Proceedings of Institute of Mathematics of NAS of Ukraine 2002, Vol. 43, Part 2, 777–781

Generalized Rayleigh–Schrödinger Perturbation Theory as a Method of Linearization of the so Called Quasi-Exactly Solvable Models

Miloslav ZNOJIL

Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic
E-mail: *znojil@ujf.cas.cz*

Sextic oscillator in D dimensions is considered as a typical quasi-exactly solvable (QES) model. Usually, the QES N–plets of energies have to be computed using the nonlinear and coupled Magyari's algebraic equations. We propose and describe an alternative linear method which works with power series (in $1/\sqrt{D}$) in integer arithmetics.

1 Introduction

Sextic Hamiltonian in D dimensions

$$H = -\triangle + a\,|\vec{r}\,|^2 + b\,|\vec{r}\,|^4 + c\,|\vec{r}\,|^6, \qquad a = a(N)$$

enters many phenomenological and methodical considerations as a "next-to-solvable" model [1]. In fact, among all the real polynomial interactions, only the *harmonic and sextic* models can generate an arbitrary N–plet of bound state wavefunctions in an elementary form. All the similar models are often called quasi-exactly solvable (QES, cf. [2]).

Unfortunately, the close parallel between the sextic and harmonic oscillator is not too robust and breaks down in practical applications [3]. For example, the Rayleigh–Schrödinger unperturbed propagator ceases to be diagonal in the sextic case [4]. Moreover, the key weakness of *any* QES model lies in the nonlinearity of its secular equation which has the polynomial form of degree N [5]. Non-numerical determination of the sextic energies is only feasible at $N \leq 4$. Otherwise, in a sharp contrast to harmonic case, the values of energies E_n are only available up to some rounding errors.

In order to refresh the parallels we shall describe a new approach to the sextic QES bound state problem. It is based on some surprising results of the symbolic manipulation experiments. They were performed in MAPLE using the technique of Groebner bases. We revealed that the QES energies become equidistant and proportional to integers in the limit of the large spatial dimensions $D \to \infty$. This feature is presented in Sections 2 and 3.

In the second step of our analysis one discovers that the systematic evaluation of the Rayleigh–Schrödinger corrections proves feasible in closed form. In spite of the non-diagonality of propagators, a merely slightly modified form of construction can be used. It gives the energy formula

$$E(\lambda) = E^{(0)} + \lambda\,E^{(1)} + \lambda^2\,E^{(2)} + \cdots + \lambda^K\,E^{(K)} + \mathcal{O}\left(\lambda^{K+1}\right), \qquad \lambda = 1/\sqrt{D}.$$

Its coefficients $E^{(k)}$ are obtainable *without any rounding errors* (cf. Sections 4 and 5 below).

2 An unusual solvable limit: Large dimensions D

All the sextic oscillator states are determined by the radial Schrödinger equation

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + a\,r^2 + b\,r^4 + c\,r^6\right]\,\psi(r) = E\,\psi(r). \tag{1}$$

It contains the dimension D and the angular momenta $k = 0, 1, \ldots$ in $\ell = k + (D-3)/2$. The elementary ansatz

$$\psi(r) = \sum_{n=0}^{\infty} h_n \, r^{2n+\ell+1} \exp\left(-\frac{1}{2}\beta\, r^2 - \frac{1}{4}\gamma\, r^4\right), \qquad c = \gamma^2 > 0, \quad b = 2\beta\gamma > 0 \tag{2}$$

converts this ordinary differential equation into the linear algebraic system characterized by the tridiagonal Hamiltonian matrix,

$$Q^{[N]}\,\vec{h} = E\,\vec{h}, \qquad Q^{[N]} = \begin{pmatrix} B_0 & C_0 & & & \\ A_1 & B_1 & C_1 & & \\ & \ddots & \ddots & \ddots & \\ & & A_{N-2} & B_{N-2} & C_{N-2} \\ & & & A_{N-1} & B_{N-1} \end{pmatrix}, \tag{3}$$

where the dimension is to be infinite, $N \to \infty$, and the matrix elements are elementary,

$$\begin{aligned} &A_n = \gamma\,(4n + 2\ell + 1) + a - \beta^2, \qquad B_n = B_n(E) = \beta\,(4n + 2\ell + 3), \\ &C_n = -2(n+1)\,(2n + 2\ell + 3), \qquad n = 0, 1, \ldots\ . \end{aligned} \tag{4}$$

The (quasi-)variational limit $N \to \infty$ gives the numerically correct spectrum [6]. For the sake of simplicity, let us now constrain our attention to the simplified model of Singh et al [5] characterized by the QES condition imposed upon the quadratic coupling $a = a(N)$,

$$a(N) = \frac{1}{4\gamma^2}\, b^2 - \gamma\,(4N + 2\ell + 1).$$

In this way one achieves the *rigorous* termination of the wavefunctions,

$$h_N = h_{N+1} = h_{N+2} = \cdots = 0. \tag{5}$$

The latter assumption merely changes the lower diagonal in equations (3) and (4) to the shorter formula $A_n = 4\gamma\,(n - N)$. Exact energies become available only at the first few integers $N \leq 4$. Beyond $N = 4$, QES solutions remain numerical. Moreover, the intrinsic asymmetry of our Hamiltonian (3) causes a loss of precision which grows quickly with the degree N [6].

In such a setting we have noticed, purely empirically, that the solutions are getting simpler when the spatial dimensions grow, $D \gg 1$. In the leading-order approximation, the corresponding matrix Schrödinger equation becomes diagonally dominated,

$$\begin{pmatrix} E-\beta D & 2D & & & \\ 4(N-1)\gamma & E-\beta D & 4D & & \\ & \ddots & \ddots & \ddots & \\ & & 6\gamma & E-\beta D & 2(N-1)D \\ & & & 4\gamma & E-\beta D \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ \vdots \\ h_{N-2} \\ h_{N-1} \end{pmatrix} = 0. \tag{6}$$

This enables us to evaluate the fully degenerate dominant eigenvalue,

$$E = \beta D - 2\sqrt{2\gamma D}\, z \tag{7}$$

where z is a constant.

3 The removal of degeneracy in sub-dominant approximation

Once we switch to the new energy variable z, we may pre-multiply equation (6) by a diagonal and regular matrix with elements ρ^j, where $\rho = \sqrt{D/(2\gamma)}$. This leads to the new, non-diagonal matrix Schrödinger equation. It determines the leading-order components of the renormalized Taylor coefficients $p_j = [D/(2\gamma)]^{j/2} h_j$ and has the following transparent form,

$$\begin{pmatrix} 0 & 1 & & & \\ (N-1) & 0 & 2 & & \\ & \ddots & \ddots & \ddots & \\ & & 2 & 0 & (N-1) \\ & & & 1 & 0 \end{pmatrix} \begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_{N-2} \\ p_{N-1} \end{pmatrix} = z \cdot \begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_{N-2} \\ p_{N-1} \end{pmatrix}. \tag{8}$$

In spite of the manifest asymmetry of this equation, all its eigenvalues remain strictly real. We computed these eigenvalues by symbolic manipulations in integer arithmetics and discovered that the underlying nonlinear secular equation is solvable exactly and completely. The N–plets of its energy roots proved nondegenerate, equidistant and extremely elementary,

$$(z_1, z_2, z_3, \ldots, z_{N-1}, z_N) = (-N+1, -N+3, -N+5, \ldots, N-3, N-1)\,. \tag{9}$$

This result is valid *at an arbitrary finite matrix size* N.

It is quite elementary to verify that also the respective left and right eigenvectors remain real. Up to their norm, all of them can be represented in terms of integers. Their components may be arranged in the rows and columns of certain square matrices,

$$P(0) = 1, \qquad P(1) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

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

$$P(4) = \frac{1}{\sqrt{16}} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & 2 & 0 & -2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & -2 & 0 & 2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix}$$

etc. These matrices $P = P(N-1)$ are all asymmetric but idempotent, $P^2 = I$.

We may summarize that in the limit $D \to \infty$, the QES sextic model may be factorized easily. After a suitable normalization, all the components of the eigenvectors are integers.

4 An adapted Rayleigh–Schrödinger perturbation recipe

At the finite values of D and *starting directly from the second-order precision of the preceding section*, the routine perturbation theory becomes applicable since the unperturbed Hamiltonian remains diagonal and all its spectrum is safely non-degenerate.

At any $D \gg 0$ the Schrödinger equation (3) is an eigenvalue problem with the perturbed Hamiltonian of the two-term form,

$$H(\lambda) = H^{(0)} + \lambda\, H^{(1)} + \lambda^2 H^{(2)}, \qquad \lambda = 1/\sqrt{D}.$$

Both the perturbations are one-diagonal matrices which depend on the value of the angular momentum k,

$$\left(H^{(1)}\right)_{nn} = \frac{\beta}{\sqrt{2\gamma}}(2n+k), \qquad n = 0, 1, \ldots, N-1,$$
$$\left(H^{(2)}\right)_{nn+1} = -(n+1)(2n+2k), \qquad n = 0, 1, \ldots, N-2.$$

We may re-write our Schrödinger equation (3) in the textbook perturbation-series representation at any N,

$$\left(H^{(0)} + \lambda\, H^{(1)} + \lambda^2 H^{(2)}\right) \cdot \left(\psi^{(0)} + \lambda\,\psi^{(1)} + \cdots + \lambda^K \psi^{(K)} + \mathcal{O}\left(\lambda^{K+1}\right)\right)$$
$$= \left(\psi^{(0)} + \cdots + \lambda^K \psi^{(K)} + \mathcal{O}\left(\lambda^{K+1}\right)\right) \cdot \left(\varepsilon^{(0)} + \cdots + \lambda^K \varepsilon^{(K)} + \mathcal{O}\left(\lambda^{K+1}\right)\right). \qquad (10)$$

Let us again concatenate the (lower-case) zero-order vectors $\vec{p} = \vec{p}^{(0)} \equiv \psi^{(0)}$ into an N by N matrix $P = P^{(0)}$, with all the eigenvalues arranged also in a diagonal matrix $\varepsilon^{(0)}$. In this way the zero-order equation $H^{(0)}\psi^{(0)} = \psi^{(0)}\varepsilon^{(0)}$ is satisfied identically. Indeed, in our compactified notation, it reads $P\varepsilon^{(0)}PP = P\varepsilon^{(0)}$ and we know that $P^2 = I$.

With the factorized $H^{(0)} = P\varepsilon^{(0)}P$, we shall use the same convention in all orders and concatenate the vectors $\vec{\psi}_j^{(k)}$, $j = 1, 2, \ldots, N$ in the square matrix $\Psi^{(k)}$. In the first order of perturbation analysis this replaces the $\mathcal{O}(\lambda)$ part of equation (10) by the matrix relation

$$\varepsilon^{(1)} + P\,\Psi^{(1)}\varepsilon^{(0)} - \varepsilon^{(0)}P\,\Psi^{(1)} = P\,H^{(1)}\,P. \qquad (11)$$

In the second order we get

$$\varepsilon^{(2)} + P\,\Psi^{(2)}\varepsilon^{(0)} - \varepsilon^{(0)}P\,\Psi^{(2)} = P\,H^{(2)}\,P + P\,H^{(1)}\,\Psi^{(1)} - P\,\Psi^{(1)}\varepsilon^{(1)} \qquad (12)$$

etc. The available expressions occur on the right-hand side of these equations while the unknown quantities stand to the left. All the higher-order formulae have the same structure.

We may summarize that the diagonal part of equations (11) or (12) determines the energy corrections $\varepsilon^{(1)}$ and $\varepsilon^{(2)}$, respectively. Non-diagonal components of these matrix relations are to be understood as a definition of the eigenvectors.

5 Merits of the method: an $N = 2$ illustration

One has to move up to the higher-order level for the elimination of the normalization ambiguities. This has been multiply clarified in the literature on perturbation theory [7]. Still, we should emphasize a user-friendliness of this normalization freedom within the framework of the present formalism. For illustration, let us consider just the s–wave problem in the $N = 2$ case. Immediately, our first-order formulae give the two energy corrections which are both equal to each other,

$$\varepsilon_{11}^{(1)} = \varepsilon_{22}^{(1)} = \beta/\sqrt{2\gamma}. \qquad (13)$$

One discovers that the $\mathcal{O}(\lambda)$ level of precision provides just an incomplete information about the norms of the first-order wave functions. This is the well known normalization freedom manifesting itself in the present setting. On the $\mathcal{O}(\lambda)$ level of precision only two constraints $\Psi_{11}^{(1)} - \Psi_{21}^{(1)} = -\beta/\sqrt{2\gamma}$ and $\Psi_{12}^{(1)} + \Psi_{22}^{(1)} = \beta/\sqrt{2\gamma}$ are imposed upon the wavefunctions. Their definition must be completed in the subsequent order.

In any higher order computation, the use of the computerized symbolic manipulations is strongly recommended. Their implementation is trivial. The algorithm can be written in integer

mathematics and generates, therefore, the perturbation series without any errors. This is our most important conclusion. One generalizes immediately the above leading-order results (7), (9) and (13) to the compact energy series for our particular sextic $k = N - 2 = 0$ illustration,

$$E_{1,2} = \frac{\beta}{\lambda^2} \pm \frac{2\sqrt{2\gamma}}{\lambda} + 2\beta \pm \frac{\beta^2}{\sqrt{2\gamma}}\,\lambda + 0 \cdot \lambda^2 \mp \frac{\beta^4}{8\gamma\sqrt{2\gamma}}\,\lambda^3 + 0 \cdot \lambda^4 + \mathcal{O}\left(\lambda^5\right). \tag{14}$$

One can observe the (complete) leading-order degeneracy of Section 2 as well as its immediate next-order removal (9) as discussed in Section 3. It is also amusing to notice the above, hand-evaluated and quite unexpected, degeneracy of the subsequent $\mathcal{O}(1)$ correction.

One can notice the existence of certain identically vanishing corrections here. In fact, their rigorous evaluation would not be possible within the standard framework of perturbation theory where the summations over the intermediate states must be computed in finite precision. Only within the present formalism which is able to work in integer arithmetics, the unusual feasibility of proving the *precise cancellation* of the series of corrections can be achieved. This is one of the less expected though most important merits of our present methodical proposal and construction.

Acknowledgements

Work supported by the GA AS CR grant Nr. A 104 8004.

[1] Znojil M., Classification of oscillators in the Hessenberg-matrix representation, *J. Phys. A: Math. Gen.*, 1994, V.27, N 14, 4945–4968.

[2] Ushveridze A.G., Quasi-exactly solvable models in quantum mechanics, Bristol, IOP, 1994 (with further references).

[3] Cannata F., Ioffe M., Roychoudhury R. and Roy P., A new class of PT-symmetric Hamiltonians with real spectra, *Phys. Lett. A*, 2001, V.281, N 5–6, 305–310 (with updated references).

[4] Znojil M., Double well model and perturbation method with triangular propagators, *Phys. Lett. A*, 1996, V.222, N 5–6, 291–298.

[5] Singh V., Biswas S.N. and Datta K., Anharmonic oscillator and the analytic theory of continued fractions, *Phys. Rev. D*, 1978, V.18, N 6, 1901–1908.

[6] Hautot A., The method of Hill determinants, *Phys. Rev. D*, 1986, V.33, N 3, 437–443.

[7] Znojil M., Numerically inspired new version of the degenerate Rayleigh–Schrödinger perturbation theory, *Czechoslovak J. Phys. B*, 1990, V.40, N 11, 1065–1078 (with further references).