On topical methods for the calculation of spectra of quantum Hamiltonians

Miloslav Znojil

OTF ÚJF Řež

seminar: 28. 4. 2003, Institute of Physics, Prague

informal continuation of the March 11 seminar for Doppler Institute,

with motto

"$q \geq 6$ is not *'hic sunt leones'* **anymore"**

and with an alternative title

'polynomial oscillators in large dimensions II'

State of the art

- calculations of spectra
  - sketchy review
    - universal, numerical methods
    - more specific techniques
  - tendency: perturbatizations
    - P + shoot = SČ, SČ + match = P'
    - P + Four = PT, PT + 1/L = P'
- P + QES (DI seminar in March)
  - zero order: $D \gg 1$
    - 1999: Mag. eq., $q = 2$, any N
  - corrections: new method
    - 2002: $q = 1$, any N
  - extrapolations in N
    - 2003: $q = 3$, any N
    - 2003: $q = 4, 5$, max $N = 6, 7$

News

- a tour in the country of lions
  - chances: small N and growing q
  - Lanczos method
    - 1991: singular V and $N = 3$
- new ideas
  - upside-down "tilding" symmetry
    - tilding-invariant variables
    - coupled polynomials
  - matching of recurrences
    - secular polynomials
- new frontiers
  - $q-$dependence clarified
    - classification: four subsets
  - Sunday April 27 preprint
    - quant-ph/0304170

MOTIVATION: Sextic QES wave functions at large dimensions, $\mu \gg 1$

Coordinate-dependence

$$\psi^{(j)}(r) = r^{\ell+1} \left(1 + \frac{r^2}{\mu}\right)^{N-j} \left(1 - \frac{r^2}{\mu}\right)^{j-1} \times$$
$$\times \exp\left(-\frac{1}{2}\alpha_0 r^2 - \frac{1}{4}\alpha_1 r^4\right) \qquad j = 1, 2, \ldots, N\,.$$

Taylor coefficients

$$p_0^{(1)} = 1, \qquad N = 1,$$

$$p_0^{(1)} = p_1^{(1)} = p_0^{(2)} = -p_1^{(2)} = 1, \qquad N = 2,$$

$$p_0^{(1)} = p_2^{(1)} = p_0^{(2)} = -p_2^{(2)} = p_0^{(3)} = p_2^{(3)} = 1,$$
$$p_1^{(1)} = -p_1^{(3)} = 2, \quad p_1^{(2)} = 0, \quad N = 3,$$

ZERO ORDER CONSTRUCTIONS: Magyari's equations

Hill-determinant method at $\mu \gg 1$ (see seminar I)

$$\begin{pmatrix} s & 1 & & & & \\ N-1 & s & 2 & & & \\ & N-2 & s & 3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 2 & s & N-1 \\ & & & & 1 & s \end{pmatrix} \begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_{N-2} \\ p_{N-1} \end{pmatrix} = 0$$

Applications (potentials)

$$V^{(1)}(r) = \Omega r^2 + b r^4 + r^6$$
$$V^{(2)}(r) = \Omega r^{-1} + b r + r^2$$
$$V^{(3)}(r) = \Omega r^{-4/3} + b r^{-2/3} + r^{2/3}$$
$$V^{(4)}(r) = \Omega r^{-3/2} + b r^{-1} + c r^{-1/2} \ .$$

Next-to-sextic potentials

$$V^{(1)}(r) = ar^2 + br^4 + \ldots + r^{10}$$
$$V^{(2)}(r) = ar^{-1} + br + \ldots + r^4$$
$$V^{(3)}(r) = ar^{-4/3} + \ldots + dr^{4/3} + r^2$$
$$V^{(4)}(r) = ar^{-3/2} + \ldots + cr^{-1/2} + dr^{1/2} + r$$
$$V^{(5)}(r) = ar^{-8/5} + \ldots + dr^{-2/5} + r^{2/5}$$
$$V^{(6)}(r) = ar^{-5/3} + \ldots + dr^{-2/3} + fr^{-1/3}$$

Magyari's matrix in general case

$$\begin{pmatrix}
s_1 & 1 & & & & \\
s_2 & s_1 & 2 & & & \\
\vdots & & \ddots & \ddots & & \\
s_q & \vdots & & s_1 & N-2 & \\
N-1 & s_q & & & s_1 & N-1 \\
 & N-2 & s_q & & \vdots & s_1 \\
 & & \ddots & \ddots & & \vdots \\
 & & & 2 & s_q & s_{q-1} \\
 & & & & 1 & s_q
\end{pmatrix}$$

Generalized secular determinants

Implicit solutions at $q = 1$

$$s^3 - 4\,s = 0, \qquad N = 3,$$
$$s^4 - 10\,s^2 + 9 = 0, \qquad N = 4,$$

etc., and at $q = 2$

$$s^6 - 7\,s^3 - 8 = 0, \qquad N = 3$$
$$s^{10} - 27\,s^7 + 27\,s^4 - 729\,s = 0, \quad N = 4$$

etc, and at $q = 3$

$$t^9 - 12\,t^5 - 64\,t = 0, \quad N = 3$$
$$t^{16} - 68\,t^{12} - 442\,t^8 - 50116\,t^4 + 50625 = 0,$$

at $N = 4$ **etc., and, say, at** $q = 5$ **and** $N = 7$

$$P(x) = x^{127} - 60071\,x^{121} + \ldots + c\,x \cdot 10^6 = 0$$

EXTRAPOLATIONS IN N

Equidistant energies at $q = 1$

$$s = s^{(j)} = -N - 1 + 2j, \qquad j = 1, 2, \ldots, N.$$

Equidistant energies at $q = 2$

$$s^{(j)} = N + 2 - 3j, \qquad j = 1, 2, \ldots, j_{max},$$

$$j_{max} = entier \left[\frac{N+1}{2} \right] \; .$$

Equidistant energies and couplings at $q = 3$

$$s = s^{(j)} = N + 3 - 4j,$$

$$r = r^{(j,k)} = t = t^{(j,k)} = -N - 3 + 2j + 2k,$$

$$k = 1, 2, \ldots, k_{max}(j),$$

$$k_{max}(j) = N + 2 - 2j \; ,$$

$$j = 1, 2, \ldots, j_{max} \; .$$

The $q = 4$, $N = 4$ puzzle

for "the simplest" anharmonic $V(r) = \ldots + r^3$

$$P(x) = (x + 3)\ P_{+\sqrt{5}}(x) \cdot P_{-\sqrt{5}}(x),$$

$$P_{\sqrt{5}}(x) = \left(2\,x + 1 + \sqrt{5}\right) \times F \times G$$

$$F = \left(x^2 + x + \sqrt{5}x + 4 + \sqrt{5}\right) > 0$$

$$G = \prod_{k=1}^{7} \left(2\,x^2 + \delta_k\,x + \gamma_k\right) > 0$$

k	γ_k	δ_k
1	18	$-3 + 3\sqrt{5}$
2	$3 + \sqrt{5}$	2
3	$3 + \sqrt{5}$	$-3 - \sqrt{5}$
4	$8 + 2\sqrt{5}$	$7 + \sqrt{5}$
5, 6	$8 + 2\sqrt{5}$	$-3 \pm \sqrt{5}$
7	$8 + 2\sqrt{5}$	$-3 - 3\sqrt{5}$

Factorization not over integers

Extrapolation in N is still feasible

$N=5$	
s_3	s_4
-1	-1
4	4
$\sqrt{5}-1$	$-\sqrt{5}-1$
$-\sqrt{5}-1$	$\sqrt{5}-1$
$(\sqrt{5}+3)/2$	$(-\sqrt{5}+3)/2$
$(-\sqrt{5}+3)/2$	$(\sqrt{5}+3)/2$
$N=6$	
s_3	s_4
0	0
5	5
$\sqrt{5}$	$-\sqrt{5}$
$-\sqrt{5}$	$\sqrt{5}$
$(\sqrt{5}+5)/2$	$(-\sqrt{5}+5)/2$
$(-\sqrt{5}+5)/2$	$(\sqrt{5}+5)/2$

Return of the YEDI at
$q = 5, \quad N = 6$

$$P(x) = x^{91} - 16120\, x^{85} + \ldots = \prod_{j=1}^{4} P_j(x)$$

$$P_1^{(6)} = x \prod_{m=1}^{5} \left(x^2 - m^2\right) \qquad \textit{can vanish}$$

$$P_2^{(6)} = \prod_{k=1}^{2} \prod_{m=-1}^{1} \left(x^2 + 3k\, m\, x + 3k^2\right) > 0$$

$$P_3^{(6)} = \prod_{k=1}^{5} \left(x^2 - k\, x + k^2\right)\left(x^2 + k\, x + k^2\right) > 0$$

$$P_4^{(6)} = \prod_{k=1}^{12} \left(x^2 - b_k\, x + c_k\right)\left(x^2 + b_k\, x + c_k\right) > 0$$

k	c_k	b_k
$1-3$	7	$1, 4, 5$
$4-6$	13	$2, 5, 7$
$7-9$	19	$1, 7, 8$
$10-12$	21	$3, 6, 9$

roots		
s_3	s_4	s_5
-5	5	-5
-3	5	-3
-1	5	-1
1	5	1
3	5	3
5	5	5
-5	-1	1
-3	-1	3
-1	-1	-1
1	-1	1
3	-1	-3
5	-1	-1
-5	2	-2
-3	2	0
-1	2	-4
-1	2	2
1	2	-2
1	2	4
3	2	0
5	2	2

$N = 7$

$$P(x) = x^{127} - 60071\,x^{121} + \ldots + c\,x \cdot 10^6 = 0$$

$$F_1^{(7)} = \left(x^2 - 6^2\right)$$

$$F_2^{(7)} = \left(x^2 - 9\,x + 27\right)\left(x^2 + 27\right)\left(x^2 + 9\,x + 27\right)$$

$$F_3^{(7)} = \left(x^2 - 6\,x + 36\right)\left(x^2 + 6\,x + 36\right)$$

$$F_4^{(7)} = \prod_{k=1}^{6} \left(x^2 - f_k\,x + g_k\right)\left(x^2 + f_k\,x + g_k\right)$$

k	f_k	g_k
$1-3$	28	$2, 8, 10$
$4-6$	31	$4, 7, 11$

New series of elementary bound states in multiply anharmonic potentials

$$V^{[q]}(x) = g_0\,x^2 + g_1\,x^4 + \ldots + g_{2q}\,x^{4q+2}$$

The more standard large-D expansions

$$V_{eff}(R+y) = \frac{\ell(\ell+1)}{(R+y)^2} + (R+y)^4 =$$

$$= 3\,R^4 + 12\,R^2 y^2 - 4\,R\,y^3 + 11\,y^4 - \frac{12}{R}\,y^5 + \frac{14}{R^2}\,y^6 + \ldots$$

$$R = [\ell\,(\ell+1)/2]^{1/6} \gg 1$$

$N = 2$ case

$$\left(\begin{array}{cc} s_1 & 1 \\ s_2 & s_1 \\ \vdots & \vdots \\ s_q & s_{q-1} \\ 1 & s_q \end{array} \right) \left(\begin{array}{c} p_0 \\ p_1 \end{array} \right) = 0\ . \qquad (1)$$

$$p_1 = 1$$
$$s_1 = a \neq 0$$
$$p_0 = -1/a$$
$$s_k = a^k$$
$$a^{q+1} = 1$$

“Tilding” symmetry

$$\begin{pmatrix} a & 1 & 0 \\ A & a & 2 \\ b & A & a \\ B & b & A \\ \vdots & \vdots & \vdots \\ \tilde{a} & \tilde{A} & \tilde{b} \\ 2 & \tilde{a} & \tilde{A} \\ 0 & 1 & \tilde{a} \end{pmatrix} \begin{pmatrix} -1/a \\ 1 \\ -1/\tilde{a} \end{pmatrix} = 0 \ . \qquad (2)$$

$$\begin{pmatrix} A_1 & a_1 & 2 \\ a_2 & A_1 & a_1 \\ A_2 & a_2 & A_1 \\ \vdots & \vdots & \vdots \\ \tilde{a}_1 & \tilde{A}_1 & \tilde{a}_2 \\ 2 & \tilde{a}_1 & \tilde{A}_1 \end{pmatrix} \begin{pmatrix} -1/a_1 \\ 1 \\ -1/\tilde{a}_1 \end{pmatrix} = 0 \ . \qquad (3)$$

The tilding-invariant solutions

$$\xi = a\,\tilde{a} = \tilde{\xi}, \ \rho = a/\tilde{a} = 1/\tilde{\rho}.$$

$$a^2 = \rho\,\xi, \qquad \tilde{a}^2 = \xi/\rho$$

$$\tilde{a}, \ \tilde{a}/a, \ \tilde{a}^2/a, \ \tilde{a}^2/a^2, \ \tilde{a}^3/a^2$$

$$\Sigma_k = \frac{A_k}{\rho^k}, \qquad \sigma_{k+1} = \frac{1}{a}\frac{a_{k+1}}{\rho^k}$$

$\Sigma_0 = 2$ **and** $\sigma_1 = 1$,

$$\Sigma_k = \xi\,\sigma_k - \Sigma_{k-1}\,, \qquad \sigma_{k+1} = \Sigma_k - \sigma_k$$

$$\Sigma_1 = \xi - 2, \;\; \sigma_2 = \xi - 3, \;\; \Sigma_2 = \xi^2 - 4\,\xi + 2, \;\; \ldots\;.$$

$\Sigma_k(\xi)$ **and** $\sigma_{k+1}(\xi)$ **of degree** k

$$A = \rho\,\Sigma_1(\xi), \;\; b = a\,\rho\,\sigma_2(\xi), \;\; B = \rho^2\,\Sigma_2(\xi), \;\ldots\;.$$

Matching conditions

$$q = 4K$$

$$\left(a_j, \; A_j\right), \;\; \left(\tilde{a}_j, \; \tilde{A}_j\right), \qquad j = 1, 2, \ldots, K\,.$$

$a_{K+1} = \tilde{A}_K$ **and** $\tilde{a}_{K+1} = A_K$

$$a\,\sigma_{K+1}\,\rho^K = \Sigma_K\,\tilde{\rho}^K\,,$$

$$\tilde{a}\,\sigma_{K+1}\,\tilde{\rho}^K = \Sigma_K\,\rho^K\,.$$

$$\rho^{4K+1} = 1$$

$$a\,\sigma_{K+1}(a^2) = \Sigma_K(a^2)$$

$q = 4K + 2$

$$\big(A_j,\ a_{j+1}\big)\,,\ \ \big(\tilde{A}_j,\ \tilde{a}_{j+1}\big)\,, \qquad j = 1, 2, \ldots, K\,.$$

$$A_{K+1} = \tilde{a}_{K+1} \textbf{ and } \tilde{A}_{K+1} = a_{K+1}$$

$$a\,\sigma_{K+1}\,\rho^{K} = \Sigma_{K+1}\,\tilde{\rho}^{K+1}$$
$$\tilde{a}\,\sigma_{K+1}\,\tilde{\rho}^{K} = \Sigma_{K+1}\,\rho^{K+1}\,.$$
$$\rho^{4K+3} = 1$$
$$a\,\sigma_{K+1}(a^2) = \Sigma_{K+1}(a^2)\,, \qquad q = 4K{+}2$$

$q = 4K + 1$

$$a_{K+1} = \tilde{a}_{K+1}$$

$$a\,\sigma_{K+1}\,\rho^{K} = \tilde{a}\,\sigma_{K+1}\,\tilde{\rho}^{K}$$
$$\rho^{2K+1} = 1$$
$$A_{K+1} = \tilde{A}_{K} \textbf{ and } \tilde{A}_{K+1} = A_{K}$$
$$\Sigma_{K+1}(\xi) = \Sigma_{K}(\xi)\,, \qquad q = 4K + 1\,.$$

$q = 4K + 3$

$$\left(a_j,\ A_j\right),\ \left(\tilde{a}_j,\ \tilde{A}_j\right), \qquad j = 1, 2, \ldots, K{+}1\,.$$

$$A_{K+1} = \tilde{A}_{K+1}$$

$$\Sigma_{K+1}\,\rho^{K+1} = \Sigma_{K+1}\,\tilde{\rho}^{K+1}$$

$$\rho^{2K+2} = 1$$

$$a_{K+2} = \tilde{a}_{K+1} \textbf{ and } \tilde{a}_{K+2} = a_{K+1}\boldsymbol{)}$$

$$\sigma_{K+2}(\xi) = \sigma_{K+1}(\xi)\,, \qquad\qquad q = 4K{+}3\,.$$

$q = 4K + 1$

$$R^{(K,-)}(\xi) = (\xi - 4)\left[\binom{2K}{0}\,\xi^K - \right.$$

$$\left. - \binom{2K-1}{1}\,\xi^{K-1} + \binom{2K-2}{2}\,\xi^{K-2} - \ldots\right]$$

Tables

Table 1. Sample solution of the matching conditions ($q = 1$ bis 10, $a = 2$ omitted).

real eigenvalues $a = a_1$		
-2		
-1		
-2		
$(\sqrt{5}-1)/2$	$-(\sqrt{5}+1)/2$	
1	-1	-2
(roots of $a^3 + a^2 - 2a - 1$)		
$\sqrt{2}$	$-\sqrt{2}$	-2
-1	(plus roots of $a^3 - 3a - 1$)	
-2	(plus values $\pm\sqrt{(3 \pm \sqrt{5})/2}$)	
(roots of $a^5 + a^4 - 4a^3 - 3a^2 + 3a + 1$)		

Table 2. Pascal-like triangle for the secular equation $\Sigma_{k=0}^{Q} a^k c_k^{(Q)} = 0$ at $q = 2Q$.

	coefficients $c_k^{(Q)}$					
$k =$ / Q	0	1	2	3	4	5
1	1	1				
2	−1	1	1			
3	−1	−2	1	1		
4	1	−2	−3	1	1	
5	1	3	−3	−4	1	1
6	−1	3	6	−4	−5	1
7	−1	−4	6	10	−5	−6
8	1	−4	−10	10	15	−6

Table 3. Secular roots

$$a_n = \sqrt{\xi_{\pm n}} = \sqrt{2 \pm \Xi_n^{[K]}}$$

.

at $q = 4K + 3$ **for** $K = 1, 2, 3, 4, 5$
[$a_0 = 0$ **at odd** K **omitted**]
[$a_3 = 2$ **at** $K = 4, 5$ **omitted**]

distance $\Xi_n^{[K]}$ of a^2 from 2	
$n = 1$	$n = 2$
2	
1	2
$\sqrt{2} \approx 1.41$	2
$(\sqrt{5} - 1)/2 \approx 0.62$	$(\sqrt{5} + 1)/2 \approx 1.62$
1	$\sqrt{3} \approx 1.73$

SUMMARY.
Large–$\mathcal{N}$ perturbation context

Hamiltonians

$$H(\lambda) = H^{(0)} + \lambda\, H^{(1)} + \lambda^2 H^{(2)} + \ldots\,,$$

with perturbations

$$\lambda = \frac{1}{\mu} = \left(\frac{2\gamma}{D}\right)^{1/(q+1)}$$

which are small in large dimensions $D \gg 1$