Spectrum in quantum mechanics and deformed periods

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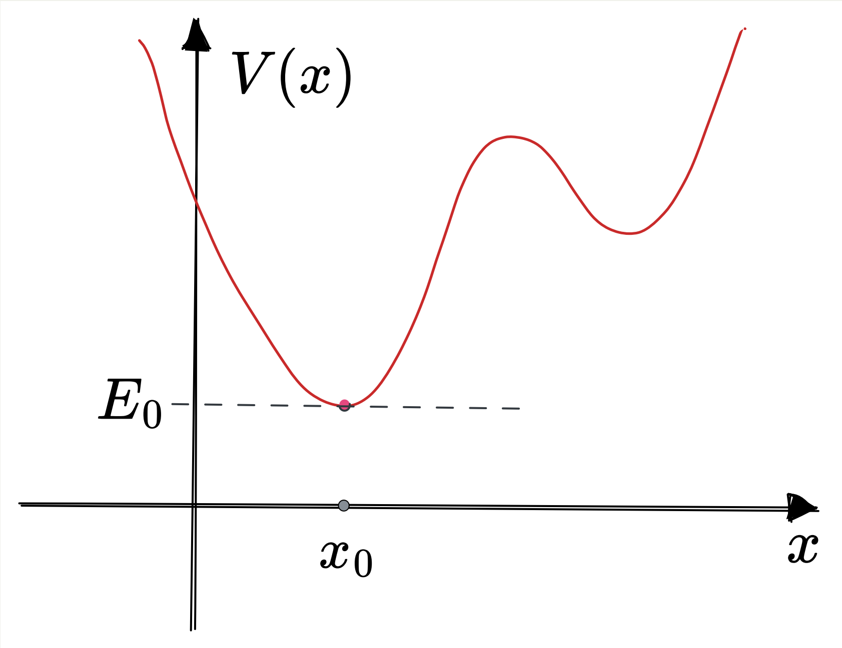
(joint work in progress with A.Soibelman)

Hamiltonian for the particle on line in the presence of a potential:

$$\hat{H} = \frac{\hat{y}^2}{2} + V(\hat{x}) = -\frac{1}{2}\left(\hbar\frac{d}{dx}\right)^2 + V(x), \quad [\hat{x}, \hat{y}] = \mathrm{i}\hbar$$

where V is a real polynomial bounded below.

If the V has only one and non-degenerate absolute minimum:



$\implies$ the eigenvalues and eigenstates for the lower part of the spectrum are close to those for the harmonic oscillator:

$$E_n = V(x_0) + (n + \frac{1}{2})\hbar\omega + O(\hbar^2), \quad n = 0, 1, 2, \dots$$

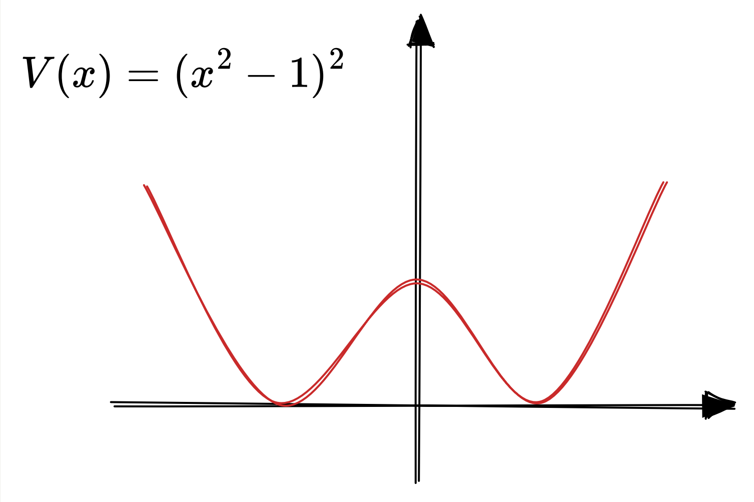
where the frequency is $\omega = \sqrt{V''(x_0)}$.

Perturbation theory: each E_n is a formal series in $\hbar$:

$$E_n \sim E_{n,0} + E_{n,1}\hbar + E_{n,2}\hbar^2 + \cdots \in \mathbb{R}[[\hbar]]$$

Fact: for any given $k \geqslant 0$ coefficient $E_{n,k}$ is a polynomial in n of degree k.

Jean Zinn-Justin for many decades was interested in the case of symmetric double-well, with two degenerate absolute minima:



He studied in this case not only the formal perturbation in $\hbar$, but also instanton corrections $\exp(-\frac{const}{\hbar})$ coming from the tunneling effect. He made several experimental observations on the structure of series, not yet understood.

The goal of my lecture: a new effective algorithm for the calculation of $\hbar$-expansion of $E_0, E_1, \ldots$, *without* quantum mechanics.

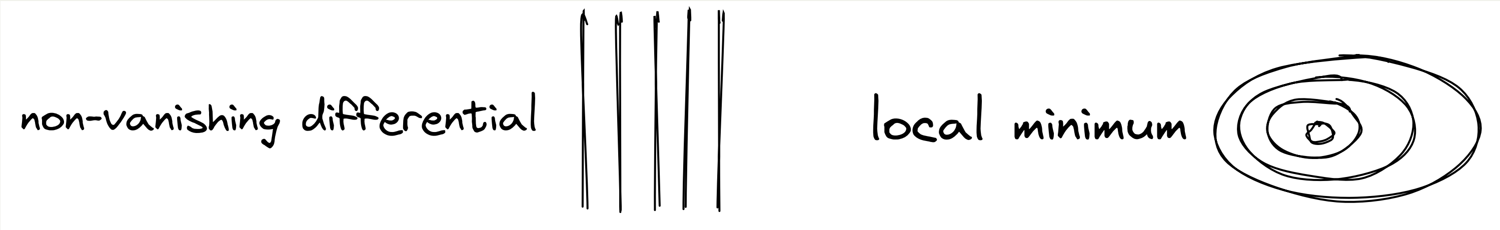
Classical and quantum Birkhoff normal forms.

Let H_{cl} be a classical Hamiltonian, which is a function on $\mathbb{R}^2_{x,y} = T^*\mathbb{R}_x$, with a unique global minimum (like $\frac{y^2}{2} + V(x) = \frac{p^2}{2} + V(q)$ in the case of the classical limit of Schrödinger operator), then after an area-preserving (=symplectic) transformation near the minimum

$$H_{cl}(x,y) = \Phi((x^2+y^2)/2)$$

$$\Phi = \Phi_0 + \Phi_1 t + \Phi_2 t^2 + \cdots \in \mathbb{R}[[t]], \quad \Phi_1 > 0$$

The only invariant of the area-element and a family of closed curves (level sets $H_{cl}^{-1}(c)$, $c \in \mathbb{R}$) is the areas of enclosed domains:



Similarly, consider a formal quantum Hamiltonian

$$\hat{H}_{formal} \in C^\infty(\hat{x}, \hat{y})[[\boldsymbol{\hbar}]] := C^\infty(\mathbb{R}^2_{x,y})[[\boldsymbol{\hbar}]],$$

an element of quantum algebra with the standard $\star$-product:

$$f \star g = \sum_{n \geqslant 0} \frac{(-\mathrm{i}\boldsymbol{\hbar}/2)^n}{n!} \partial_y^n(f)\partial_x^n(g)$$

Then the formally self-adjoint quantum Hamiltonian $\hat{H}_{formal}$ such that its classical limit $H_{cl} := \left(\hat{H}_{formal}\right)_{|\boldsymbol{\hbar}=0}$ has non-degenerate absolute minimum, can be transformed by an automorphism of $\star$-product on $\mathbb{C}[[\hat{x}, \hat{y}, \boldsymbol{\hbar}]]$ to

$$\hat{H}_{formal} = \sum_{i,j \geqslant 0} c_{i,j} \hat{H}^i_{osc} \boldsymbol{\hbar}^j, \quad \hat{H}_{osc} := \frac{1}{2}(\hat{x}^2 + \hat{y}^2)$$

Then for any (pseudo)-differential operator $\hat{H}$ with the asymptotic expansion $\hat{H}_{formal}$, the low part of the spectrum of $\hat{H}$ is

$$E_n = \sum_{i,j \geqslant 0} c_{i,j}(n + \frac{1}{2})^i \, \boldsymbol{\hbar}^{i+j}$$

In particular, the coefficient of $\boldsymbol{\hbar}^k$ is a polynomial in n of degree $\leqslant k$.

This result is a particular case of a general theorem by J.Sjöstrand which is valid for the deformation quantization of arbitrary symplectic manifold (arbitrary number of degrees of freedom). For a moment I will be concentrated on the case of operators in *one* variable.

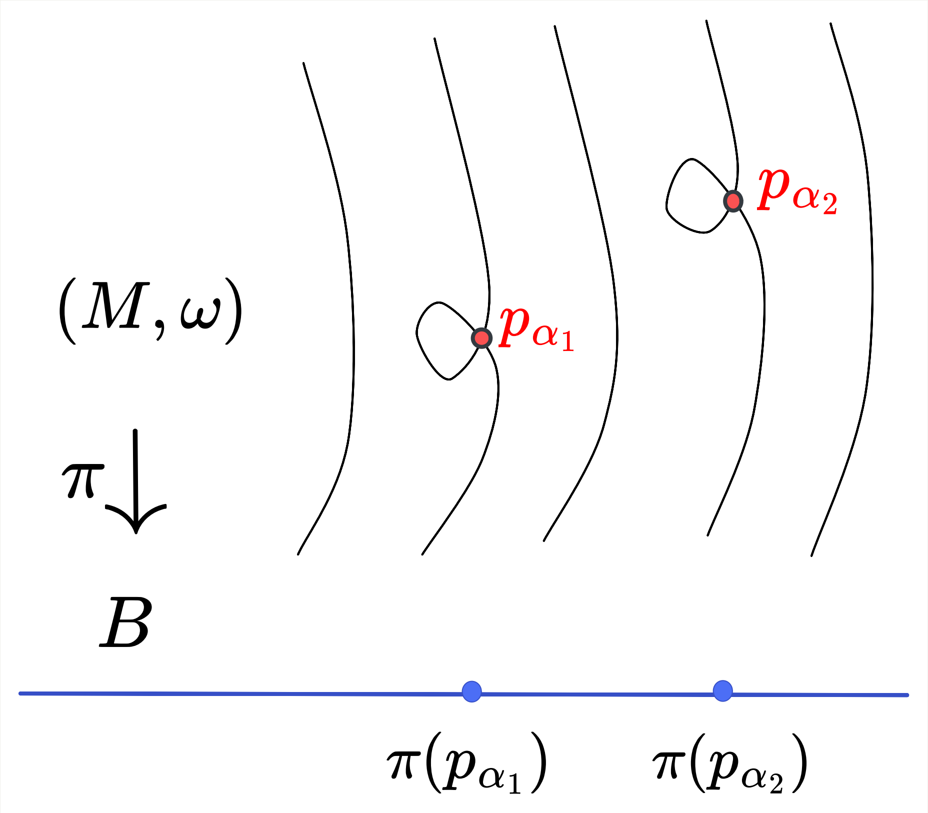
The theory of classical/quantum normal forms near Morse critical point in 2 dimensions is completely algebraic, works over any field of characteristic zero (e.g.. $\mathbb{C}$).

We see that the problem of calculating $\hbar$-expansion of eigenvalues "close to the ground state" makes sense near every critical point.

From now on I forget about real numbers, consider general Hamiltonians $\hat{H} \in \mathbb{C}[\hat{x}, \hat{y}, \hbar] = \mathbb{C}[x, -\frac{i\hbar d}{dx}, \hbar]$ (with the *polynomial* dependence on $\hbar$).

Each complex critical point p_α of the corresponding classical Hamiltionian gives a series in two variables $\Phi_\alpha \in \mathbb{C}[[\hat{H}_{osc}, \hbar]]$ and hence the formal definition of the perturbative spectrum "near" this point.

Classical limit: projection π from $(M, \omega) = (\mathbb{C}^2_{x,y}, dx \wedge dy)$ to the base $B = \mathbb{C}_t$ with Lagrangian fibers.



Assume: all critical points are *Morse*, with *distinct* critical values.

Classical Hamiltonian gives a polynomial map

$$\pi : \mathbb{C}^2_{x,y} \to \mathbb{C}_t, \quad \pi : (x,y) \mapsto t = H_{cl}(x,y)$$

(e.g. $(x,y) \mapsto t = \frac{y^2}{2} + (x^2-1)^2$ in Zinn-Justin's example).

It is formally a classical integrable system, a map from a symplectic manifold $(M,\omega) = (\mathbb{C}^2_{x,y}, dx \wedge dy)$ to a base $B = \mathbb{C}_t$ with Lagrangian fibers.

It fibers are non-compact spectral curves $C_t := \pi^{-1}(t)$ (possibly singular), not necessarily of genus 1. Denote by $\mathcal{H}^1$ the bundle on B whose fiber at $t \in B$ is $H^1(C_t, \mathbb{C})$ (Deligne extension at singular fibers). It carries natural Gauss-Manin connection ∇ with integral monodromy. The dual bundle contains the lattice of integer homology $H_1(C_t, \mathbb{Z})$.

Symplectic form $\omega \in \Omega^2(M)$ can be integrated over cycles in $H_1(C_t, \mathbb{Z})$ giving 1-forms on the base. Hence, we obtain a section $\boldsymbol{s}_{(cl)}$ of the bundle $\mathcal{H}^1 \otimes T^*_B$ with singularities.

Claim: any *formal* quantum Hamiltonian $\in \mathbb{C}[\hat{x}, \hat{y}][[\boldsymbol{\hbar}]]$ gives a deformation $\boldsymbol{s} = \boldsymbol{s}_{(q)}$ of section $\boldsymbol{s}_{(cl)}$ depending formally on $\boldsymbol{\hbar}$ and having poles at the locus of critical values $\{t_\alpha = \pi(p_\alpha)\} \subset B$:

$$\boldsymbol{s} = \boldsymbol{s}_0 + \boldsymbol{s}_1 \boldsymbol{\hbar} + \boldsymbol{s}_2 \boldsymbol{\hbar}^2 + \cdots \in \Gamma(B - \{t_\alpha\}, \mathcal{H}^1 \otimes T^*_B)[[\boldsymbol{\hbar}]]$$

where $\boldsymbol{s}_0 = \boldsymbol{s}_{(cl)}$.

Explanation: *outside of the critical locus* $\{p_\alpha\} \subset M$ we have an equivalence:

$$\boxed{\text{classical integrable systems}/\mathbb{C}[[\hbar]] \iff \text{quantum i.s.}}$$

Local models: classical/quantum Darboux coordinates, $H_{cl} = const + x$ up to transformations $(x, y) \mapsto (x, y + f(x))$, or $\hat{H}_{formal}$ up to transformations $(\hat{x}, \hat{y}) \mapsto (\hat{x}, \hat{y} + f(\hat{x}, \hbar))$ - ***the same group!!***

Therefore, quantization gives a deformation of the *punctured* integrable system

$$(M - \{p_\alpha\}, \omega) \to B$$

Formal deformation theory of a complex surface *minus* finitely many points is *infinite-dimensional*: $H^1(\mathbb{C}^2 - (0,0), \mathcal{O}) \sim x^{-1}y^{-1}\mathbb{C}[x^{-1}, y^{-1}]$

Alternative viewpoint: in classical mechanics, in a neighborhood of a given simple loop $\gamma \subset C_t \subset M$ we have (non-canonical) conjugate action-angle coordinates (I, θ) where θ is multivalued with monodromy $\theta \to \theta + 2\pi$. Coordinate I is in fact well-defined up to a shift, $dI = s_{(cl)}(\gamma) \in \Omega^1_{closed,B}$.

The conditions $\{I, \theta\} = 1$ and θ is defined up to $2\pi\mathbb{Z}$ mean that $Z = e^{\mathrm{i}\theta}$ is well-defined *invertible* function and $\{I, Z\} = \mathrm{i}Z$.

Quantum version: there exists a unique (up to shift) quantum action coordinate $\hat{I}$ in a neighborhood of $\gamma \subset M$ such that

1. $[\hat{I}, \hat{H}] = 0$ (means that $\hat{I}$ belongs to the commutative subalgebra generated by $\hat{H}$)

2. there exists an invertible element $\hat{Z}$ in the neighborhood of γ such that

$$[\hat{I}, \hat{Z}] = \hbar \hat{Z}$$

Properties of quantum deformation s of section $s_{(cl)}$

Near each critical value $t_\alpha \in B$ choose a basis $(\gamma_1, \gamma_2, \dots)$ of cycles in nearby fiber such that the local monodromy is

$$\gamma_1 \mapsto \gamma_1, \quad \gamma_2 \mapsto \gamma_2 + \gamma_1, \quad \gamma_i \mapsto \gamma_i \ \forall \boldsymbol{i} \geqslant \mathbf{3}$$

(i.e. γ_1 is the vanishing cycle and γ_2 intersect γ_1 once). Then we have

1. Regularity constraint: $\int_{\gamma_i} \boldsymbol{s}$ has no poles at $t = t_\alpha$ for $i = 1, 3, 4, \dots$.
Reason: loop γ_i for $i \neq 2$ can be chosen to be well-defined even in the singular fiber C_{t_α}.

2. Relation to the quantum normal form.

The non-singular 1-form $\int_{\gamma_1} \boldsymbol{s}$ with values in $\mathbb{C}[[\boldsymbol{\hbar}]]$ is the differential of certain function

$$T_{can,\alpha} \in \mathbb{C}[[(t - t_\alpha), \boldsymbol{\hbar}]]$$

such that if we write coordinate t as a series $t = \Phi_\alpha(T_{can,\alpha}, \boldsymbol{\hbar})$ then Φ_α is exactly the series appearing in the quantum normal form near p_α.

So, we see that section $\boldsymbol{s}$ determine *almost uniquely* series Φ_α controlling asymptotic expansion of spectra. The ambiguity in the reconstruction of $T_{can,\alpha}$ is a series in $\boldsymbol{\hbar}$ for each critical value t_α :

$$(T_{can,\alpha})_{|t=t_\alpha} = b_{1,\alpha}\boldsymbol{\hbar} + b_{2,\alpha}\boldsymbol{\hbar}^2 + \cdots \in \boldsymbol{\hbar}\,\mathbb{C}[[\boldsymbol{\hbar}]]$$

.

3. Bernoulli constraint

1-form $\int_{\gamma_2} \boldsymbol{s}$ can be written *modulo regular terms* as

$$\left(\log(T_{can,\alpha}) + \sum_{n\geqslant 1} \frac{B_{2n}(1/2)}{2n}\left(\frac{\mathrm{i}\hbar}{T_{can,\alpha}}\right)^{2n}\right) dT_{can,\alpha}$$

Reason: $\log(z) + \log(\frac{d}{dz}) = \psi(z\frac{d}{dz})$ where $\psi(u) = \frac{\Gamma'(u)}{\Gamma(u)}$.

A reformulation: introduce locally functions t_A, t_B on the base such that $dt_A = \boldsymbol{s}(\gamma_1), dt_B = \boldsymbol{s}(\gamma_2)$ (in classical mechanics integrals of $d^{-1}\omega$ over "A-cycle" γ_1 and "B-cycle" γ_2). Then write $t_B = \partial\mathcal{F}_0/\partial t_A$ (special geometry). Bernoulli constraint says that $\mathcal{F}_0 = \log(\Gamma_2)(t_A/\hbar)$+unknown regular term, (cf. perturbative part in Nekrasov-Shatashvili limit).

4.Constraint at infinity

Up to now, any quantum Hamiltonian $\hat{H} \in \mathbb{C}[\hat{x}, \hat{y}]\,[[\boldsymbol{\hbar}]]$ with the given classical limit will satisfy all the previous local constraints. Here we can can have a series in $\boldsymbol{\hbar}$ whose coefficients are differential operators of *growing* degrees. Even for a *bounded* degrees, i.e. for $\hat{H} \in \mathbb{C}[[\boldsymbol{\hbar}]]\,[\hat{x}, \hat{y}]$ we still have an infinite ambiguity.

Experimental observation (should be easily provable): for a *polynomial* $\hat{H} \in \mathbb{C}[\hat{x}, \hat{y}, \boldsymbol{\hbar}]$ the corresponding section $\boldsymbol{s}$ has the property that its expansion at $t \to \infty$ has

1. no poles in an appropriate trivialization of $\mathcal{H}^1 \otimes T_B^*$ at infinity,
2. for every $j \geqslant 0$ the j-th Taylor coefficient of $\boldsymbol{s}$ in coordinate t^{-1} is a ***polynomial*** in $\boldsymbol{\hbar}$, with coefficients depending polynomially on coefficients of $\hat{H}$.

$\Longrightarrow$ One can easily calculate several such coefficients, and get an *overdetermined system* fixing uniquely section s *and* ambiguities $b_{1,\alpha}\hbar + b_{2,\alpha}\hbar^2 + \ldots$ in the reconstruction of canonical coordinates.

Surprise (for me): some control at the limit $\hbar \to \infty$! The whole story is applicable also to q-difference equations, via a control at $q \to 0, q \to \infty$.

All this generalizes immediately to the higher-dimensional case, for quantum integrable systems given by the collection of N commuting differential operators in N variables. In general, we get a formal deformation of a section of the sheaf

$$H^1(fibers) \otimes \Omega^1_{closed,base}$$

uniquely characterized by constraints at the discriminant and at infinity.

Example: $\hat{H} = \left(\frac{\hbar d}{dx}\right)^2 + \frac{x^3}{3} - x$, critical values $t_{1,2} = \pm\frac{2}{3}$.

Connection on the bundle $\mathcal{H}^1$: $\nabla = d + \frac{1}{9t^2-4}\begin{pmatrix} -\frac{3t}{2} & 1 \\ -1 & \frac{3t}{2} \end{pmatrix}$

Section $\boldsymbol{s}$ of $\mathcal{H}^1 \otimes T^*_{base\ \ B=\mathbb{C}_t}$ is

$$\boldsymbol{s} = \boldsymbol{s}_0 + \boldsymbol{\hbar}^2 \boldsymbol{s}_2 + \dots = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} + \boldsymbol{\hbar}^2 \begin{pmatrix} -\frac{3t}{2(4-9t^2)^2} \\ -\frac{28+45t^2}{48(4-9t^2)^2} \end{pmatrix} + \dots$$

Unique solution for regularity/Bernoulli constraints on $\boldsymbol{s}_{2n}$ having poles of order $\leqslant 2n$ at $t = \pm\frac{2}{3}$ and vanishing of order $O(t^{-2})$ at $t \to \infty$ for $n = 1, 2, \dots$.