Quantum Geometry in Semiclassical Approximations

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1. Adiabatic slow-fast systems

Consider a quantum system with a Hamiltonian

$$\widehat{H} = H(x, -\mathrm{i}\varepsilon\nabla_x)$$

given by the Weyl quantization of an operator valued symbol

$$H : \mathbb{R}^{2n} \to \mathcal{L}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}}) \quad \text{acting on} \quad \mathcal{H} = L^2(\mathbb{R}^n_x) \otimes \mathcal{H}_{\mathrm{f}} = L^2(\mathbb{R}^n_x; \mathcal{H}_{\mathrm{f}})\,.$$

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- Concrete realizations of this setting are for example particles with spin, molecules and Bloch electrons in weak fields.

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Let $e : \mathbb{R}^{2n} \to \mathbb{R}$ be an isolated eigenvalue band of H, i.e.

$$H(q,p)\,P_0(q,p) = e(q,p)\,P_0(q,p) \qquad \text{for all } (q,p) \in \mathbb{R}^{2n}\,,$$

and $P_0 : \mathbb{R}^{2n} \to \mathcal{L}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ the corresponding spectral projection.

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States in the range of $\widehat{P}_0 \in \mathcal{L}_{\mathrm{sa}}(\mathcal{H})$ behave “semiclassical” with respect to the classical Hamiltonian function $e(q,p)$.

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E.g.

$$\mathrm{Tr}\left(\widehat{P}_0\, f(\widehat{H}\,)\,\widehat{a}\right) \approx \frac{1}{(2\pi\varepsilon)^n}\int_{\mathbb{R}^{2n}} a(q,p)\, f(e(q,p))\,\mathrm{d}q\mathrm{d}p$$

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States in the range of $\widehat{P}_0 \in \mathcal{L}_{\mathrm{sa}}(\mathcal{H})$ behave "semiclassical" with respect to the classical Hamiltonian function $e(q,p)$.

or

$$\widehat{P}_0\, \mathrm{e}^{\mathrm{i}\widehat{H}\frac{t}{\varepsilon}}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{H}\frac{t}{\varepsilon}}\, \widehat{P}_0 \;\approx\; \widehat{P}_0\, \widehat{a \circ \Phi^e_t}\, \widehat{P}_0$$

2. Superadiabatic subspaces

Adiabatic perturbation theory:[1]

Under suitable technical conditions there exists an orthogonal projection $\widehat{P}$ with symbol

$$P(q,p) = P_0(q,p) + \mathcal{O}(\varepsilon)$$

such that

$$[\widehat{P}\,,\widehat{H}\,] = \mathcal{O}(\varepsilon^{\infty})\,.$$

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Hence, $\widehat{H}$ is almost block-diagonal with respect to $\widehat{P}$,

$$\widehat{H} = \widehat{P}\,\widehat{H}\,\widehat{P} + (1-\widehat{P})\widehat{H}(1-\widehat{P}) + \mathcal{O}(\varepsilon^\infty)$$

while for $\widehat{P}_0$ one only has

$$\widehat{H} = \widehat{P}_0\widehat{H}\,\widehat{P}_0 + (1-\widehat{P}_0)\widehat{H}(1-\widehat{P}_0) + \mathcal{O}(\varepsilon)$$

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2. Superadiabatic subspaces

Goal in the following:

Expand contributions from superadiabatic subspaces to equilibrium expectation values

$$\mathrm{Tr}\left(\widehat{P}\ f(\widehat{H})\,\widehat{a}\right) = \frac{1}{(2\pi\varepsilon)^n}\left(\int_{\mathbb{R}^{2n}} a(q,p)\,f(e(q,p))\,\mathrm{d}q\mathrm{d}p \;+\; \mathcal{O}(\varepsilon)\right)$$

or to Heisenberg operators

$$\widehat{P}\ \mathrm{e}^{\mathrm{i}\widehat{H}\,\frac{t}{\varepsilon}}\,\widehat{a}\,\mathrm{e}^{-\mathrm{i}\widehat{H}\,\frac{t}{\varepsilon}}\ \widehat{P} = \widehat{P}\ \widehat{a\circ\Phi^{e}_{t}}\ \widehat{P}\ +\ \mathcal{O}(\varepsilon)$$

in powers of $\varepsilon \ll 1$ and express as much as possible in terms of a

ε-dependent classical Hamiltonian system.

3. A modified Hamiltonian system

The family of projections $P_0(q,p)$ defines a line-bundle over the classical phase space $\mathbb{R}^{2n}$ that inherits a connection from the trivial vector bundle $\mathbb{R}^{2n} \times \mathcal{H}_{\mathrm{f}}$,

$$\nabla^{\mathrm{B}} := P_0 \nabla \, ,$$

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The components of the associated curvature form $\omega^{(0)} = \omega^{(0)}_{ij} \mathrm{d}z^i \wedge \mathrm{d}z^j$ are

$$\omega^{(0)}_{ij}(z) = 2 \operatorname{Im} \operatorname{tr}_{\mathcal{H}_{\mathrm{f}}} \Big(P_0(z) \, \partial_i P_0(z) \, \partial_j P_0(z) \Big) \,.$$

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The components of the "quantum metric" $g = g_{ij}\, \mathrm{d}z^i \otimes \mathrm{d}z^j$ are

$$g_{ij}(z) := \mathrm{Re}\,\mathrm{tr}_{\mathcal{H}_{\mathrm{f}}} \Big(P_0(z)\, \partial_i P_0(z)\, \partial_j P_0(z) \Big) \,.$$

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Finally define the skew-symmetric matrix

$$M_{ij}(z) = \mathrm{Im}\;\mathrm{tr}_{\mathcal{H}_\mathrm{f}}\Big(\partial_i P_0(z)\,\big(H(z) - e(z)\big)\,\partial_j P_0(z)\Big)\,.$$

3. A modified Hamiltonian system

With an isolated simple energy band e of an adiabatic slow-fast system we associate the classical Hamiltonian

$$h^{(1)}(z) := e(z) - \frac{\varepsilon}{2}\,\mathrm{tr}_{\mathbb{R}^{2n}}\big(J\,M(z)\big)$$

and the symplectic form

$$\Omega^{(1)} := J + \varepsilon\,\omega^{(0)}\,,$$

where

$$J = \begin{pmatrix} 0 & E_n \\ -E_n & 0 \end{pmatrix}\,.$$

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This Hamiltonian system appeared already in Littlejohn-Flynn '91 in the context of Bohr-Sommerfeld quantization for coupled wave equations.

4. Results: first order

Theorem (Stiepan, Teufel; CMP 320, 2013)

Under suitable technical conditions it holds that

$$\mathrm{Tr}\left(\widehat{P}\ f(\widehat{H})\,\widehat{a}\right) = \frac{1}{(2\pi\varepsilon)^n}\left(\int_{\mathbb{R}^{2n}} \mathrm{d}\lambda^{(1)}\ a(z)\, f\left(h^{(1)}(z)\right)\ +\ \mathcal{O}(\varepsilon^2\|a\|_{L^1})\right)$$

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and

$$\left\| \widehat{P}\; \left(\mathrm{e}^{\mathrm{i}\widehat{H}\,\frac{t}{\varepsilon}}\, \widehat{a}\; \mathrm{e}^{-\mathrm{i}\widehat{H}\,\frac{t}{\varepsilon}} - \mathrm{Weyl}^{\varepsilon}\left(a \circ \Phi_t^{(1)}\right)\right) \widehat{P} \right\| = \mathcal{O}(\varepsilon^2)$$

uniformly on bounded time intervals.

Here $\lambda^{(1)}$ is the Liouville measure of $\Omega^{(1)}$ and $\Phi_t^{(1)}$ the Hamiltonian flow.

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For $h(q,p) = \frac{1}{2}|p|^2 + V(q)$ he showed that

$$\mathrm{Tr}\left(\mathrm{e}^{-\beta\widehat{h}}\,\widehat{a}\right) \approx \frac{1}{(2\pi\varepsilon)^n}\int_{\mathbb{R}^{2n}} \mathrm{d}q\mathrm{d}p\; a(q,p)\,\mathrm{e}^{-\beta h(q,p)}\,\left(1+\varepsilon^2 c(q,p)\right)$$

where

$$c(q,p) = \frac{\beta^3}{24}\left(|\nabla V(q)|^2 + \langle p, \nabla^2 V(q) p\rangle_{\mathbb{R}^n} - \frac{3}{\beta}\,\mathrm{tr}\nabla^2 V(q)\right)$$

4. What about the next order?

For more general Hamiltonians and distributions

$$h : \mathbb{R}^{2n} \to \mathbb{R}\,, \quad \widehat{h} = h(x, -\mathrm{i}\varepsilon\nabla_x)\,, \quad f : \mathbb{R} \to \mathbb{C}\,,$$

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$$\mathrm{Tr}\left(\widehat{a}\, f(\widehat{h})\right) = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^{2n}} \mathrm{d}q\mathrm{d}p\; a(q,p)\, f^{\varepsilon}(q,p)\,,$$

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where (by standard pseudo-differential calculus)

$$f^{\varepsilon} := \mathrm{Symb}\left(f(\widehat{h})\right) = f \circ h + \varepsilon^2 f_2 + \mathcal{O}(\varepsilon^3)$$

with

$$f_2 = \tfrac{1}{12}\left(f'''(h) \sum_{|\alpha+\beta|=2} \frac{(-1)^{\beta}}{\alpha!\beta!} (\partial_q^{\alpha}\partial_p^{\beta} h)(\partial_q h)^{\beta}(\partial_p h)^{\alpha} + f''(h)\,\{h,h\}_2 \right)$$

5. Results: second order

Theorem (Gaim, Teufel; 2016)

There is a classical Hamiltonian $h^{(2)} = h^{(1)} + \varepsilon^2 h_2$ and a symplectic form $\Omega^{(2)} = \Omega^{(1)} + \varepsilon^2 \Omega_2$ such that for all observables a and distributions f (satisfying suitable technical conditions)

$$\mathrm{Tr}\left(\widehat{P}\, f(\widehat{H})\,\widehat{a}\right) = \frac{1}{(2\pi\varepsilon)^n}\left(\int_{\mathbb{R}^{2n}} \mathrm{d}\lambda^{(2)}\, a(z)\left(f(h^{(2)}(z)) + \varepsilon^2 Q(z)\right) + \mathcal{O}(\varepsilon^3 \|a\|_{L^1})\right)$$

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where $\lambda^{(2)}$ is the Liouville measure of $\Omega^{(2)}$.

The "quantum corrections" are

$$\begin{aligned} Q &= \tfrac{1}{2} f''(e)\, \|J\nabla e\|_g^2 \\ &\quad - \mathrm{tr}_{\mathbb{R}^{2n}}\left(J\nabla\left(f'(e)\, g\, J\nabla e\right)\right) \\ &\quad + \text{Wigner terms} \end{aligned}$$

5. The “superadiabatic” Hamiltonian system

The classical Hamiltonian is uniquely fixed by the following

Lemma There is a unique scalar semiclassical symbol $h(\varepsilon, q, p)$ such that

$$\widehat{P}\ \widehat{H}\ \widehat{P} = \widehat{P}\ \widehat{h}\ \widehat{P} + \mathcal{O}(\varepsilon^{\infty})\,.$$

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The symplectic form is constructed as follows:

There is a "natural" pointwise projection $\Pi(\varepsilon, z) = P_0(z) + \mathcal{O}(\varepsilon)$ related to the Moyal projection $P(\varepsilon, z) = P_0(z) + \mathcal{O}(\varepsilon)$ defining a line-bundle over phase space such that the modified Berry connection

$$\nabla^{\Pi} = \Pi\nabla$$

has the curvature form

$$\omega = \omega^{(0)} + \varepsilon\,\mathrm{d}S\,.$$

The "superadiabatic" symplectic form is then

$$\Omega := J + \varepsilon\omega\,.$$

6. Application: Fermions in periodic media

In tight binding models for a single particle in a periodic background the Hamiltonian fibers in crystal-momentum representation as

$$(\widehat{H}\,\psi)(k) = H(k)\psi(k)\,, \quad \text{where } \psi \in L^2(\mathbb{B}, \mathbb{C}^N) \text{ and } H : \mathbb{B}_k \to \mathcal{L}(\mathbb{C}^N)$$

with $\mathbb{B}$ the Brillouin torus.

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When adding external non-periodic potentials $A : \mathbb{R}^d \to \mathbb{R}^d$ and $\phi : \mathbb{R}^d \to \mathbb{R}$ the Hamiltonian changes into

$$\widehat{H} = H(k - A(\mathrm{i}\varepsilon\nabla_k)) + \phi(\mathrm{i}\varepsilon\nabla_k)\mathbf{1}_{N\times N}\,.$$

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We can now use the semiclassical formulas to compute currents and free energies for systems of non-interacting fermions in equilibrium states.

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Quantum Hall current at zero temperature:

Let $d = 2$, include a constant magnetic field B_0 with rational flux in the periodic Hamiltonian and set $A(x) = \frac{1}{2} b \wedge x$ and $\phi(x) := \mathcal{E} \cdot x$. Take $f(x) := \mathbf{1}_{(-\infty,\mu)}(x)$ to be the Fermi-Dirac distribution with Fermi energy μ and consider the current operator $\widehat{J} := \frac{\mathrm{i}}{\varepsilon}[\widehat{H}, x]$.

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$$j(b, \mathcal{E}) := \mathrm{Tr}\Big(f(\widehat{H}) \, \widehat{J} \Big)$$

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$$j(b, \mathcal{E}) := \mathrm{Tr}\Big(f(\widehat{H})\,\widehat{J}\Big) = \sum_{n=1}^{m} \mathrm{Tr}\Big(\widehat{P}_n f(\widehat{H})\,\widehat{J}\Big)$$

6. Application: Fermions in periodic media

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Note that our theorems also hold for the phase space $T^*\mathbb{B}$ with nontrivial topology where eigen-bundles can be non-trivializable.

6. Application: Fermions in periodic media

The free energy of a such a Fermi gas at positive temperature is

$$p(b, \beta, \mu) := \beta^{-1} \mathrm{Tr} \ln \left(1 + \mathrm{e}^{-\beta \left(\widehat{H}^{b} - \mu \right)} \right).$$

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We can write also this as a sum of contributions from all Bloch bands:

$$p(b,\beta,\mu) \quad = \quad \frac{1}{\beta}\sum_{n}\int_{\mathbb{B}}\left[\ln\left(1+\mathrm{e}^{-\beta\left(h_n^{(2)}(k)-\mu\right)}\right)+Q_n(k)\right]\lambda_n^{(2)}(\mathrm{d}k)+\ \mathcal{O}(b^3)$$

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$$\begin{aligned} S(\beta,\mu) \;&:=\; \partial_b^2\, p(b,\beta,\mu)|_{b=0} \\ &=\; \frac{2}{\beta}\sum_{n}\int_{\mathbb{B}}\Big[\, f(e_n(k))\,\lambda_{2,n}(k) \\ &\quad + f'(e_n(k))\big(m_n(k)\,\omega_n(k)+h_{2,n}(k)\big) \\ &\quad + f''(e_n(k))\Big(\tfrac{1}{2}m_n(k)^2+\|\nabla e_n(k)^{\perp}\|^2_{g_n(k)} \\ &\qquad -\tfrac{1}{24}\varepsilon_{jk}\varepsilon_{kl}(\nabla^2 e_n)_{jk}(k)(\nabla^2 e_n)_{li}(k)\Big)\Big]\,\mathrm{d}k \end{aligned}$$

where $f(x)=\ln(1+\exp(-\beta(x-\mu)))$.

Thanks for your attention!