Effective dynamics for constrained quantum systems

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To Shelly’s 60th Birthday

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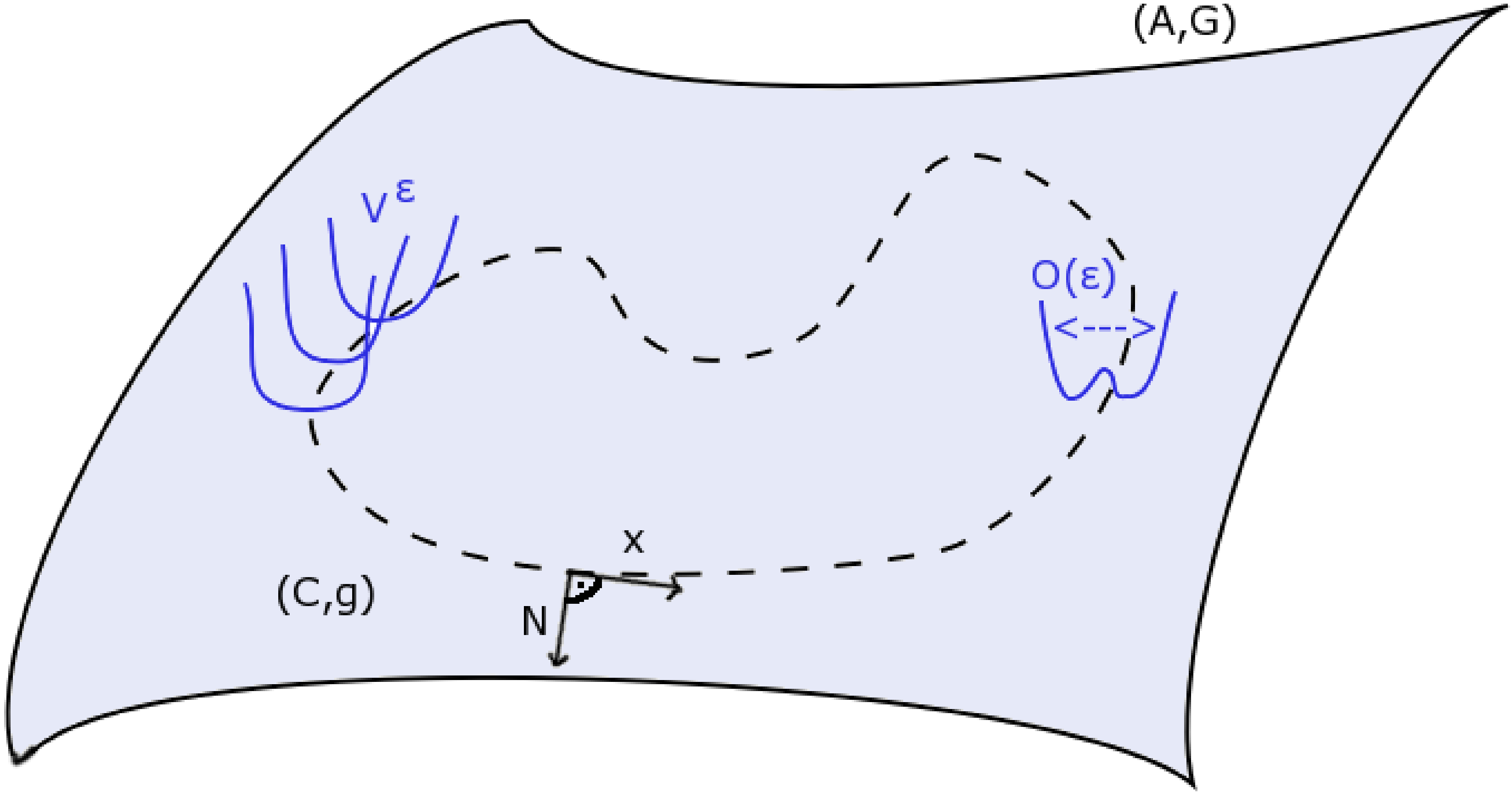
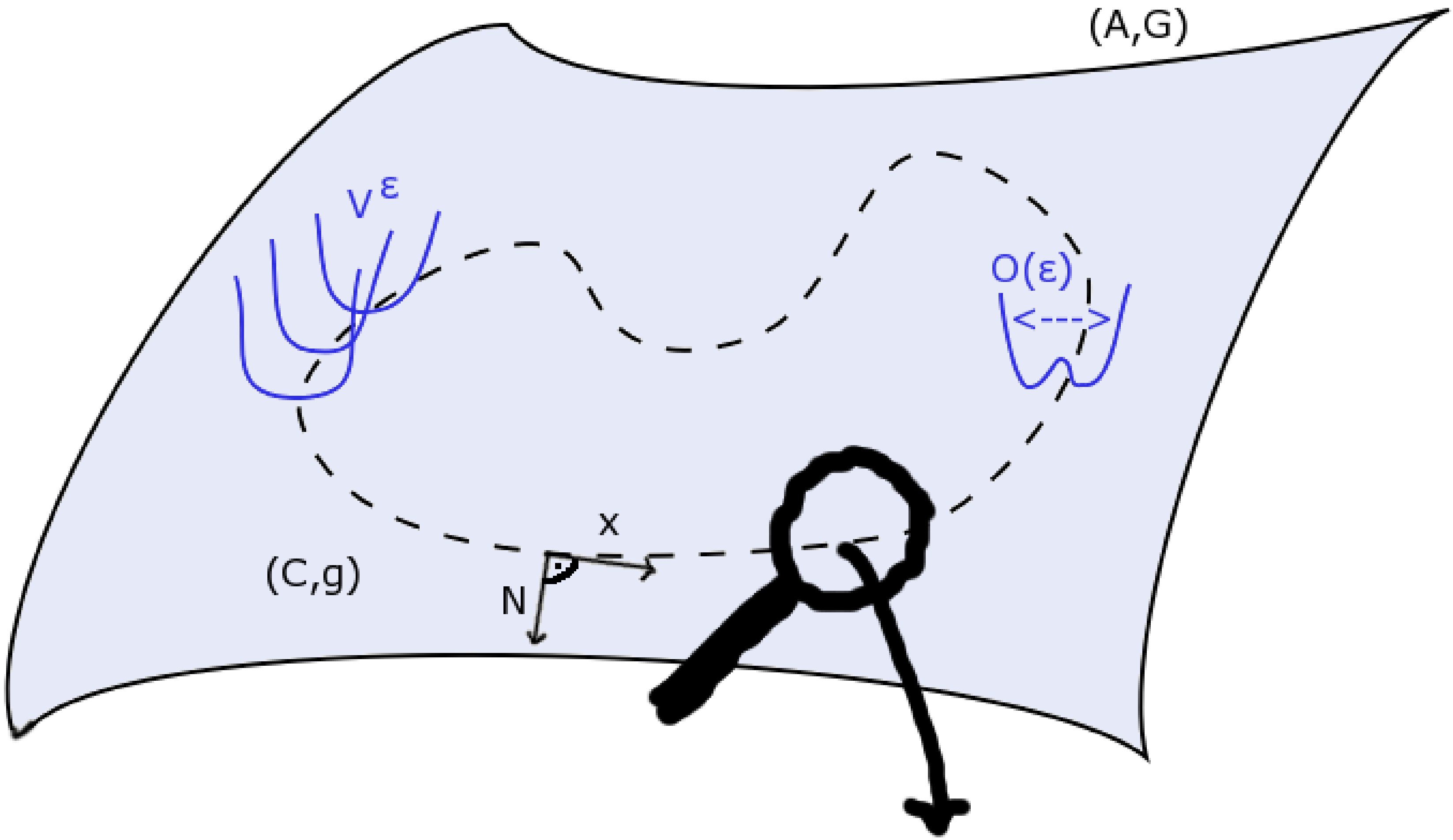
Jointly with Jakob Wachsmuth

Macroscopic picture

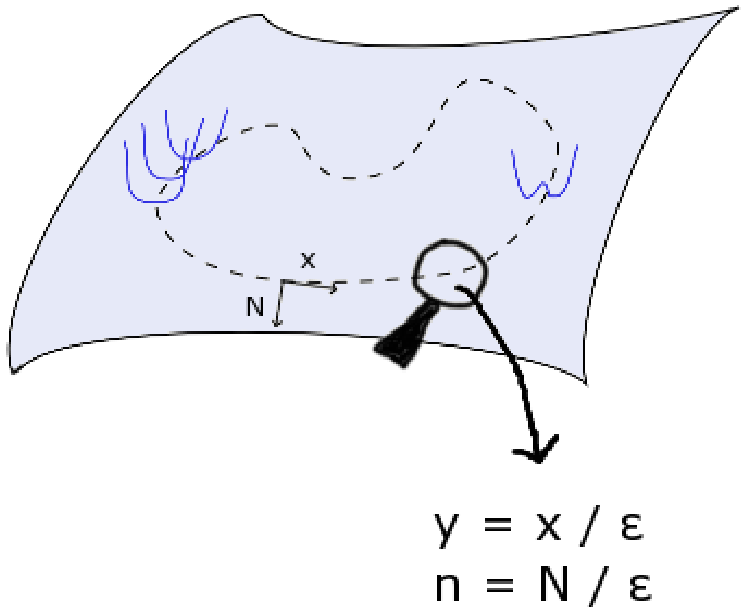


Schrödinger equation on a Riemannian manifold $(\mathcal{A}, G)$ with a Potential $V^\varepsilon : \mathcal{A} \to \mathbb{R}$ that approximately confines to a submanifold $(\mathcal{C}, g)$.

Macroscopic picture



Rescaling to the microscopic variables
$y = x/\varepsilon$ and $n = N/\varepsilon$ yields



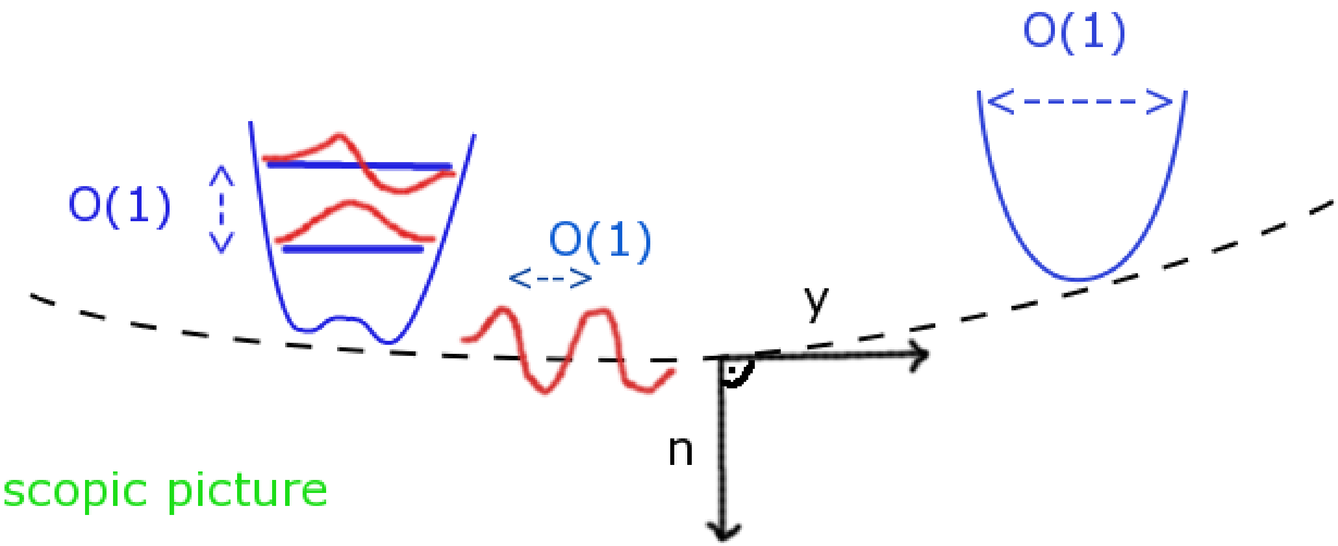
In the **microscopic variables**

-the width of the potential is $\mathcal{O}(1)$,

-derivatives of the solution are $\mathcal{O}(1)$,

-derivatives of the metric are $\mathcal{O}(\varepsilon)$,

-derivatives of the potential tangent to $\mathcal{C}$ are $\mathcal{O}(\varepsilon)$,



Microscopic picture

In the microscopic variables (y, n) the Schrödinger equation thus reads

$$\mathrm{i}\,\partial_t \Psi = -\Delta_{G^\varepsilon}\Psi + V(\varepsilon\, y, n)\Psi \quad .$$

Going back to macroscopic variables $(x = \varepsilon\, y, N = \varepsilon\, n)$ one finds

$$\mathrm{i}\,\partial_t \Psi^\varepsilon = -\varepsilon^2 \Delta_G \Psi^\varepsilon + V(x, N/\varepsilon)\Psi^\varepsilon \quad .$$

For $\varepsilon \ll 1$ the solutions of this equation concentrate on the submanifold $\mathcal{C}$.

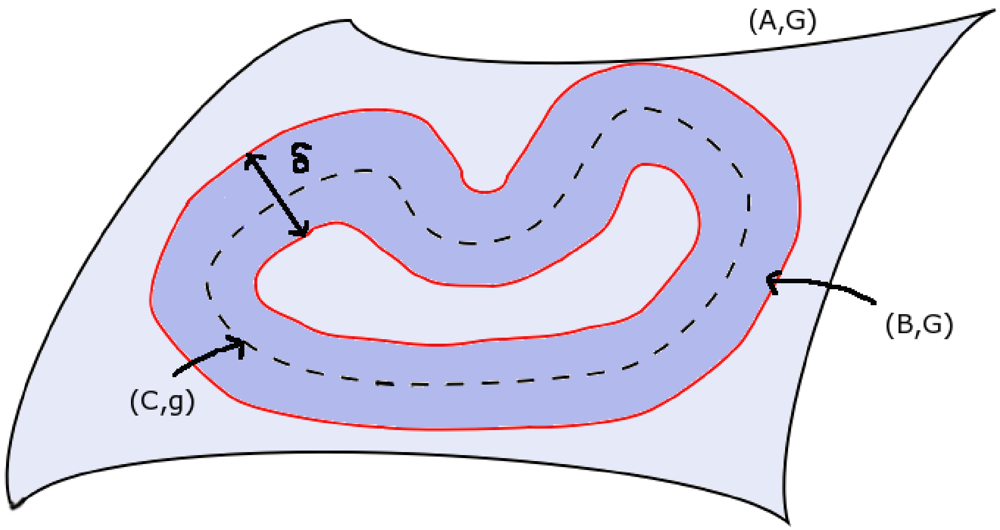
Our goal is to derive an effective Schrödinger equation on $\mathcal{C}$ such that the solutions $\psi^\varepsilon(t)$ of the effective equation approximate the solutions $\Psi^\varepsilon(t)$ of the full equation in a suitable sense.

Applications

Molecular dynamics: In the Born-Oppenheimer approximation the nuclei move in an effective potential given by the electronic energy surfaces. Such surfaces often have pronounced valleys of the type considered here.

Quantum wave guides: Wave guides for single atoms with adiabatically varying potentials are considered theoretically and recently also experimentally.

- $(\mathcal{A}, G)$ is a Riemannian manifold of dimension dim$\mathcal{A} = n + m$.
- $\mathcal{C} \subset \mathcal{A}$ is a submanifold without boundary of dimension dim$\mathcal{C} = n$.
- $(\mathcal{C}, g = G|_{\mathcal{C}})$ is called the constraint manifold.
- $\mathcal{B}_\delta$ is a closed, non-self-intersecting δ-tube around $\mathcal{C}$.



We construct a diffeomorphism

$$\phi : \mathcal{B}_\delta \to N\mathcal{C} \,,$$

which is an isometry on $\mathcal{B}_{\delta/2}$.

For $\delta \gg \varepsilon > 0$ the solution lives in $\mathcal{B}_{\delta/2}$ up to exponentially small terms.

Assumption 1:

Let $V : N\mathcal{C} \to \mathbb{R}$ satisfy a number of technical conditions.

Problem:

Find approximate solutions of the Schrödinger equation

$$\mathrm{i}\,\partial_t \Psi^\varepsilon = -\varepsilon^2 \Delta_G \Psi^\varepsilon + V(x, N/\varepsilon)\Psi^\varepsilon =: H^\varepsilon \Psi^\varepsilon$$

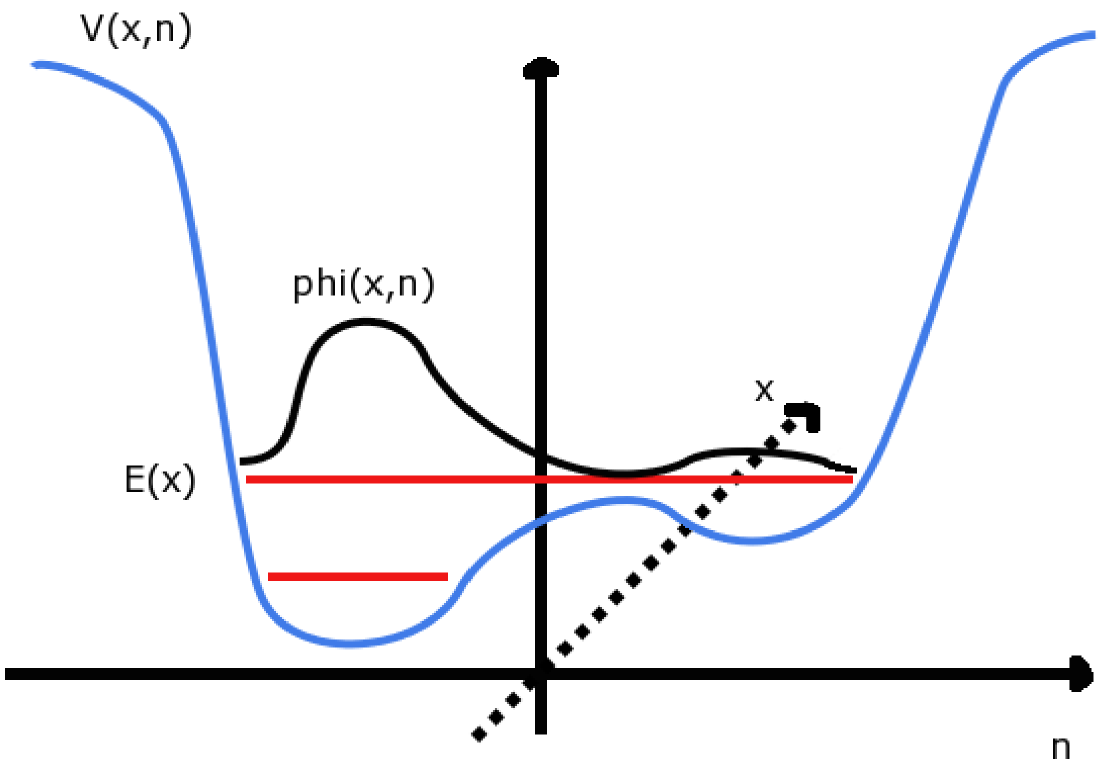
on $\mathcal{H} = L^2(N\mathcal{C})$.

Basic idea: For $x \in \mathcal{C}$ define the local normal Hamiltonian as

$$H_{\mathsf{f}}(x) := -\Delta_n + V(x,\cdot) \qquad \text{on} \quad \mathcal{D}(H_{\mathsf{f}}(x)) \equiv \mathcal{D}(H_{\mathsf{f}}) \subset L^2(\mathbb{R}^m)$$

and let $\varphi(x,n)$ be a normalized eigenfunction,

$$H_{\mathsf{f}}(x)\,\varphi(x,\cdot) = E(x)\,\varphi(x,\cdot)\,.$$



<u>Basic idea:</u> For $x \in \mathcal{C}$ define the local normal Hamiltonian as

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Then states in the subspace

$$\mathcal{P}_0 := \{\psi(x)\varphi(x,n) : \psi \in L^2(\mathcal{C},g)\} \subset L^2(N\mathcal{C})$$

should be approximately invariant in the sense that for $\Psi_0^\varepsilon = \psi_0^\varepsilon\varphi$ the solution of the SE satisfies

$$\Psi^\varepsilon(t,x) \approx \psi^\varepsilon(t,x)\varphi(x,n)\,,$$

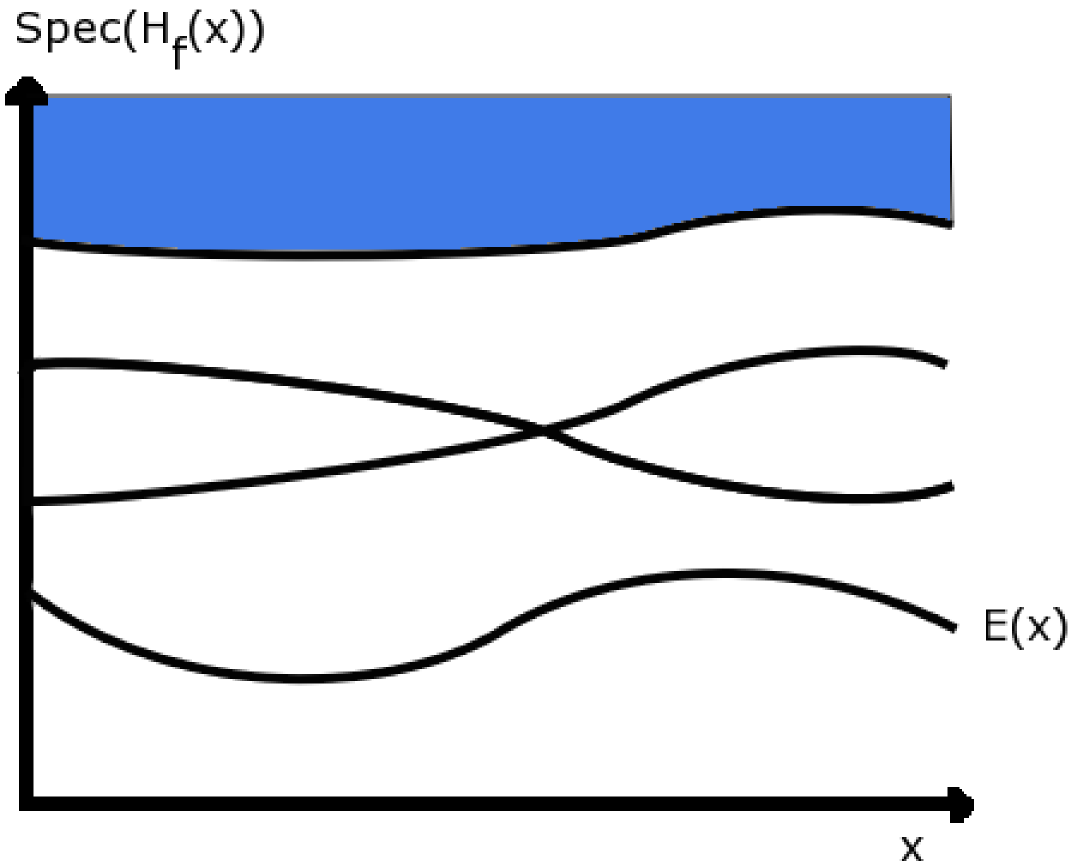
where $\psi^\varepsilon(t,x)$ solves an effective SE on $\mathcal{C}$,

$$\mathrm{i}\,\partial_t\psi^\varepsilon(t,x) = -\varepsilon^2\Delta_g\psi^\varepsilon(t,x) + E(x)\psi^\varepsilon(t,x) \quad .$$

Assumption 2:

$H_{\mathsf{f}}(x)$ has a simple eigenvalue $E(x)$ such that

$$\inf_{x\in\mathcal{C}} \mathrm{dist}(E(x), \mathrm{Spec}(H_{\mathsf{f}}(x)) \setminus E(x)) \geq c > 0\,.$$



Theorem 1: Let $E_{\text{max}} < \infty$. There exist a Riemannian metric g_{eff} on $\mathcal{C}$, a unitary mapping

$$\mathcal{U}_0 : \mathcal{P}_0 \to L^2(\mathcal{C}, g_{\text{eff}}),$$

a self-adjoint operator H_{eff} on $L^2(\mathcal{C}, g_{\text{eff}})$, $C < \infty$ and $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$

$$\left\| \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t} - \mathcal{U}_0^* \, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\text{eff}} t} \, \mathcal{U}_0 \right) P_0 \, \chi_{(-\infty, E_{\text{max}}]}(H^\varepsilon) \right\| < C \, \varepsilon \, (\varepsilon |t| + 1) .$$

The effective Hamiltonian is given by the quadratic form

$$\langle \psi, \, H^\varepsilon_{\text{eff}} \, \psi \rangle = \int_{\mathcal{C}} \left(g^*_{\text{eff}}(p^\varepsilon_{\text{eff}} \, \psi, \, p^\varepsilon_{\text{eff}} \, \psi) + E|\psi|^2 \right) \mathrm{d}g_{\text{eff}} \, ,$$

where

$$\begin{aligned} p^\varepsilon_{\text{eff}} &= \mathrm{i}\varepsilon \mathrm{d} + \varepsilon \mathrm{i} \langle \varphi, \tilde{\mathrm{d}} \varphi \rangle \, , \\ g_{\text{eff}} &= g + \varepsilon II(\langle \varphi, n^\alpha \varphi \rangle) \, , \end{aligned}$$

$$\mathcal{U}_0^* : L^2(\mathcal{C}, g_{\text{eff}}) \to \mathcal{H} \, , \qquad \psi(x) \mapsto \psi(x) \varphi(x, n) \cdot \sqrt{\frac{\sqrt{\det G(x,n)}}{\sqrt{\det g_{\text{eff}}(x)}}}$$

Theorem 2: Let $E_{\mathrm{max}} < \infty$. There exist a Riemannian metric g_{eff} on $\mathcal{C}$, a unitary mapping

$$\mathcal{U}_\varepsilon : \mathcal{P}_\varepsilon \to L^2(\mathcal{C}, g_{\mathrm{eff}}) \,,$$

a self-adjoint operator H_{eff} on $L^2(\mathcal{C}, g_{\mathrm{eff}})$, $C < \infty$ and $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$

$$\left\| \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t} - \mathcal{U}_\varepsilon{}^* \, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{eff}} t} \, \mathcal{U}_\varepsilon \right) P_\varepsilon \, \chi_{(-\infty, E_{\mathrm{max}}]}(H^\varepsilon) \right\| < C \, \varepsilon^3 \, |t| \,.$$

The effective Hamiltonian is given by the quadratic form

$$\begin{aligned} \langle \psi, \, H^\varepsilon_{\mathrm{eff}} \, \psi \rangle \; &= \; \int_{\mathcal{C}} \Big(g^*_{\mathrm{eff}}(p^\varepsilon_{\mathrm{eff}} \, \psi, \, p^\varepsilon_{\mathrm{eff}} \, \psi) + E|\psi|^2 \\ &\quad + \varepsilon^2 \, \mathcal{M}(p\psi, p\psi) + \varepsilon^2 \, (V_{\mathrm{BH}} + V_{\mathrm{geom}}) \, |\psi|^2 \Big) \, \mathrm{d}g_{\mathrm{eff}} \end{aligned}$$

where, e.g.,

$$V_{\mathrm{geom}} = -\tfrac{1}{4}|\tau|^2 + \tfrac{1}{2}\kappa_{\mathcal{C}} \,.$$

Mitchell (Phys. Rev. A 2001); Froese, Herbst (CMP 2001):

(earlier Jensen, Koppe '71; da Costa '81–'86)

These authors assume that

- the kinetic energy in the tangential direction is small, i.e. that

$$\| \varepsilon \mathrm{d}_x \Psi^\varepsilon \|^2 = \mathcal{O}(\varepsilon^2)\,.$$

- up to orthogonal transformations the confining potential is constant along the manifold, i.e. that

$$V^\varepsilon(x,N) = V^\varepsilon(x_0, \phi(N)) \qquad \text{for some} \quad \phi \in SO(m)\,;$$

Dell'Antonio, Tenuta (J. Phys. A 2006):

They construct approximate solutions having the form of sharply peaked Gaussian wave packets for a slightly different scaling.

Our result for small kinetic energies and constant eigenvalue:

For $E \equiv$ const. and $\|\varepsilon \mathrm{d}\psi\|^2 = \mathcal{O}(\varepsilon^2)$ the Hamiltonian

$$\begin{aligned}\langle \psi,\, H^{\varepsilon}_{\mathrm{eff}}\, \psi\rangle \;&=\; \int_{\mathcal{C}} \Big(g^{*}_{\mathrm{eff}}(p^{\varepsilon}_{\mathrm{eff}}\,\psi,\, p^{\varepsilon}_{\mathrm{eff}}\,\psi) + E|\psi|^2 \\ &\quad + \varepsilon^2\, \mathcal{M}(p^{\varepsilon}\psi, p^{\varepsilon}\psi) + \varepsilon^2\, (V_{\mathrm{BH}} + V_{\mathrm{geom}})\, |\psi|^2 \Big)\, \mathrm{d}g_{\mathrm{eff}}\end{aligned}$$

is reduced to

$$\langle \psi,\, H^{\varepsilon}_{\mathrm{eff}}\, \psi\rangle = \varepsilon^2 \int_{\mathcal{C}} \Big(g^{*}(p^{0}_{\mathrm{eff}}\psi, p^{0}_{\mathrm{eff}}\psi) + V_{\mathrm{geom}}|\psi|^2 \Big)\, \mathrm{d}g + \mathcal{O}(\varepsilon^3)\,,$$

which corresponds to the result of Mitchell.

Rubin and Ungar '57 find for the effective Hamiltonian function of a classical particle

$$H_{\text{eff}}(q^{\|}, p^{\|}) = g^*(p^{\|}, p^{\|}) + V_{\text{eff}}(q^{\|})$$

with

$$V_{\text{eff}}(q^{\|}) = \sum_{j=1}^{m} \theta_j(q_0, p_0)\, \omega_j(q^{\|})\,.$$

Here $\omega_j(q^{\|})$ are the normal frequencies of the confining harmonic potential and $\theta_j(q_0, p_0)$ is the initial action in this mode,

$$\theta_j(q, p) = \frac{1}{\omega_j(q^{\|})} g^*(p_j^{\perp}, p_j^{\perp}) + \frac{\omega_j(q^{\|})}{\varepsilon^4} \langle q_j^{\perp}, q_j^{\perp} \rangle_{\mathbb{R}^m}\,.$$

The main steps of the proof are

1. Expand metric locally near $\mathcal{C}$ and use exponential decay of normal eigenfunctions.

2. Apply adiabatic perturbation theory in local coordinates
   [Martinez-Nenciu-Sordoni, Panati-Spohn-T]

3. Identify geometric terms in order to patch together local results

Thank you!