A posteriori, one may expect an efficient numerical summability of this series by the standard Padé-resummation techniques. We skip here the really amusing possibility of a backward comparison of the resulting rational approximations with their available initial versions (24).
3.5 Expansions at an arbitrary matrix dimension $N$

In a way which is outlined in Table 1 and which may be tested on the further non-numerical QES constructions (with dimensions $N = 7 - N = 9$, i.e., up to quartic-polynomials) as well as at any higher $N$, we have reached the stage where the overall structure of secular polynomials is clear,

$$\mathcal{P}(\Omega) = \mathcal{P}_0(\Omega) + \mu^2 \mathcal{P}_1(\Omega) + \ldots + \mu^{2K} \mathcal{P}_K(\Omega), \quad K = \text{entier} \left[ \frac{N}{4} \right]. \quad (26)$$

The routine analysis confirmed our expectations that at any $N$, the large parameters \( \ell \) or $D$ entering the measure of smallness $\mu$ as defined by eq. (13) are “optimally shifted”. This assertion is supported by the following four reasons at least.

- All the odd powers of $\mu$ disappear from the polynomial forms of the secular determinants as well as from the perturbation expansions of the observable quantities (energies).

- Up to the dimension $N = 9$ which is already fairly large, the degree of our “optimalized” secular polynomials does not exceed four; this means that their factorization may be made non-numerically.

- At all the larger $N > 9$, a partial (i.e., asymptotic, $D \to \infty$) factorization is still feasible non-numerically in zero order. As a consequence, all the higher-order $O(\mu^2)$ corrections may be generated in the form which, in many a respect, generalizes the analytic continued fraction.

Surprisingly enough, the use of our present generalizations of continued fractions has led to a very transparent alternative to Cardano formulae at dimension as low as $N = 6$. Similarly, at $N = 7$ we eliminate the trivial root $E = 0$ and get the rule

$$-2304 E + 784 E^3 - 56 E^5 + E^7 + 40320 \mu^2 E - 4320 \mu^2 E^3 = 0$$

and the parallel update of eq. (21),

$$\left( \Omega - 2^2 \right) \left( \Omega - 4^2 \right) \left( \Omega - 6^2 \right) = 1440 \mu^2 (-28 + 3 \Omega). \quad (27)$$
We need not repeat the extraction of the conclusions similar to the ones in section 3.4. A not too dissimilar remark may be added concerning $N = 8$ with

$$
(\Omega - 1^2)(\Omega - 3^2)(\Omega - 5^2)(\Omega - 7^2) = 360 \mu^2 \left( 1225 - 682 \Omega + 33 \Omega^2 \right) + 1587600 \mu^4.
$$

(28)

This equation illustrates both the emergence of the higher powers of $\mu^2$ on the right-hand side and the parallels with the $N = 9$ secular equation

$$
(\Omega - 2^2)(\Omega - 4^2)(\Omega - 6^2)(\Omega - 8^2) =
$$

$$
= 288 \mu^2 \left( 22016 - 3740 \Omega + 99 \Omega^2 \right) + 24385536 \mu^4
$$
as well as an unexpectedly smooth character of transition to the “first unsolvable” $N = 10$ example

$$
-893025 + 1057221 \, E^2 - 172810 \, E^4 + 8778 \, E^6 - 165 \, E^8 + E^{10} +
$$

$$
+ 71442000 \mu^2 - 48647664 \mu^2 E^2 + 3809520 \mu^2 E^4 - 61776 \mu^2 E^6 -
$$

$$
- 914457600 \mu^4 + 199148544 \mu^4 E^2.
$$
does not bring, in full accord with the scheme of Table 1, anything new, indeed.

The general pattern indicated in Table 1 works and remains valid for all the matrix dimensions $N = 4K, 4K + 1, 4K + 3$ and $4K + 3$ with any auxiliary $K = 1, 2, \ldots$.

On this basis, we are permitted to pay attention to any root $\tilde{\Omega}$ of our zero-order secular polynomial $P_0(\Omega) = (\tilde{\Omega} - \Omega) Q(\Omega)$. As long as this root is an integer, it is extremely easy to study its small vicinity by the insertion of the ansatz $\Omega = \tilde{\Omega} + \mu^2 \omega(\mu^2)$ into the exact secular equation $P(\Omega) = 0$. The resulting new form of our secular equation reads

$$
\mu^2 \omega(\mu^2) = \frac{1}{Q_0(\Omega)} \left[ \mu^2 P_1(\Omega) + \ldots + \mu^{2K} P_K(\Omega) \right].
$$

(29)

On the basis of this formula we may consider a sequence $\omega_j(\mu^2)$ of approximate corrections initiated by $\omega_{-1}(\mu^2) = \omega_{-2}(\mu^2) = \ldots = 0$. The use of the abbreviations
\[ \Omega_j = \tilde{\Omega} + \mu^2 \omega_j (\mu^2) \]
re-interprets finally our secular equation (29) as an innovated and most important recurrent relation

\[ \omega_j (\mu^2) = \frac{P_1 (\Omega_{j-1})}{Q_0 (\Omega_{j-1})} + \ldots + \mu^{2K-4} \frac{P_{K-1} (\Omega_{j-K+1})}{Q_0 (\Omega_{j-K+1})} + \mu^{2K-2} \frac{P_K (\Omega_{j-K})}{Q_0 (\Omega_{j-K})}, \quad j = 0, 1, \ldots. \]  

(30)

At \( K = 1 \) and \( N = 4 \) or \( N = 5 \) this recipe returns us back to the current definition of the analytic continued fractions. Similarly, at \( N = 6 \) and \( N = 7 \) we get their branched alternative. At all the higher \( N \geq 8 \), our recurrences (30) offer just an immediate rational generalization of the latter two concepts.

4 Interpretation and outlook

4.1 Zero-order Schrödinger equation

We have seen that once we switch to the rescaled energy variable \( E \) in eq. (11) and to the Hamiltonian (12), the zero-order diagonalization of \( H(0) \) becomes unexpectedly easy at any \( N \). In spite of the manifest asymmetry of the Schrödinger QES equation in the limit \( \ell \to \infty \),

\[
\begin{pmatrix}
0 & 1 & & & \\
(2N-2) & 0 & 2 & & \\
& \ddots & \ddots & \ddots & \\
2 & 0 & (N-1) & & \\
1 & 0 & & & \\
\end{pmatrix}
\begin{pmatrix}
p_0 \\
p_1 \\
\vdots \\
p_{N-2} \\
p_{N-1} \\
\end{pmatrix}
= E
\begin{pmatrix}
p_0 \\
p_1 \\
\vdots \\
p_{N-2} \\
p_{N-1} \\
\end{pmatrix},
\]  

(31)

all its eigenvalues remain strictly real, equal to integers and equidistant,

\[
(E_1, E_2, E_3, \ldots, E_{N-1}, E_N) = (-N+1, -N+3, -N+5, \ldots, N-3, N-1).
\]  

(32)

It is quite elementary to verify that also the respective left and right eigenvectors of \( H(0) \) remain real. Up to their norm, all of them can be represented in terms of integers as well. Their components may be arranged in the rows and columns of the
following \( N \) by \( N \) square matrices \( P = P(N) \),

\[
P(1) = 1, \quad P(2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},
\]

\[
P(3) = \frac{1}{\sqrt{4}} \begin{pmatrix} 1 & 1 & 1 \\ 2 & 0 & -2 \\ 1 & -1 & 1 \end{pmatrix}, \quad P(4) = \frac{1}{\sqrt{8}} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 3 & 1 & -1 & -3 \\ 3 & -1 & -1 & 3 \\ 1 & -1 & 1 & -1 \end{pmatrix},
\]

\[
P(5) = \frac{1}{\sqrt{16}} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & 2 & 0 & -2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & -2 & 0 & 2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix}, \ldots
\]

All these matrices are asymmetric but idempotent, \( P^2 = I \). This implies that the Hamiltonian in our zero-order QES sextic Schrödinger equation \( H^{(0)} \vec{p}^{(0)} = \vec{p}^{(0)} E^{(0)} \) need not be diagonalized at all. Indeed, as long as the \( N \)-plets of the zero-order (lower-case) vectors \( \vec{p}^{(0)} \) are concatenated into the above-mentioned (upper-case) \( N \) by \( N \) matrices \( P = P^{(0)} \), we may also collect all the pertaining eigenvalues \( E^{(0)} \) in a diagonal matrix \( \varepsilon^{(0)} \). In this arrangement, the unperturbed Hamiltonian is factorized, \( H^{(0)} = P \varepsilon^{(0)} P \). As a consequence, the zero-order equation is an identity since, in our compactified notation, it reads \( P \varepsilon^{(0)} PP = P \varepsilon^{(0)} \) and we know that \( P^2 = I \). In the next section we show that and how similar notation may be used in all orders.

### 4.2 Rayleigh-Schrödinger perturbation recipe revisited

We have seen that

At any finite value of the spatial dimension \( D \) we have seen in section 3 that the routine power-series ansatz of perturbation theory becomes applicable even though the unperturbed Hamiltonian \( H(\mu) \) itself is non-diagonal. We may write

\[
H(\lambda) = H^{(0)} + \lambda H^{(1)}, \quad \lambda = \mu^2
\]
where the perturbation is an asymmetric one-diagonal matrix in our particular illustrative example. Even without the latter constraint we arrive at the textbook perturbative representation of our matrix Schrödinger equation,

\[
(H^{(0)} + \lambda H^{(1)}) \cdot (p^{(0)} + \lambda p^{(1)} + \ldots + \lambda^K P^{(K)} + O(\lambda^{K+1}))
= (p^{(0)} + \ldots + \lambda^K P^{(K)} + O(\lambda^{K+1})) \cdot (E^{(0)} + \ldots + \lambda^K E^{(K)} + O(\lambda^{K+1})).
\]  

(33)

The sets of the vectors for corrections \( \vec{p}_j^{(k)} \), \( j = 1, 2, \ldots, N \) may be concatenated in the square matrices \( \Psi^{(k)} \). This enables us to re-write the first-order \( O(\lambda) \) part of eq. (33) in the particularly compact matrix form

\[
\varepsilon^{(1)} + P \Psi^{(1)} \varepsilon^{(0)} - \varepsilon^{(0)} P \Psi^{(1)} = P H^{(1)} P.
\]  

(34)

In the second order we get

\[
\varepsilon^{(2)} + P \Psi^{(2)} \varepsilon^{(0)} - \varepsilon^{(0)} P \Psi^{(2)} = P H^{(2)} P + P H^{(1)} \Psi^{(1)} - P \Psi^{(1)} \varepsilon^{(1)}
\]  

(35)

etc. This is a hierarchy of equations representing their source (33) order-by-order in \( \lambda \). Their new merit lies in their recurrent character. Their “old” or “input” data occur on the right-hand side of these equations, while the “new” or “unknown” quantities stand to the left. All the higher-order prescriptions have the same structure. In all of them, the diagonal part of each equation (i.e., of (34) or (35) etc) determines the diagonal matrices containing energy corrections (i.e., \( \varepsilon^{(1)} \) or \( \varepsilon^{(2)} \) etc, respectively). Non-diagonal components of these matrix relations are to be understood as definitions of the eigenvectors, with an appropriate account of the well known normalization freedom which has been thoroughly discussed elsewhere [21].

All these relations just re-tell the story of our preceding section but after an appropriate modification they may also be used for the evaluation of separate corrections in some more complicated QES systems [10].

In the conclusion, we may emphasize that the practical reliability of any perturbation prescription is, mostly, determined by the quality of the zero-order approximation. In this sense, our present study offers also a broadening of their menu. In the light of our results one will be forced to make a more careful selection between the ES
and QES $V^{[QES]}(|\vec{r}|)$. Indeed, in each of these respective extremes one encounters different difficulties. Still, the simpler ES-based choice of $V_0(|\vec{r}|)$ is predominantly preferred in practice. Almost without exceptions, such a decision is being made for one of the following three apparently good reasons.

- Up to now, many QES-based constructions stayed within the mere lowest-order perturbation regime since the majority of the naive implementations of the Rayleigh-Schrödinger perturbation scheme becomes complicated in the high orders [8].

- A priori, any available set of the QES bound states $\psi_0$ is, by definition, incomplete. This makes the matrix form of the pertaining propagators non-diagonal and, hence, not too easy to use even in the lowest orders.

- Last but not least, many ambitious QES models cannot be used as eligible for perturbations because they are almost frighteningly complicated even in zero order [6, 9].

Within our new perturbation prescription, all these shortcomings were at least partially weakened. At the same time, the appeal of the ES-based perturbation constructions should at least slightly be re-evaluated as well: (i) the class of the available $V^{[ES]}(|\vec{r}|)$ is really extremely narrow for many practical purposes; (ii) several important (e.g., double-well) models lead to a perturbation which is not “sufficiently small” in the sense of Kato [22]; (iii) one needs to go to the really very high perturbations in many cases of practical interest [23].

In such a setting we showed that the technical treatment of the QES-type zero-order approximations can be significantly simplified. This could help, say, in situations where we have to deal with a phenomenological potential $V(r)$ which cannot be well approximated by any available exactly solvable $V^{[ES]}(|\vec{r}|)$ while there exists an exceedingly good approximation of $V(r)$ by a partially solvable $V^{[QES]}(|\vec{r}|)$. Under this assumption we may recommend the present construction as a guide to new applications of the old large-$\ell$ expansion idea [24], especially when a very high order
$N$ characterizes the polynomial part of the QES wave function $\psi^{[N]}(r)$, which would makes the simple-minded zero-order construction prohibitively complicated by itself.

5 Summary

The problem of construction of large QES multiplets has been addressed here within the framework of the so called large $-\ell$ expansion method. Its key idea is very popular and re-emerges whenever radial Schrödinger equation is considered at a large angular momentum $\ell$. Originally, this attracted our attention because in all these recipes there exists an obvious ambiguity in a free choice between alternative small parameters $\lambda = 1/\ell$ and $\lambda_{shifted} = 1/(\ell + \beta)$. We should remind the reader that there exist in fact many alternative shifted-large $-\ell$ versions of the expansions which use this freedom in different ways [25] but, mostly, this parameter plays a certain not too essential variational role. In this context, the position of our present approach may be exceptional; in QES context the role of our "optimal" and unique $\beta$ happened to be much more essential, influencing not only the rate of convergence but also, directly, the form of the perturbation series itself.

Thus, although in most cases the transition to a shifted large $-\ell$ expansion is being designed to extend its practical applicability, we imagined that the construction of the $N$–plets of quasi-exact sextic-oscillator bound states $\psi^{[N]}_n(r)$ does not admit any free choice of the shift $\beta$ at all. On the contrary, our approach has been shown to prefer the unique, "optimal" definition of the shift $\beta = \beta(N)$ which leads to one of the best available constructions of the QES spectrum. This is our main result.

Our secondary motivation stemmed from the fact that whenever one moves beyond the first few trivial multiplet dimensions $N$, the practical appeal of QES solutions fades away. In this sense we have verified once more that one of the most efficient strategies of solving “difficult” Schrödinger equation is provided by the standard Rayleigh-Schrödinger perturbation series [22] and by many of its various practical modifications and alternative implementations [4]. We succeeded in developing a prescription with several merits described throughout the text.
In a broader methodical setting we were guided by the idea that the quality of perturbative results depends on the two decisive factors, viz., on the number of the available perturbation corrections and on the rate of convergence of their series. In both these aspects our new approach passes the test very well. We have seen that in comparison with the standard approach summarized for our present purposes in section 2.2, we arrived at the more compact and, presumably, most easily generated representation of our QES energies. Moreover, in a sharp contrast to the manifest divergence of the former (though, admittedly, more universal) recipe [15], our algebraic approach represents the QES spectra by convergent infinite series.

Our new implementation of some old ideas of perturbation theory looks promising and will definitely serve as a guide to the more complicated QES constructions in the future. For the sake of simplicity we have chosen just one of the simplest models where the sextic oscillator is not even complemented by a quartic force and admits merely a quadratic repulsion near the origin. This simplified many technicalities and strengthened our belief that any future transition to models with more parameters may and will proceed along the same lines.

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Table 1. QES secular polynomials $\mathcal{P}(\Omega) = \mathcal{P}_0(\Omega) + \mu^2 \mathcal{P}_1(\Omega) + \ldots + \mu^{2K} \mathcal{P}_K(\Omega)$ (the trivial factor $E$ ignored at odd $N$).

| dimension | perturbation       | degree of $\mathcal{P}_j(\Omega)$ |
|-----------|--------------------|-------------------------------------|
| $N$       | in $\mathcal{P}(\Omega)$ | $j = 0$ | $j = 1$ | $j = 2$ | $j = 3$ |
| 0 and 1   | absent ($K = 0$)    | 0      | -      | -      | -      |
| 2 and 3   | absent ($K = 0$)    | 1      | -      | -      | -      |
| 4 and 5   | linear ($K = 1$)    | 2      | 0      | -      | -      |
| 6 and 7   | linear ($K = 1$)    | 3      | 1      | -      | -      |
| 8 and 9   | quadratic ($K = 2$) | 4      | 2      | 0      | -      |
| 10 and 11 | quadratic ($K = 2$) | 5      | 3      | 1      | -      |
| 12 and 13 | cubic ($K = 3$)     | 6      | 4      | 2      | 0      |
| ...       | ...                | ...    | ...    | ...    | ...    |