.

Inverse Feshbach's effective Hamiltonian problem

(reconstruction of Hamiltonians from the effective ones)

Miloslav Znojil

The Czech Academy of Sciences, Nuclear Physics Institute, Hlavní 130, 250 68 Řež, Czech Republic, e-mail: znojil@ujf.cas.cz

.

.

AAMP XXI, Prague, August 27 - 31, 2024

1. Effective Hamiltonians

. **a. Idea: simplification**

. **b. Model-building strategies**

2. Inverse problem

. **a. Motivation**

. **b. Results**

3. Applications

. **a. Open systems: Why?**

. **b. Open systems: How?**

.

.

.

.

1. effective Hamiltonians

.

.

.

1.a. idea: the (Feshbach's) model space

.

.

References

[1] H. Feshbach, *Unified theory of nuclear reactions*, Ann. Phys. (NY) **5**, 357-390, 1958.

[2] P.-O. Löwdin, *Studies in Perturbation Theory. IV. Solution of Eigenvalue Problem by Projection Operator Formalism*, J. Math. Phys. **3**, 969982, 1962.

the projection-operator RECIPE:

.
.

- **consider** projector P on a suitable **model space** and
- **split** the "big" Hilbert space into two subspaces, i.e.,
- **partition** Schrödinger equation $(P+Q)\,H\,(P+Q)\,|\psi\rangle = E\,(P+Q)\,|\psi\rangle$
- **exclude**, via projector $Q = 1 - P$, the would-be "environment",

$$Q\,|\psi\rangle = Q\,\left[E\,I - Q\,H\,Q\right]^{-1}\,Q\,H\,|\phi\rangle\,, \qquad |\phi\rangle = P\,|\psi\rangle$$

- **end up** with the reduced problem $H_{eff}(E)\,|\phi\rangle = E\,|\phi\rangle$ where

$$H_{eff}(E) = PHP + PHQ\,\left[E - QHQ\right]^{-1} QHP\,.$$

an intuitive guide: the **split** of space ($P + Q = I$, $\dim P = 3$)

.

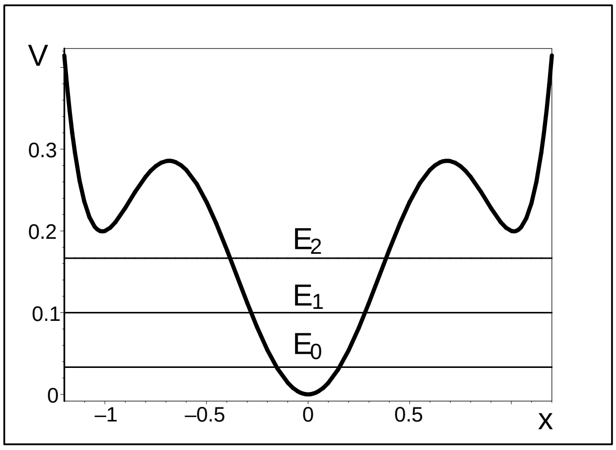

Figure 1: The decoupling of environment in sextic $\mathfrak{v}(x) = x^6 - \boxed{56}/25\, x^4 + 36/25\, x^2$.

.

.

1.b. practical implementations

.

.

.

a typical practical model-building strategy

the most common forms of $H_{eff}(E)$:

.

♡ the choice of **a candidate** for $H_{eff}(E)$: ansatz plus fit

♢ trial and error **amendments**

References

[1] H. Feshbach, *A unified theory of nuclear reactions II*, Ann. Phys. (NY) **19**, 287-313, 1962;

[2] MZ, *Non-selfadjoint operators in quantum physics: ideas, people and trends*, in "Non-Selfadjoint Operators in Quantum Physics: Mathematical Aspects", Eds. F. Bagarello et al, John Wiley & Sons, Hoboken, July 2015, pp. 7 - 58.

the **model space** separation:

♠. a **full-space** dynamical information (Hamiltonian)

.

$$H = \begin{pmatrix} H_{1,1} & H_{1,2} & \dots \\ H_{2,1} & H_{2,2} & \dots \\ \dots & \dots & \dots \end{pmatrix}$$

♣ is **partitioned** using the **split** $P + Q = I$ $(\dim P = N)$:

.

$$H = \left(\begin{array}{ccc|cc} H_{1,1} & \dots & H_{1,N} & H_{1,N+1} & \dots \\ H_{2,1} & \dots & H_{2,N} & H_{2,N+1} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ H_{N,1} & \dots & H_{N,N} & H_{N,N+1} & \dots \\ \hline H_{N+1,1} & \dots & H_{N+1,N} & H_{N+1,N+1} & \dots \\ \dots & \dots & \dots & \dots & \dots \end{array}\right) = \begin{pmatrix} H_{PP} & H_{PQ} \\ H_{QP} & H_{QQ} \end{pmatrix}$$

Jacobi-rotation *alias* Lanczos' **partial tridiagonalization** trick:

$\diamondsuit$ = a **tridiagonal** H_{QQ} $\boxed{\&}$ a **single-element** couplings H_{PQ} and H_{QP} in

$$H = \left(\begin{array}{cccc|cccc} H_{1,1} & \ldots & & H_{1,N} & 0 & \ldots & & \\ \vdots & & & \vdots & \vdots & & & \\ H_{N-1,1} & \ldots & & H_{N-1,N} & 0 & \ldots & & \\ H_{N,1} & \ldots & & H_{N,N} & H_{N,N+1} & 0 & \ldots & \\ \hline 0 & \ldots & 0 & H_{N+1,N} & H_{N+1,N+1} & H_{N+1,N+2} & 0 & \ldots \\ \vdots & & \vdots & 0 & H_{N+2,N+1} & H_{N+2,N+2} & H_{N+2,N+3} & \ddots \\ & & & \vdots & 0 & H_{N+3,N+2} & H_{N+3,N+3} & \ddots \\ & & & & \vdots & \ddots & \ddots & \ddots \end{array} \right)$$

$\heartsuit$ = the information about the $Q-$projected environment is **compactified** physical interpretation of $|N\rangle$: **doorway** state

$$H = \left[\begin{array}{ccc|c||ccccc}
H_{11} & \dots & H_{1N-1} & H_{1N} & 0 & \dots & & \dots & 0 \\
\vdots & & \vdots & \vdots & \vdots & & & & \vdots \\
H_{N-11} & \dots & H_{N-1N-1} & H_{N-1N} & 0 & \dots & & \dots & 0 \\
\hline
H_{N1} & \dots & H_{NN-1} & H_{NN} & H_{NN+1} & 0 & \dots & \dots & 0 \\
\hline\hline
0 & \dots & 0 & H_{N+1N} & a_1 & b_1 & 0 & \dots & 0 \\
0 & \dots & \dots & 0 & c_2 & a_2 & b_2 & \ddots & \vdots \\
\vdots & & & \vdots & 0 & \ddots & \ddots & \ddots & 0 \\
\vdots & & & \vdots & \vdots & \ddots & c_{K-1} & a_{K-1} & b_{K-1} \\
0 & \dots & \dots & 0 & 0 & \dots & 0 & c_K & a_K
\end{array}\right].$$

Lemma 1 *Under our assumptions, the exact effective Schrödinger operator has the N by N matrix form*

$$H_{\mathit{eff}}(E) - E = \left[\begin{array}{cccc} H_{11} - E & \dots & H_{1N-1} & H_{1N} \\ \vdots & \ddots & \vdots & \vdots \\ H_{N-11} & \dots & H_{N-1N-1} - E & H_{N-1N} \\ H_{N1} & \dots & H_{NN-1} & \mathcal{G}(E) \end{array} \right] .$$

Proof. The insertion of semi-tridiagonal H in the definition of $H_{eff}(E)$. □

Operator $H_{\mathit{eff}}(E)$ only differs from its approximate truncated analogue PHP in a single matrix element which is a nonlinear, environment-representing function of the energy,

$$\mathcal{G}(E) = H_{NN} - E + \left[H\, Q \, \frac{Q}{E - Q\, H\, Q} \, Q\, H \right]_{NN} .$$

.

.

.

.

2. inverse problem

2.1. key trick: continued fractions (CF)

Lemma 2 *With $f_{K+1} = 0$ and with CF recurrences*

$$f_k = \frac{1}{a_k - E - b_k f_{k+1} c_{k+1}}, \qquad k = K, K-1, \ldots, 3, 2, (1)$$

we can factorize $Q\,(H-E)\,Q = \mathcal{U}\,\mathcal{F}\,\mathcal{L}$, with elements $1/f_k(E)$ forming diagonal matrix $\mathcal{F}$, and with

$$\mathcal{U} = \begin{bmatrix} 1 & b_1 f_2 & 0 & \ldots & 0 \\ 0 & 1 & b_2 f_3 & \ddots & \vdots \\ 0 & 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1 & b_{K-1} f_K \\ 0 & \ldots & 0 & 0 & 1 \end{bmatrix}, \qquad \mathcal{L} = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ f_2 c_2 & 1 & 0 & \ldots & 0 \\ 0 & f_3 c_3 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 & 0 \\ 0 & \ldots & 0 & f_K c_K & 1 \end{bmatrix}.$$

Lemma 3 *At any $K \leq \infty$, the necessary $Q-$subspace matrix inversion (i.e., the* **construction of** $H_{eff}(E)$) is **trivial** since, with $\alpha_{k+1} = -b_k f_{k+1}$ and $\beta_j = -c_j f_j$,

$$\mathcal{U}^{-1} = \begin{bmatrix} 1 & \alpha_2 & \alpha_2\alpha_3 & \dots & \alpha_2\alpha_3\dots\alpha_K \\ 0 & 1 & \alpha_3 & \ddots & \vdots \\ 0 & 0 & \ddots & \ddots & \alpha_{K-1}\alpha_K \\ \vdots & \ddots & \ddots & 1 & \alpha_K \\ 0 & \dots & 0 & 0 & 1 \end{bmatrix}$$

$$\mathcal{L}^{-1} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \beta_2 & 1 & 0 & \dots & 0 \\ \beta_3\beta_2 & \beta_3 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 & 0 \\ \beta_K\dots\beta_3\beta_2 & \dots & \beta_K\beta_{K-1} & \beta_K & 1 \end{bmatrix}$$

2.2. the **CF-based formulation** of inverse problem:

.

- **assume** the knowledge of $\boxed{\text{function}}$ $\mathcal{G}(E)$

  (= an "experimental" **input** information about dynamics)

- **abbreviate** $H_{NN} = a_0$, $H_{NN+1} = b_0$ and $H_{N+1N} = c_1$

- **recall** Lemma 1 and Lemma 2 and notice the consequence:

$$\mathcal{G}(E) = a_0 - E - b_0 f_1(E) c_1 = 1/f_0(E)$$

- **reconstruct** all of the unknown elements of H in recurrent manner.

(for proof, **recall** just the triple partitioning),

$$
H = \left[\begin{array}{ccc||c|ccccc}
H_{11} & \dots & H_{1N-1} & H_{1N} & 0 & \dots & & \dots & 0 \\
\vdots & & \vdots & \vdots & \vdots & & & & \vdots \\
H_{N-11} & \dots & H_{N-1N-1} & H_{N-1N} & 0 & \dots & & \dots & 0 \\
\hline\hline
H_{N1} & \dots & H_{NN-1} & a_0 & b_0 & 0 & \dots & \dots & 0 \\
\hline
0 & \dots & 0 & c_1 & a_1 & b_1 & 0 & \dots & 0 \\
0 & \dots & \dots & 0 & c_2 & a_2 & b_2 & \ddots & \vdots \\
\vdots & & & \vdots & 0 & \ddots & \ddots & \ddots & 0 \\
\vdots & & & \vdots & \vdots & \ddots & c_{K-1} & a_{K-1} & b_{K-1} \\
0 & \dots & \dots & 0 & 0 & \dots & 0 & c_K & a_K
\end{array}\right].
$$

.

in this notation, our present **main message** is the proposal of

.

= **the existence** of a $\boxed{\text{closed-form}}$ $\underline{\text{reconstruction}}$ of matrices

$$Q^{(+)}HQ^{(+)} = \left[\begin{array}{c|cccccc} a_0 & b_0 & 0 & \ldots & \ldots & 0 \\ \hline c_1 & a_1 & b_1 & 0 & \ldots & 0 \\ 0 & c_2 & a_2 & b_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 0 & c_{K-1} & a_{K-1} & b_{K-1} \\ 0 & \ldots & 0 & 0 & c_K & a_K \end{array} \right]$$

.

i.e., of the **environment-describing** "missing" submatrix of H

strictly speaking, just the <u>unique</u>, renormalized solutions are/can be sought

$$\mathcal{D}\,Q^{(+)}HQ^{(+)}\,\mathcal{D}^{-1} = \begin{bmatrix} a_0 & \rho_0 & 0 & \dots & \dots & 0 \\ 1 & a_1 & \rho_1 & 0 & \dots & 0 \\ 0 & 1 & a_2 & \rho_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 0 & 1 & a_{K-1} & \rho_{K-1} \\ 0 & \dots & 0 & 0 & 1 & a_K \end{bmatrix} = \mathcal{S}^{(K)}_{(reconstructed)}$$

.

where $\rho_j = b_j c_{j+1}$, $j = 0, 1, \dots, K-1$ (cf. CFs)
with diagonal $\mathcal{D}$ s.t. $\mathcal{D}_{00} = 1$, $\mathcal{D}_{11} = 1/c_1$, $\mathcal{D}_{22} = 1/(c_1 c_2)$, $\dots$

-
-
-
-

3. results

MAIN GOAL:

the reconstruction of $\mathcal{S}^{(K)}_{(reconstructed)}$
using "input info" numbers

$$\{E_\alpha\,,\mathcal{G}(E_\alpha)\,(\equiv\;G_\alpha)\}\,,\quad \alpha=0,1,\ldots,J$$

.

will be done by **solving** the

$\boxed{\text{coupled set of nonlinear algebraic equations}}$

$$f_0(E_\alpha)=1/G_\alpha\,,\quad \alpha=0,1,\ldots J\,,\qquad J=2K$$

for the unknown environment-representing elements $\boxed{a_0,\ \rho_0,\ a_1,\ \rho_1,\ \ldots a_K}$.

A. warm up: $K = 1$

$$\mathcal{S}^{(1)} = \left[\begin{array}{cc} a_0 & \rho_0 \\ 1 & a_1 \end{array} \right]$$

THE TASK = solve the three coupled polynomial equations

$$E_\alpha{}^2 + G_\alpha\, E_\alpha - E_\alpha\, (a_0 + a_1) - G_\alpha\, a_1 + a_0 a_1 - \rho_0 = 0\,, \qquad \alpha = 0, 1, 2$$

= tool: **LINEARIZATION** via the change of variables

$$-a_0 - a_1 = x_1\,, \quad a_1 = y_1\,, \quad a_0 a_1 - \rho_0 = x_2$$

= and **CONVERSION** to the matrix inversion,

$$G_\alpha\, y_1 - E_\alpha\, x_1 - x_2 = E_\alpha{}^2 + G_\alpha E_\alpha\,, \qquad \alpha = 0, 1, 2\,.$$

.

closed-form **SOLUTION** at $K = 1$

Lemma 4. *The inversion of mapping* $\{a_0, a_1, \rho_0\} \to \{x_1, x_2, y_1\}$ *has the following nonlinear but compact form,*

$$a_1 = y_1\,, \qquad a_0 = -x_1 - y_1\,, \qquad \rho_0 = -x_1 y_1 - x_2 - {y_1}^2\,.$$

Remark 5. *For negative* ρ_0 $(= b_0 c_1 < 0)$ *the* $K = 1$ *solution* H *is quasi-Hermitian.*

Illustrative example 6. *At* $K = N = 1$ *the quasi-Hermitian* H *with negative* $\rho_0 = -1$ *has real spectrum* $\{\pm\sqrt{3}\}$. *Reconstructed* $a_0 = -2$ *and* $a_1 = 2$ *are obtained from* $\mathcal{G}(E) = (E^2 - 3)/(2 - E)$ *yielding intermediate* $x_1 = 0$, $x_2 = -3$ *and* $y_1 = 2$.

.

B. the next case: $K = 2$

.

$$\mathcal{S}^{(2)} = \begin{bmatrix} a_0 & \rho_0 & 0 \\ 1 & a_1 & \rho_1 \\ 0 & 1 & a_2 \end{bmatrix} .$$

THE SET = **COMPACTIFIED** and **LINEARIZED**

$$-{E_\alpha}^3+(a_2 + a_0 + a_1 - G_\alpha)\, E_\alpha^2+((a_1 + a_2)\, G_\alpha - a_0a_1 - a_1a_2 - a_0a_2 + \rho_0 + \rho_1)\, E_\alpha+$$
$$+\,(-a_1a_2 + \rho_1)\, G_\alpha + a_0a_1a_2 - \rho_0a_2 - \rho_1a_0 = 0\,, \qquad \alpha = 1, 2, 3, 4, 5$$

$$a_0 + a_1 + a_2 = x_1\,, \quad -a_0a_1 + \rho_0 - a_1a_2 - a_0a_2 + \rho_1 = x_2\,,$$
$$a_0a_1a_2 - \rho_0a_2 - a_0\rho_1 = x_3\,, \quad -a_1 - a_2 = y_1\,, \quad a_1a_2 - \rho_1 = y_2$$

$${E_\alpha}^2 x_1 + E_\alpha\, x_2 + x_3 - G_\alpha\, E_\alpha\, y_1 - G_\alpha\, y_2 = {E_\alpha}^3 + G_\alpha\, E_\alpha\,, \qquad \alpha = 1, 2, 3, 4, 5\,.$$

the problem is STANDARDIZED

.

♠ by amending the input (i.e., physical information),

$$\{E_1, E_2, \ldots, E_5, G_1, G_2, \ldots, G_5\} \quad \to \quad \{x_1, x_2, x_3, y_1, y_2\}$$

♣ and by abbreviations

$$p_1 = a_0 + a_1 + a_2\,, \quad p_2 = -a_0a_1 + \rho_0 - a_1a_2 - a_0a_2 + \rho_1$$
$$p_3 = a_0a_1a_2 - \rho_0a_2 - a_0\rho_1\,, \quad q_1 = -a_1 - a_2\,, \quad q_2 = a_1a_2 - \rho_1$$

yielding $2K + 1$ equations, i.e., *five* at $K = 2$,

$$p_1(a_0, a_1, a_2) = x_1\,, \quad p_2(a_0, a_1, a_2, \rho_0, \rho_1) = x_2\,, \quad p_3(a_0, a_1, a_2, \rho_0, \rho_1) = x_3$$
$$q_1(a_1, a_2) = y_1\,, \quad q_2(a_1, a_2, \rho_1) = y_2$$

FINAL SOLUTION at $K=2$

Lemma 7. *At $K=2$ we have*

$$a_0 = y_1 + x_1\,, \quad \rho_0 = -{y_1}^2 - y_1x_1 + y_2 + x_2\,,$$

$$a_1 = -\frac{-2\,y_2y_1 - y_2x_1 + x_3 + {y_1}^3 + {y_1}^2x_1 - y_1x_2}{{y_1}^2 + y_1x_1 - y_2 - x_2}\,, \quad a_2 = -\frac{y_2y_1 + y_2x_1 - x_3}{{y_1}^2 + y_1x_1 - y_2 - x_2}\,,$$

$$\rho_1 = -\frac{C}{\left({y_1}^2 + y_1x_1 - y_2 - x_2\right)^2}$$

$$C = {y_2}^2y_1x_1 - 3\,y_2y_1x_3 + {y_2}^2{x_1}^2 - 2\,y_2x_1x_3 + {x_3}^2 +$$

$$+{y_1}^3x_3 + {y_1}^2x_1x_3 - {y_1}^2x_2y_2 - y_1x_2y_2x_1 - y_1x_2x_3 + {y_2}^3 + 2\,{y_2}^2x_2 + y_2{x_2}^2\,.$$

.

.

$\boxed{\textbf{C.}\text{ the }\textbf{FINAL SOLUTIONS}\text{ at }K = 3\text{ and }K = 4}$

.

.

Remark 8 *At present, the reconstruction of the whole* H *was performed up to* $K = 4$ *and also, for some elements, up to all* K*.*

.

(formulae available, in pdf format, on demand; too long to be displayed here)

Table 1: Complete reconstructions as available, in closed form, at present.

K	input info	matrix elements
0	x_1	a_0
1	x_1, x_2, y_1	a_0, a_1, ρ_0
2	x_1, x_2, x_3 y_1, y_2	a_0, a_1, a_2 ρ_0, ρ_1
3	x_1, x_2, x_3, x_4 y_1, y_2, y_3	a_0, a_1, a_2, a_3 ρ_0, ρ_1, ρ_2
4	x_1, x_2, x_3, x_4, x_5 y_1, y_2, y_3, y_4	a_0, a_1, a_2, a_3, a_4 $\rho_0, \rho_1, \rho_2, \rho_3$

.

.

.

D. PARTIAL SOLUTIONS at arbitrary $K < \infty$

.

.

(sampled in a few Tables, P. T. O.)

Table 2: Matrix elements $H_{MM} = a_0 = a_0(K)$ as reconstructed at all K.

K	0	1	2	3	4	5	...
a_0	x_1	$-x_1 - y_1$	$x_1 + y_1$	$-x_1 - y_1$	$x_1 + y_1$	$-x_1 - y_1$	...

Table 3: Reconstructed $H_{M,M+1}H_{M+1,M} = \rho_0(K)$ with $a_0 = a_0(K) = (-1)^K(x_1+y_1)$ (cf. Table 2).

K	1	2	3	4	5	...
ρ_0	$-x_2 + a_0\, y_1$	$x_2 + y_2 - a_0\, y_1$	$-x_2 - y_2 + a_0\, y_1$	$x_2 + y_2 - a_0\, y_1$	$-x_2 - y_2 + a_0\, y_1$	...

.

. Table 4: $H_{M+1,M+1} = a_1(K)$ – see Tables 2 and 3 for $a_0 = a_0(K)$ and $\rho_0 = \rho_0(K)$, respectively.

K	a_1
1	y_1
2	$-y_1 + (x_3 - a_0\, y_2)/\rho_0$
3	$y_1 - (x_3 + y_3 - a_0\, y_2)/\rho_0$
4	$-y_1 + (x_3 + y_3 - a_0\, y_2)/\rho_0$
5	$y_1 - (x_3 + y_3 - a_0\, y_2)/\rho_0$
6	$-y_1 + (x_3 + y_3 - a_0\, y_2)/\rho_0$
7	$y_1 - (x_3 + y_3 - a_0\, y_2)/\rho_0$
8	$-y_1 + (x_3 + y_3 - a_0\, y_2)/\rho_0$
$\vdots$	$\vdots$

.

$\boxed{\text{what is expected in the \textbf{GENERAL case}}}$

.

Conjecture 9 *The inversion of mapping* $\mathcal{S}^{(K)} \to \{x_1, x_2, \ldots, x_{K+1}, y_1, y_2, \ldots, y_K\}$ *has a closed rational-function form at any* K*.*

.

.

.

.

4. Physics of open quantum systems

.

QM: particle in a potential

.

unitary-evolution ("closed-system") scenario in 1D:

$$\mathrm{i}\,\frac{d}{dt}\,|\psi(t)\succ = \mathfrak{h}\,|\psi(t)\succ \;\;, \qquad \mathfrak{h} = -\frac{d^2}{dx^2} + \mathfrak{v}(x)\,, \qquad x \in \mathbb{R}$$

.

or in dD:

$$\mathrm{i}\,\frac{d}{dt}\,|\psi(t)\succ = \mathfrak{h}\,|\psi(t)\succ \;\;, \qquad \mathfrak{h} = -\triangle + \mathfrak{v}(x)\,, \qquad x \in \mathbb{R}^d$$

environment? why? interplay between subsystems!

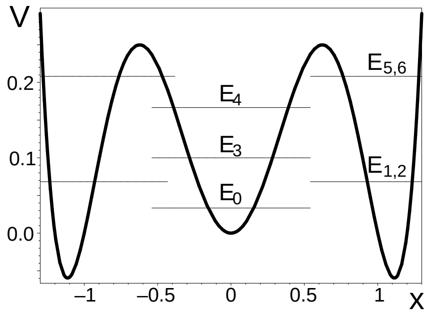

Figure 2: Different domains of bound states in 1D triple-well $\mathfrak{v}(x) = x^6 - \boxed{\mathbf{61}}/25\,x^4 + 36/25\,x^2$ (see MZ, "Arnolds potentials and **quantum catastrophes**", Ann. Phys. 413 (2020) 168050).

technical difficulties: cf. the **dD coupled wells**

.

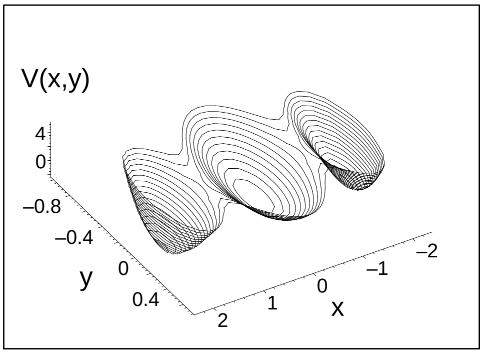

Figure 3: 2D problem – MZ, **"Relocalization switch** in a triple quantum dot molecule in 2D", Mod. Phys. Lett. B. 34 (2020) 2050378.

.

.

.

.

summary

$\boxed{\text{the } Q\text{-projected } \textbf{environment} \text{ are often just the } \textbf{weakly coupled} \text{ states}}$

$\boxed{\text{so that their reconstruction may make sense}}$

.

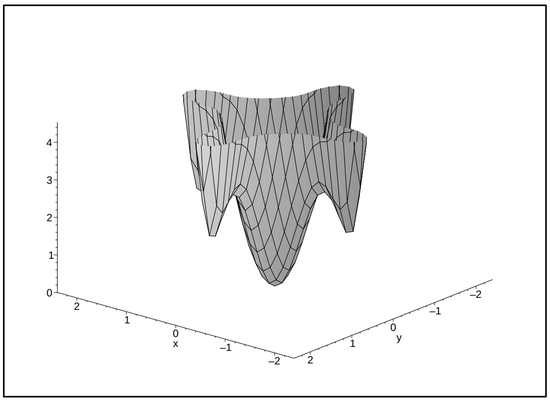

Figure 4: **Our last "realistic application" example** (MZ, Polynomial potentials and **coupled quantum dots** in two and three dimensions, Ann. Phys. 416 (2020) 168161).

.

.

.

.

.

thanks for attention