Effective dynamics for constrained quantum systems

Jakob Wachsmuth

Mathematical Institute, University of Tübingen

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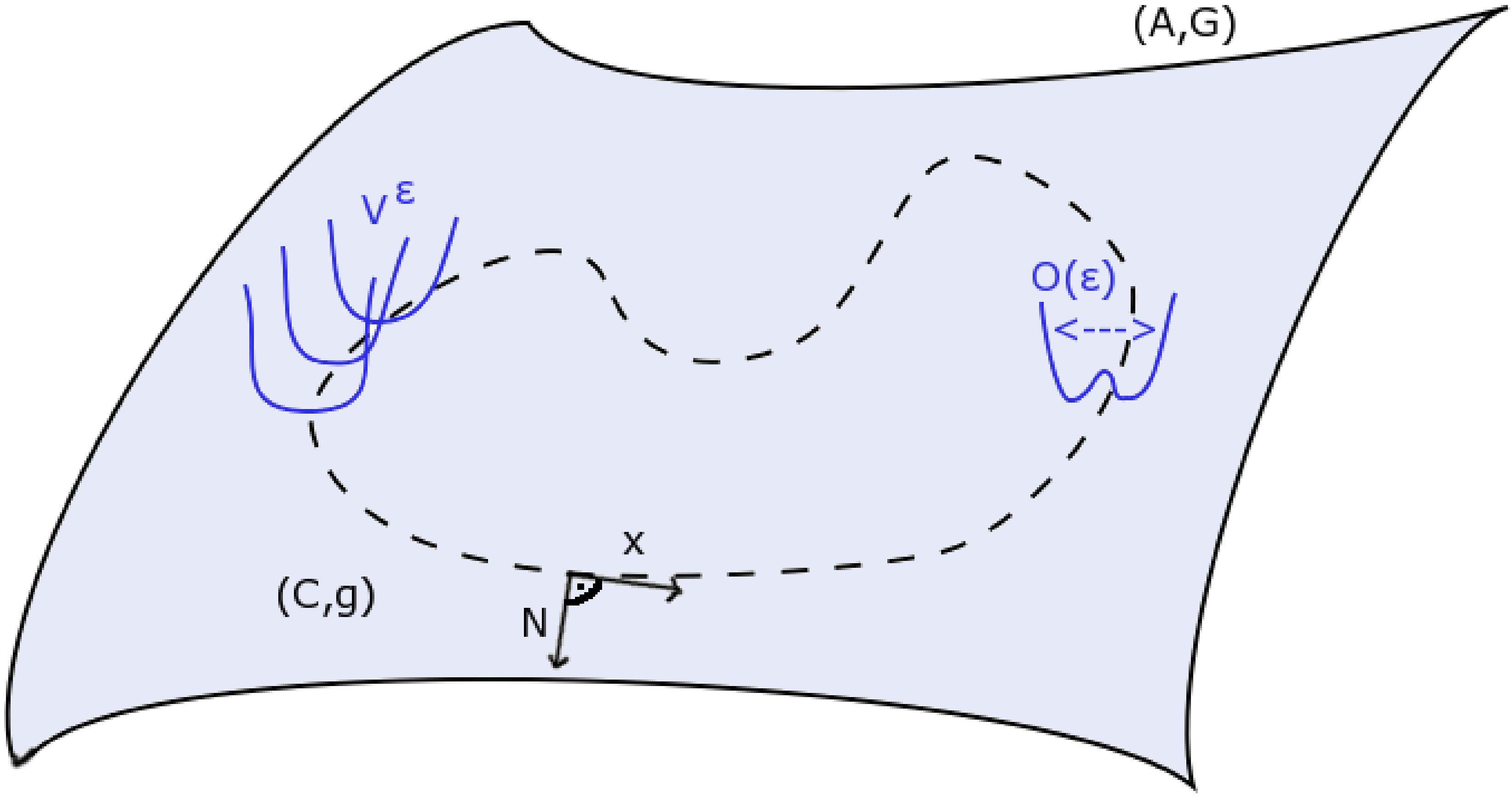
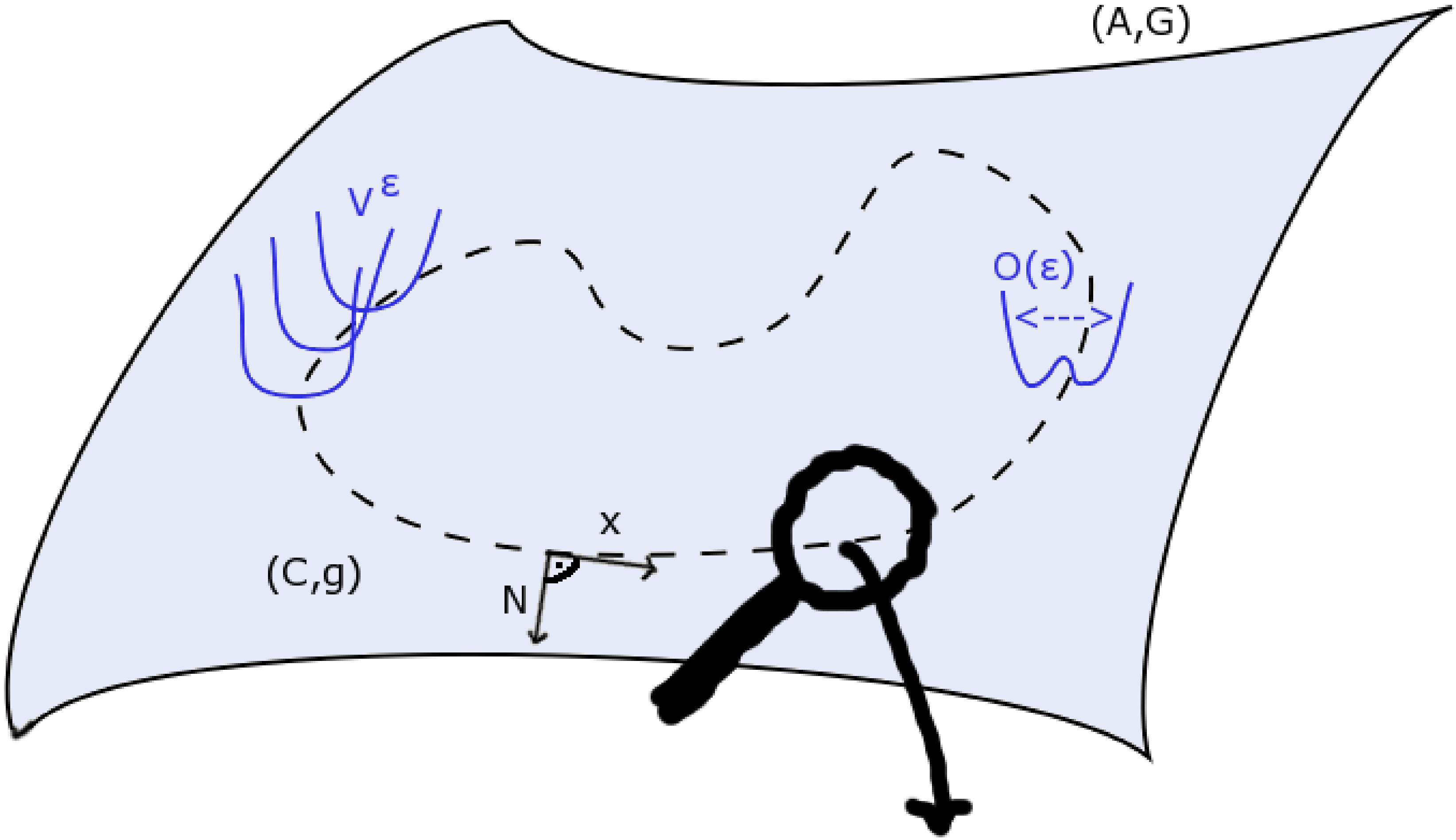
Jointly with Stefan Teufel

Macroscopic picture

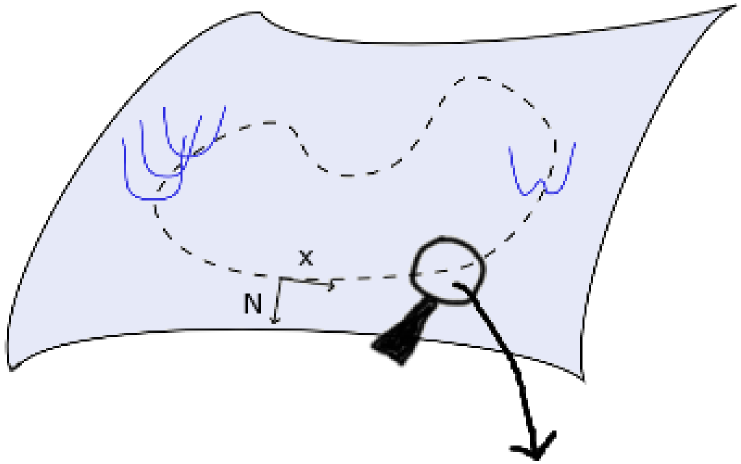


Schrödinger equation on a Riemannian manifold $(\mathcal{A}, G)$ with a Potential $V^\varepsilon : \mathcal{A} \to \mathbb{R}$ that approximately confines to a submanifold $(\mathcal{C}, g)$.

Macroscopic picture



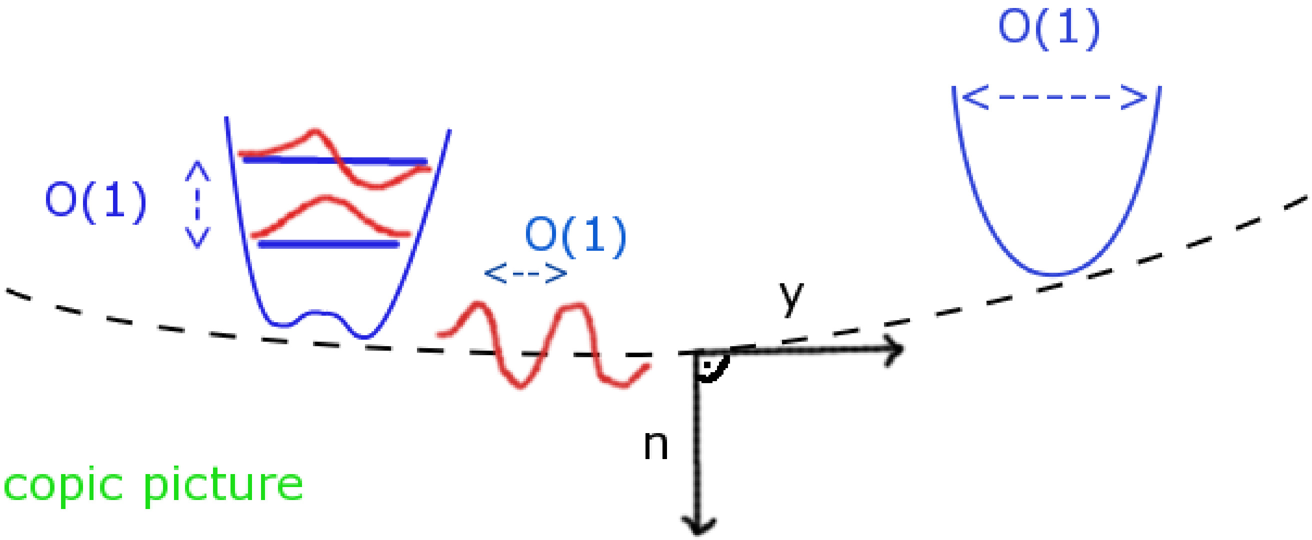
Rescaling to the microscopic variables
$y = x/\varepsilon$ and $n = N/\varepsilon$ yields



y = x / ε
n = N / ε

In the **microscopic variables**

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



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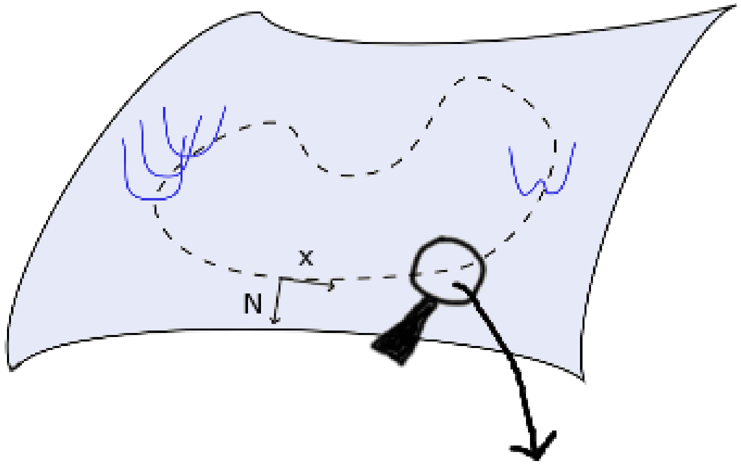
-derivatives of the solution are $\mathcal{O}(1)$,



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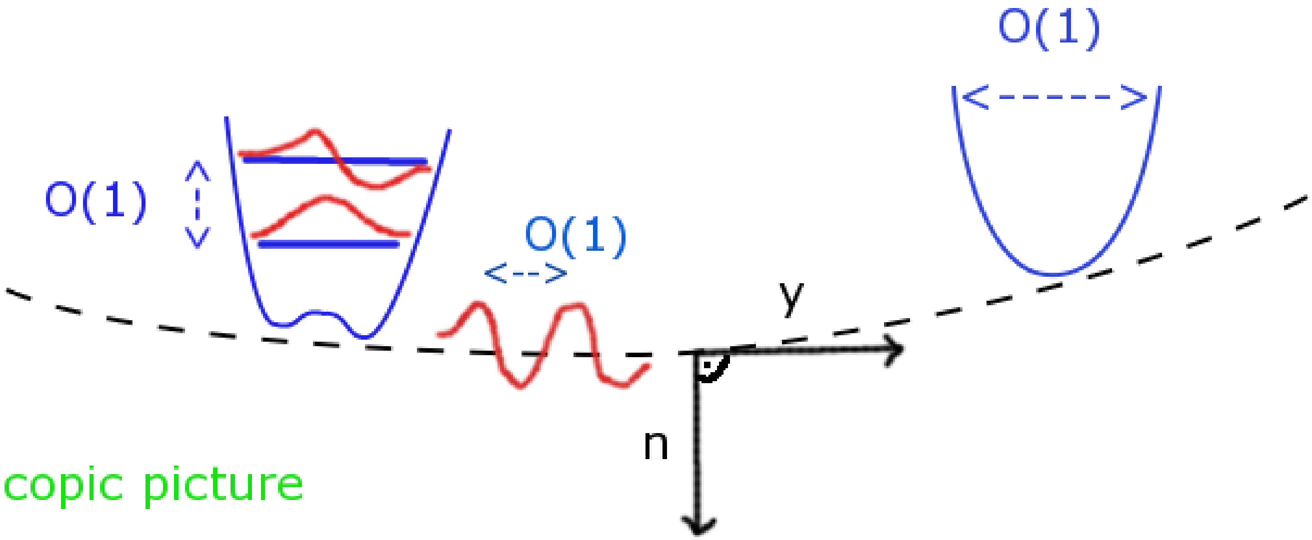

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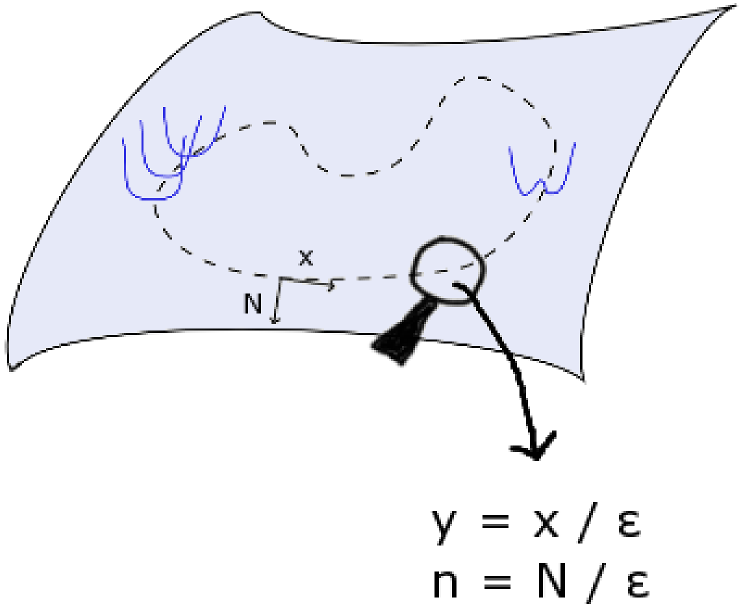

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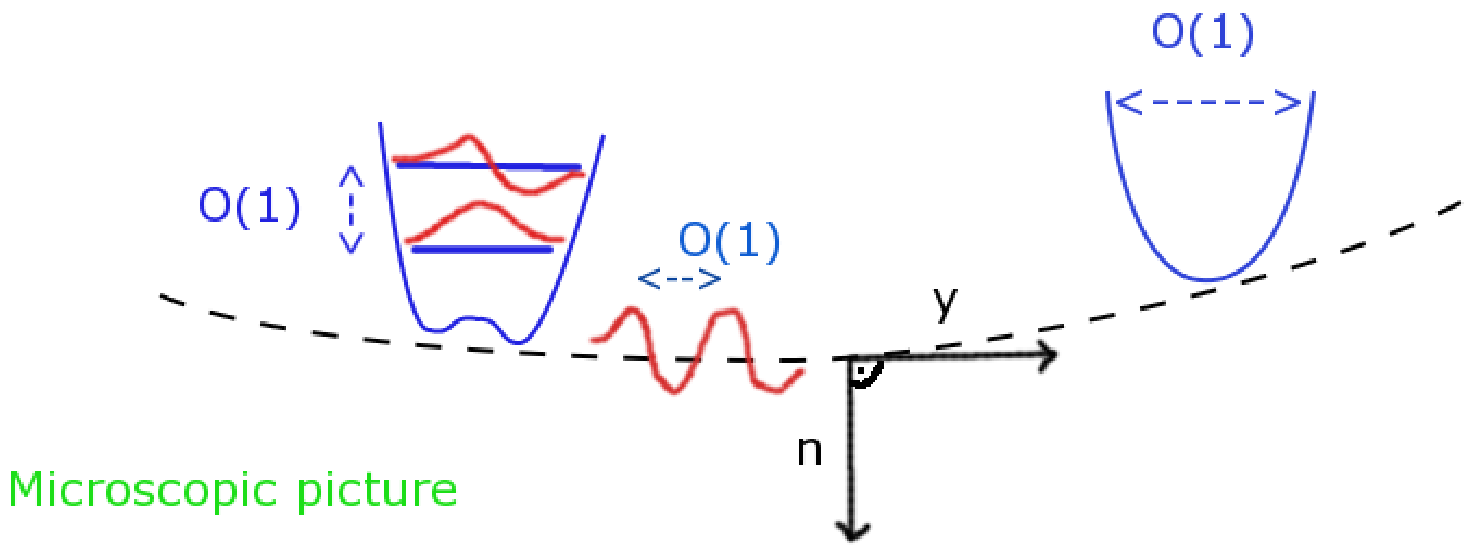

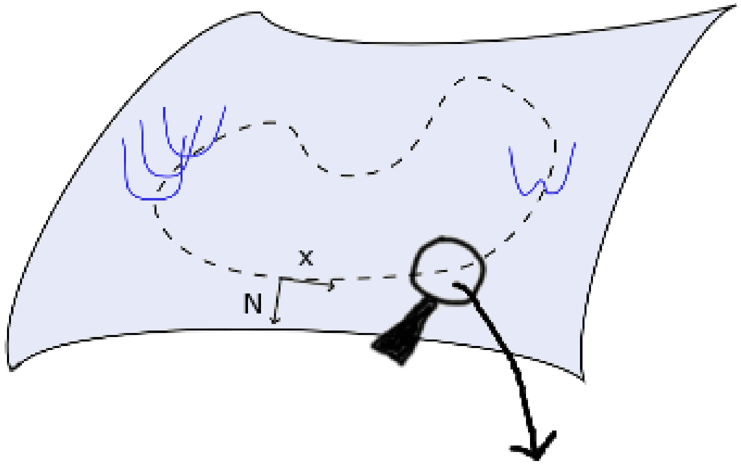

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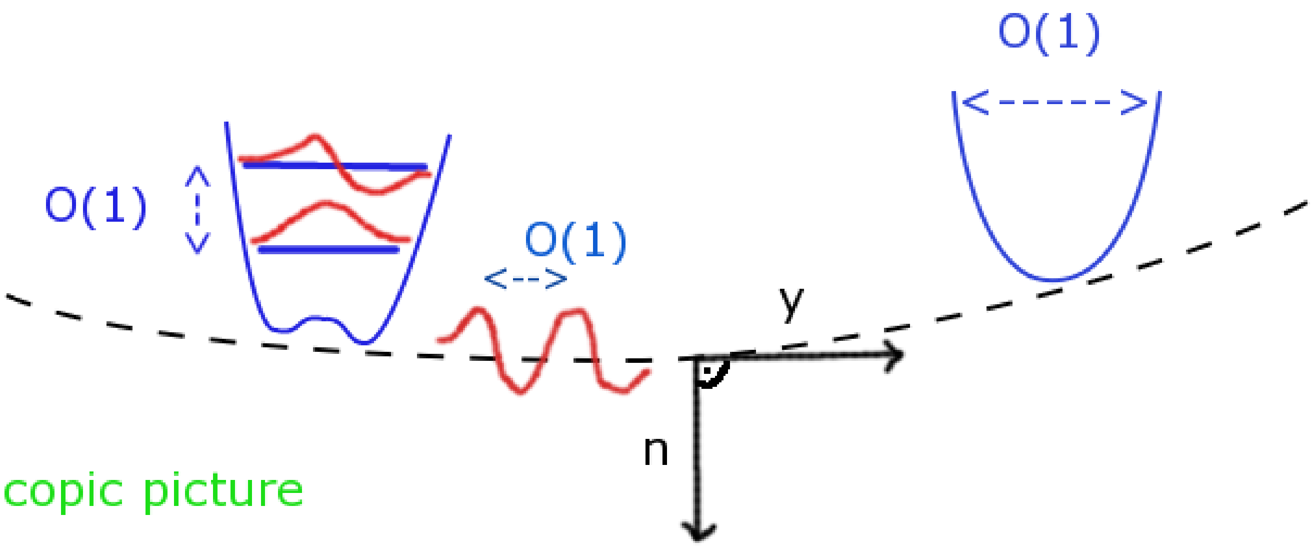

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In the microscopic variables (y, n) the Schrödinger equation thus reads

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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.

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- $(\mathcal{A}, G)$ is a Riemannian manifold of dimension $\dim \mathcal{A} = d + k$.
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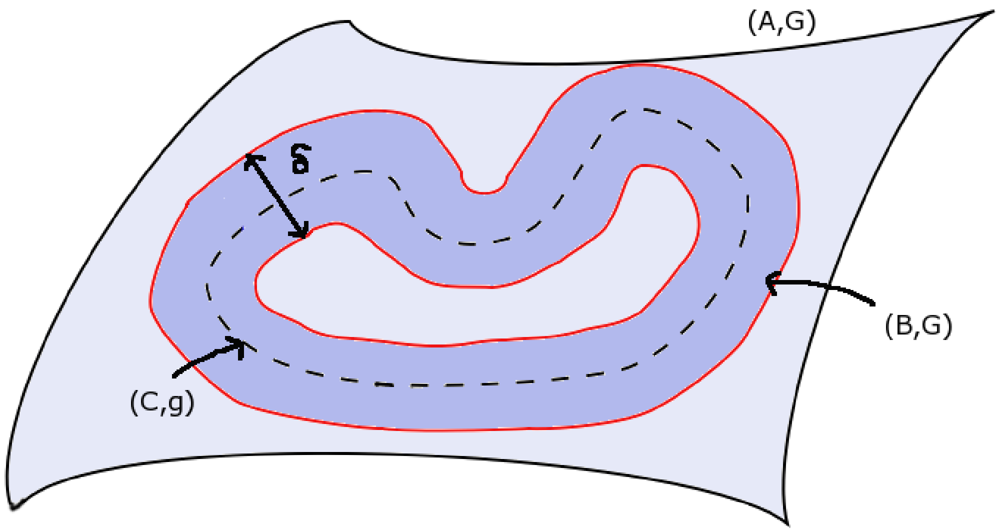

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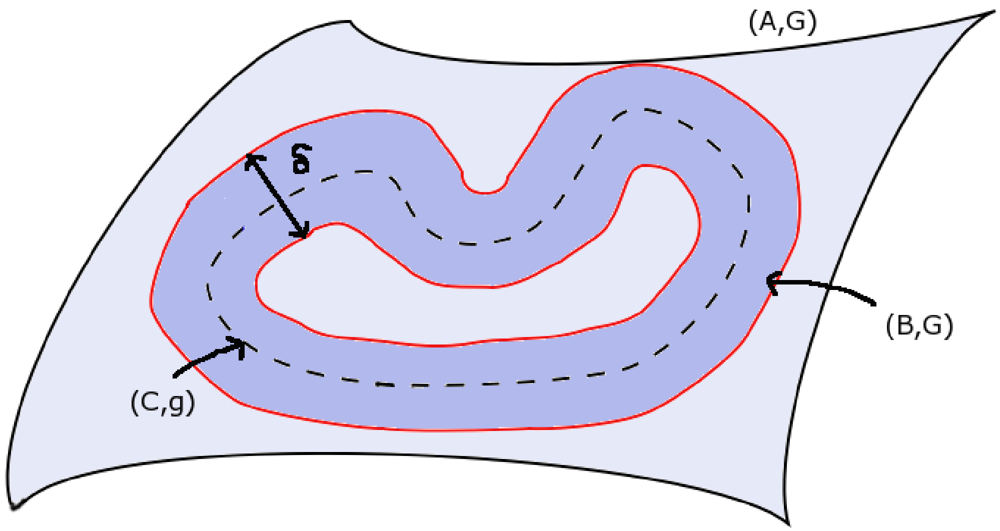

We construct a diffeomorphism

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

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.

Problem:

Find approximate solutions of the Schrödinger equation

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

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Assumption 1:

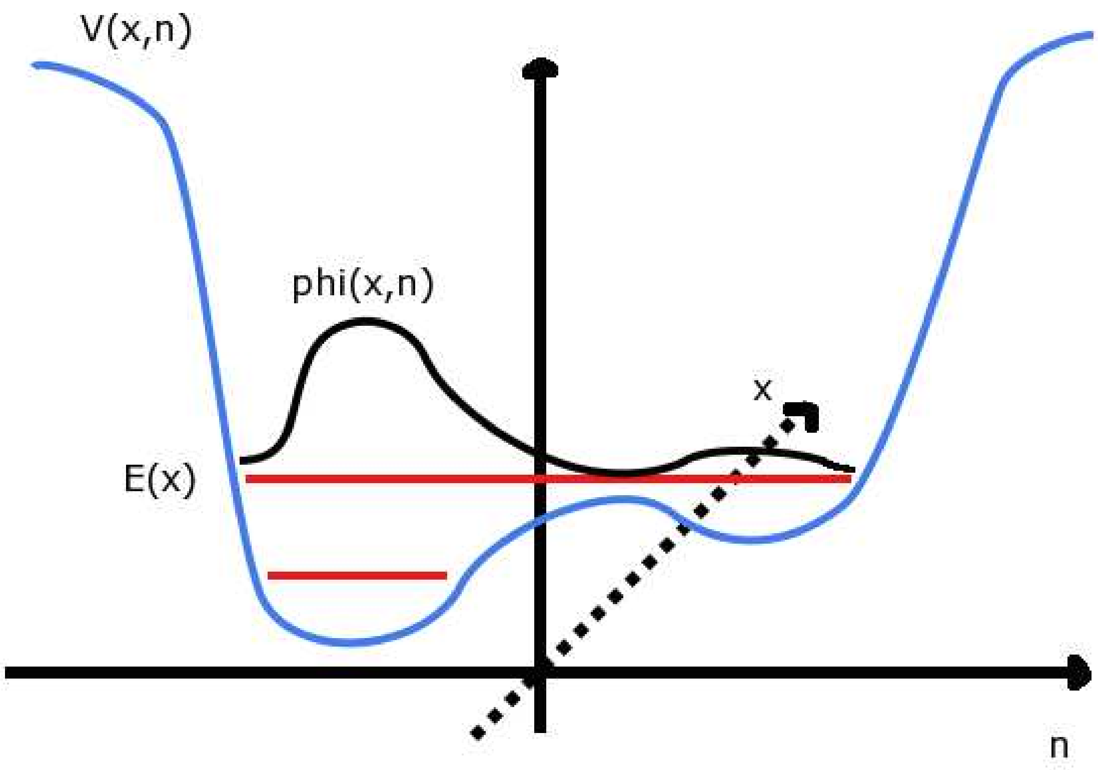
Let $V : N\mathcal{C} \to \mathbb{R}$ satisfy a number of technical conditions.

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

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

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

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



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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 $\Psi^\varepsilon|_{t=0} = \psi^\varepsilon|_{t=0}\,\varphi$ the solution of the SE satisfies

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

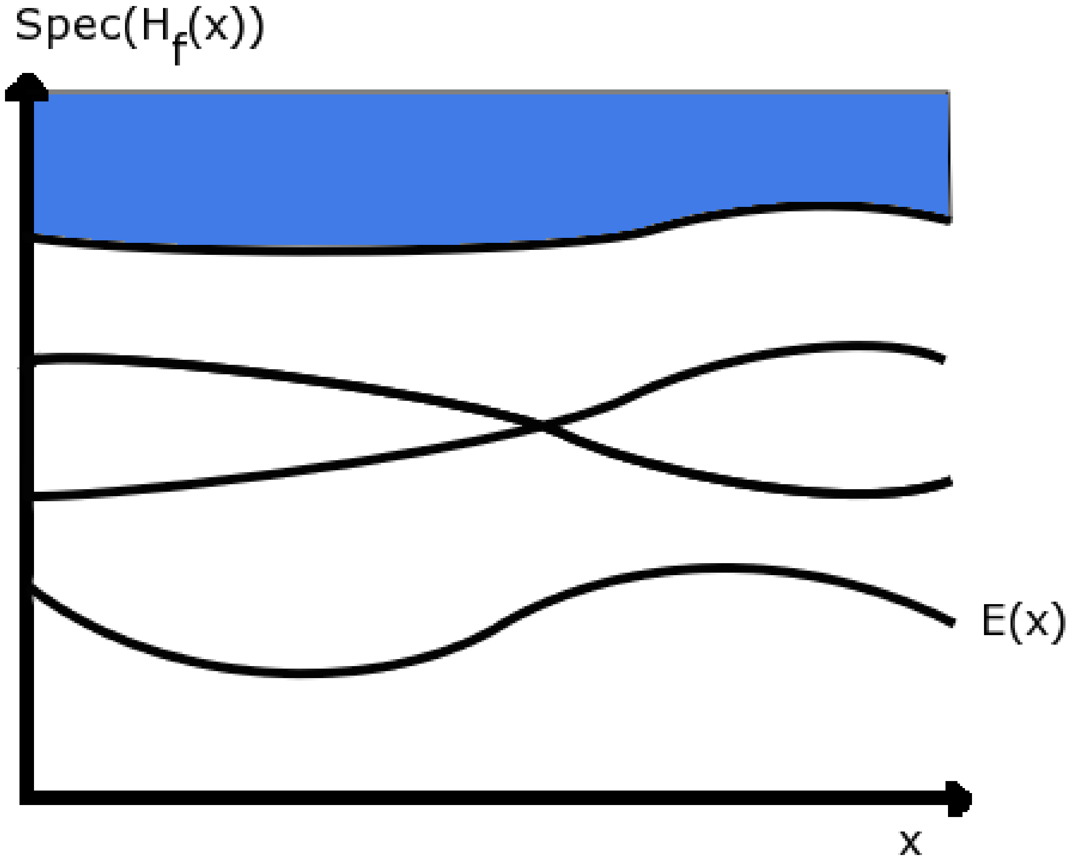
where $\psi^\varepsilon(t,x)$ solves an effective SE on $\mathcal{C}$,

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

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 $E_{\mathsf{max}} < \infty$. There exist a Riemannian metric $g^\varepsilon_{\mathsf{eff}}$ on $\mathcal{C}$, a unitary mapping

$$\mathcal{U}_0 : \mathcal{P}_0 \to L^2(\mathcal{C}, g^\varepsilon_{\mathsf{eff}})\,,$$

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

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

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The effective Hamiltonian is given by the quadratic form

$$\langle \psi, \, H^{\varepsilon}_{\mathrm{eff}} \, \psi \rangle = \int_{\mathcal{C}} \Big(g^{\varepsilon}_{\mathrm{eff}} \big(\overline{p^{\varepsilon}_{\mathrm{eff}} \, \psi}, \, p^{\varepsilon}_{\mathrm{eff}} \, \psi \big) + E |\psi|^2 \Big) \, d g^{\varepsilon}_{\mathrm{eff}}\,,$$

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where

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

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

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$$\begin{aligned} \langle \psi,\, H^{\varepsilon}_{\mathsf{eff}}\, \psi \rangle \;&=\; \int_{\mathcal{C}} \Big(g^{\varepsilon}_{\mathsf{eff}}(\overline{p^{\varepsilon}_{\mathsf{eff}}\, \psi},\, p^{\varepsilon}_{\mathsf{eff}}\, \psi) + E|\psi|^2 \\ &\qquad + \varepsilon^2\, \mathcal{M}(\overline{p\psi}, p\psi) + \varepsilon^2\, (V_{\mathsf{BH}} + V_{\mathsf{geom}})\, |\psi|^2 \Big)\, dg_{\mathsf{eff}} \end{aligned}$$

where, e.g.,

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

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

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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

$$\langle\psi,\, H^{\varepsilon}_{\text{eff}}\,\psi\rangle \;=\; \int_{\mathcal{C}} \Big(g^{\varepsilon}_{\text{eff}}\big(\overline{p^{\varepsilon}_{\text{eff}}\,\psi},\, p^{\varepsilon}_{\text{eff}}\,\psi\big) + E|\psi|^2 + \varepsilon^2\, \mathcal{M}\big(\overline{p^{\varepsilon}\psi}, p^{\varepsilon}\psi\big) + \varepsilon^2\, (V_{\text{BH}} + V_{\text{geom}})\, |\psi|^2 \Big)\, \mathrm{d}g_{\text{eff}}$$

is reduced to

$$\langle\psi,\, H^{\varepsilon}_{\text{eff}}\,\psi\rangle = \varepsilon^2 \int_{\mathcal{C}} \Big(g\big(\overline{p^1_{\text{eff}}\psi}, p^1_{\text{eff}}\psi\big) + (V_{\text{BH}} + V_{\text{geom}})\, |\psi|^2 \Big)\, \mathrm{d}g + \mathcal{O}(\varepsilon^3)\,,$$

which corresponds to the result of Mitchell.

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

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

with

$$V_{\mathrm{eff}}(q^{\|}) = \sum_{j=1}^{k} I_j(q_0, p_0)\, \omega_j(q^{\|})\,.$$

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

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

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