Application of quantum Hamilton equations

Michael Beyer[1], Jeanette Köppe[1], Markus Patzold[1], Wilfried Grecksch[2], Wolfgang Paul[1]

[1]Institute for physics
Martin-Luther-Universität Halle-Wittenberg

[2]Institute for mathematics
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Outline

- Nelson's stochastic mechanics
- Stochastic Mechanics as an optimal control problem (Derivation of quantum Hamilton equations)
- Numerical algorithm
- Results for stationary problems
  - Double-well potential
  - Excited states
  - Simple multidimensional systems

Analogy between classical and quantum mechanics

Classical mechanics

Hamilton principle

$S[x] = \int_0^T \left\{ \frac{1}{2} m v(t) - V(x,t) \right\} \mathrm{d}t$

Hamilton-Jacobi equation

$\partial_t S(x,t) - V(x,t) - \frac{1}{2m} (\nabla_x S(x,t))^2 = 0$

Newton's equations

$\dot{x}(t) = v(t)\,, \quad m\, a(t) = F = -\nabla_x V(x,t)$

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Quantum Hamilton principle

$$J[x] = \mathbb{E}\left[\int_0^T \left\{\frac{1}{2} m (v - \mathrm{i}u)^2 - V(x,t)\right\} \mathrm{d}t + \Phi_0(x_0)\right]$$

*M. Pavon, J. Math. Phys., 36: 6774-6800, **1995***

Schrödinger equation

$$\mathrm{i}\hbar\,\partial_t \Psi(x,t) = \left[-\frac{\hbar^2}{2m}\Delta + V(x,t)\right]\Psi(x,t)$$

$$v(x,t) = \frac{\nabla_x \mathfrak{Im}[\ln\Psi]}{m}\,, \quad u(x,t) = \frac{\hbar}{m}\nabla_x \mathfrak{Re}[\ln\Psi]$$

Kinematic equations

$$\mathrm{d}x(t) = [v(x,t) + u(x,t)]\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\mathrm{d}W_f(t)\,, \qquad \mathbb{E}[ma(t)] = F$$

$$\mathrm{d}x(t) = [v(x,t) - u(x,t)]\mathrm{d}t + \sqrt{\frac{\hbar}{m}}\mathrm{d}W_b(t)$$

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Forward backward stochastic differential equations (FBSDE)

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Nelson: particles subjected to conservative Brownian motion (diffusion process) where **interaction with the environment** can not be neglected

diffusion coefficient $\sigma^2 = \frac{\hbar}{m}$ $\qquad \mathbb{E}[ma] = -\partial_x V(x,t)$

- equivalent to Schrödinger equation, if wavefunction has the form

$$\psi(x,t) = \exp\left\{R(x,t) + i\,S(x,t)\right\}$$

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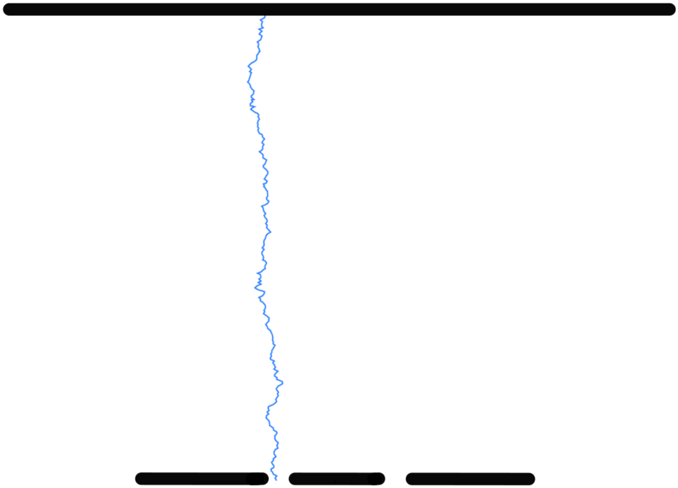
Example: double slit (electrons)

with known v and u → create realizations of quantum point particles

$$N = 1$$



Example: double slit (electrons)

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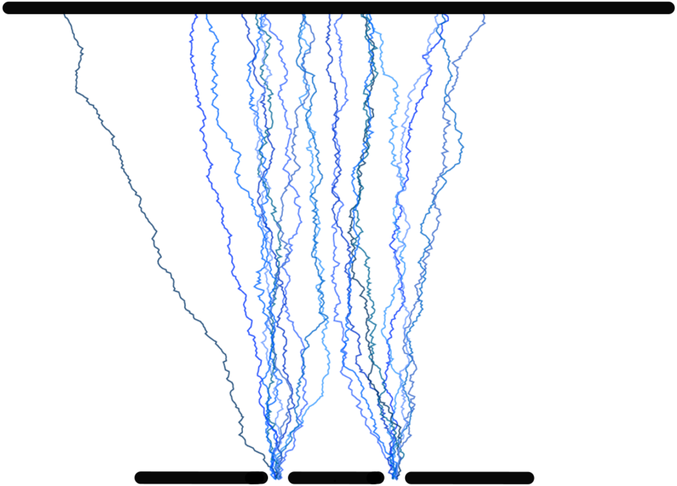
$$N = 20$$



Example: double slit (electrons)

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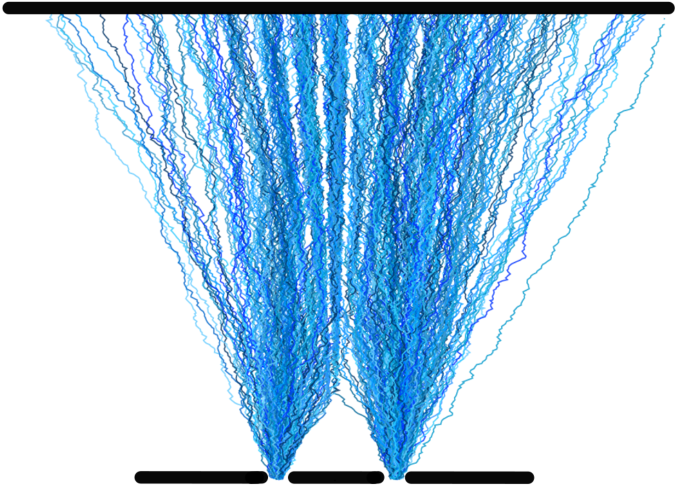
$$N = 400$$



Example: double slit (electrons)

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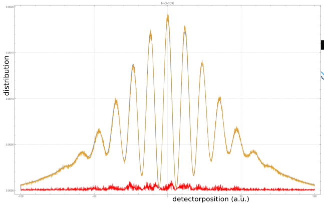
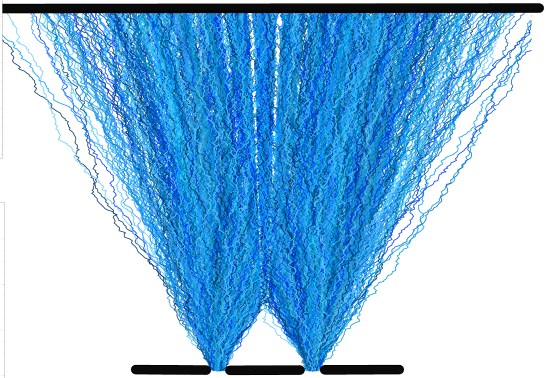
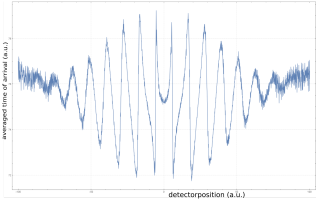
$N = 800$







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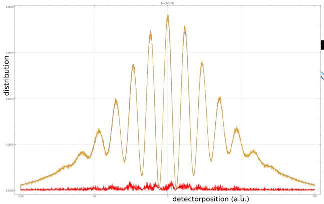

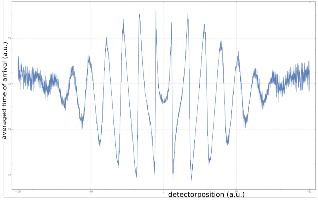

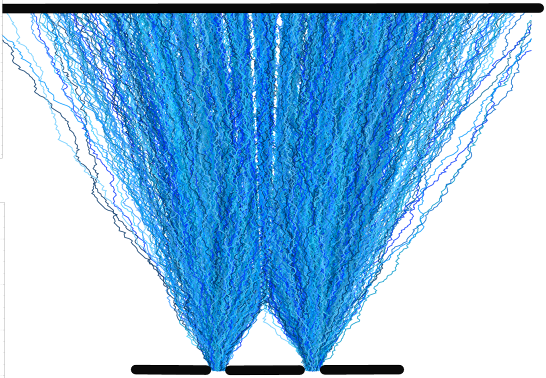

problem: solution of Schrödinger equation is needed to get the velocities v, u

Stochastic optimal control problem

Hamilton's principle: extremize action functional w. r. t. x

$$J[x] = \int_0^T \mathcal{L}(t, x(t), \dot{x}(t))\, dt \qquad \text{Lagrangian} \quad \mathcal{L} = T - V$$

Quantum Hamilton principle as stoch. optimal control problem [3, 1]:

- maximization of cost function J with $\mathcal{L}$ as (stochastic) Lagrange function

$$J[v_q] = \mathbb{E}\left[\int_0^T \mathcal{L}(t, x(t), v_q(t, x(t)))\mathrm{d}t + \Phi(x_0) \right]$$

- subject to the constraint (controlled equation)

$$\mathrm{d}x(t) = v_q(t, x(t))\mathrm{d}t + \frac{1}{2}\sigma\big((1+\mathrm{i})\mathrm{d}W(t) + (1-\mathrm{i})W_*(t)\big)\,, \quad x(0) = x_0$$

- v_q is the quantum velocity $v_q = v - \mathrm{i}\,u$ and the optimal feedback control to $x(t)$

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Quantum Hamilton equations

J. Koeppe *et. al*, *Derivation and application of quantum Hamilton equations of motion. Annalen der Physik* **529**, *1600251 (2017)*

coupled forward backward SDEs [1]

$$dx(t) = [v(t,x) + u(t,x)]dt + \sigma dW(t)$$
$$dx(t) = [v(t,x) - u(t,x)]dt + \sigma dW_*(t)$$
$$m\,d[v(t,x) + u(t,x)] = \partial_x V(x,t)dt + q(t)\,dW_*(t)$$

- taking the classical limit $(u, \hbar/m \to 0)$

$$dx(t) = v(x,t)dt\ ,\ \ mdv = -\partial_x V(x,t)dt$$

- taking the expectation value one recovers Ehrenfest's theorem

$$d\mathbb{E}[x(t)] = \mathbb{E}[v(x,t)]dt\ ,\ \ md\mathbb{E}[v(t)] = -\mathbb{E}[\partial_x V(x,t)]dt$$

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Towards a numerical solution

→ problem: four unknown stochastic processes x, v, u, q

- consider stationary case $v \equiv 0$, all information is stored in u, e. g.

$$\rho(x) = \exp\left[\frac{2}{\sigma^2}\int_{\mathcal{C}} u(x')\cdot \mathrm{d}x'\right]$$

- discretize time axis, e. g. using Euler–Mayurama Scheme

$$x^\pi(t_{i+1}) = x^\pi(t_i) + u^\pi(x^\pi(t_i))\Delta t + \sigma\Delta W(t_i)$$
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- due to Markov property the backward equation can be calculated with the help of **conditional expectation**

$$u^\pi(x^\pi(t_i)) = \mathbb{E}[u^\pi(x^\pi(t_{i+1}))|x^\pi(t_i)] - \partial_x V(x^\pi(t_i))\Delta t$$

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Iteration scheme

Iteration scheme for u

0. choose starting value $u(x) \equiv 0$
1. use u to generate N paths with n_t steps
2. integrate u backward in time
3. average $u(x(t_i))$ over intervals $\rightarrow u(x) = \langle u(x(t_i)) \rangle_{\text{cube}}$
4. go to 1

1D harmonic oscillator

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

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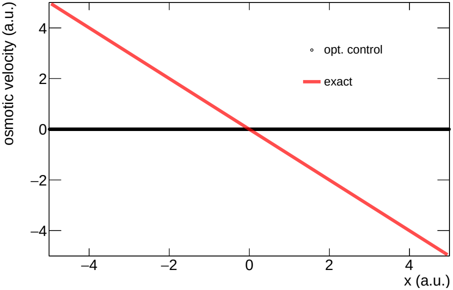

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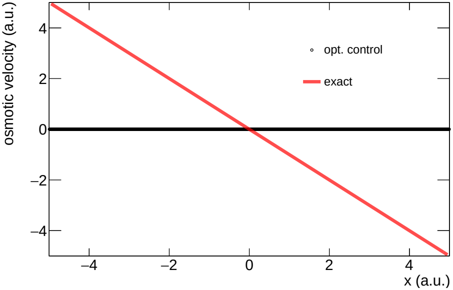

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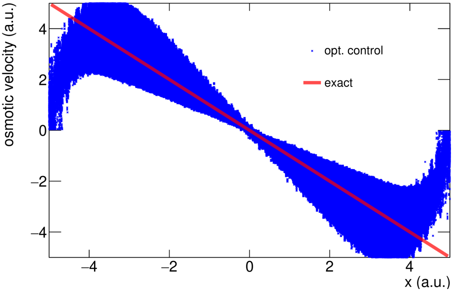

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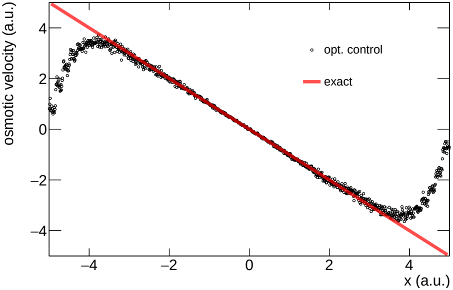

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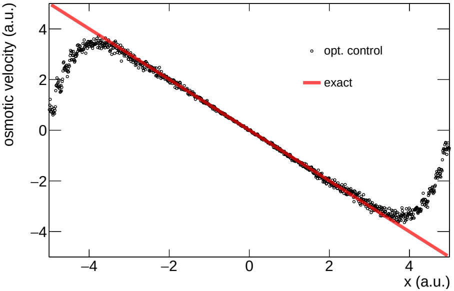

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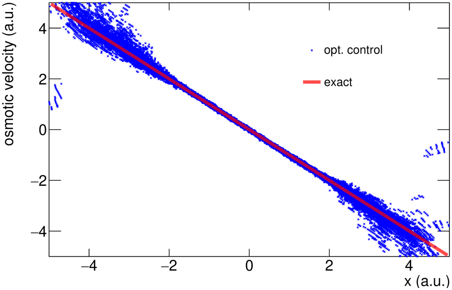

Iteration scheme

Iteration scheme for u

0 choose starting value $u(x) \equiv 0$
1 use u to generate N paths with n_t steps
2 integrate u backward in time
3 average $u(x(t_i))$ over intervals $\rightarrow u(x) = \langle u(x(t_i)) \rangle_{\text{cube}}$
4 go to 1

1D harmonic oscillator

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

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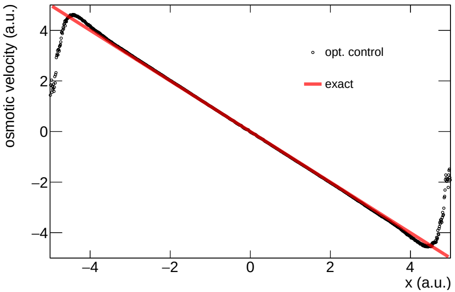

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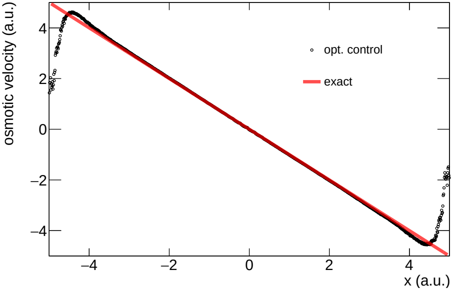

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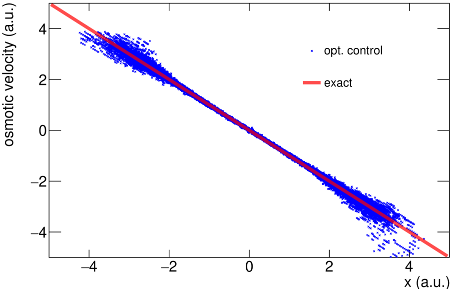

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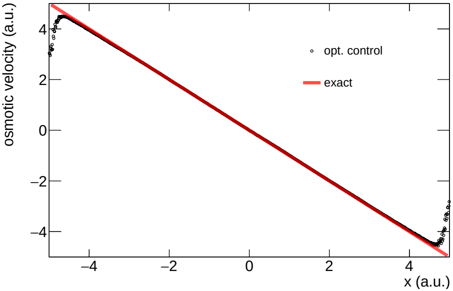

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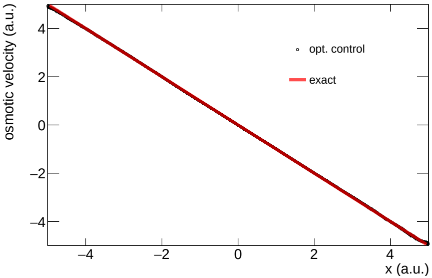
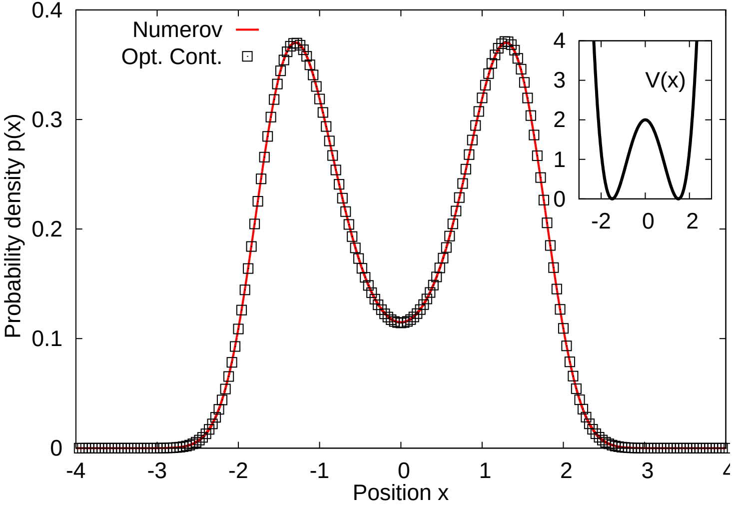
$u(x)$ after 50 iterations



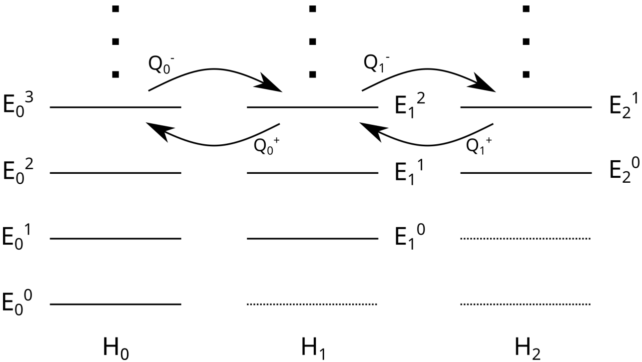
Double well: ground state

$V(x) = \frac{V_0}{a^4}(x^2 - a^2)^2 \quad V_0 = 2, \ a = 1.5$



SUSY in stochastic mechanics

$$\mathcal{H}_0 = \boldsymbol{Q}_0^+ \cdot \boldsymbol{Q}_0^- + E_0 \;\rightarrow\; \mathcal{H}_1 = \boldsymbol{Q}_0^- \circ \boldsymbol{Q}_0^+$$

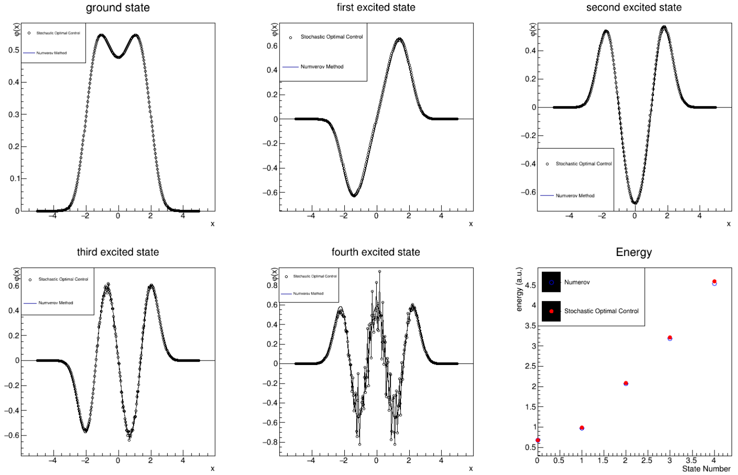


e. g. for the Hamiltonian $\mathcal{H}_i$ in cartesian coordinates

$$\boldsymbol{Q}_i^\pm = \mp\nabla - \boldsymbol{u}_i$$

Double well: excited states

$$V(x) = \frac{V_0}{a^4}(x^2 - a^2)^2 \qquad V_0 = 1,\ a = 1.5$$



- Tunnel splitting is given by the mean first passage time
- Perturbation theory prediction for the splitting is not correct

} → Poster

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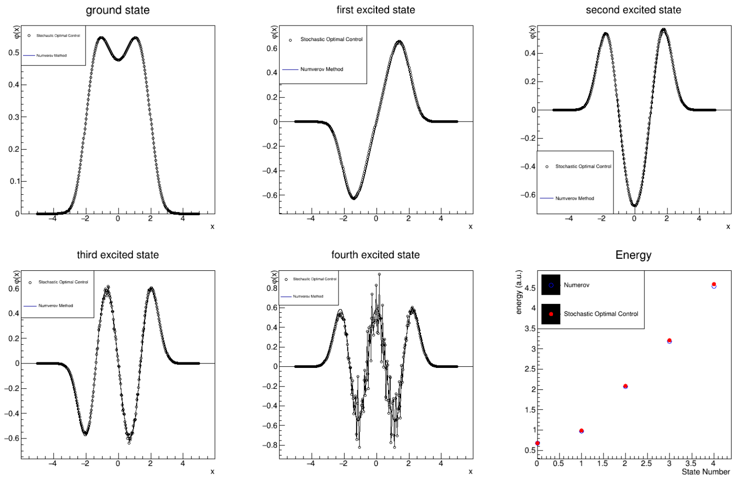

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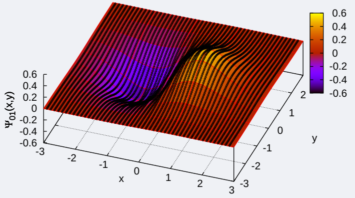
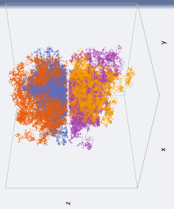
Higher dimensional systems

2D isotropic harmonic oscillator



3D hydrogen atom

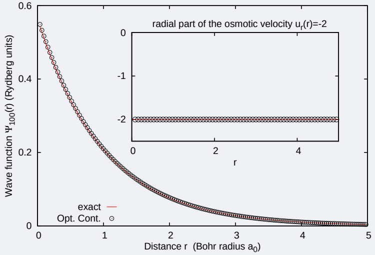


Spherical problems

$$\mathrm{d}r = \left(u_r + \frac{\sigma^2}{r}\right)\mathrm{d}t + \sigma \mathrm{d}W$$

$$\mu \mathrm{d}u_r = \frac{1}{r^2}\left(\hbar u_r + \partial_r V(r)\right)\mathrm{d}t + (q\mathrm{d}\boldsymbol{W}_*)_r$$

hydrogen atom



Summary

- Derivation of kinematic and dynamic equations for non-relativistic quantum system → **quantum Hamilton equations**
- Numerical algorithm to solve these stochastic equations in the stationary case without using the Schrödinger equation
- Solution to (simple) problems in higher dimensions
- Determination of all excited eigenstates of the Schrödinger equation

Future work

> Solving non-stationary problems numerically
> Extending to relativistic particles and spin

Literature I

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Derivation and application of quantum hamilton equations of motion.
Annalen der Physik, 529(3):1600251–n/a, 2017.
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Edward Nelson.
Derivation of the schrödinger equation from newtonian mechanics.
Physical Review, 150(4):1079, 1966.

Michele Pavon.
Hamilton's principle in stochastic mechanics.
Journal of Mathematical Physics, 36(12):6774–6800, 1995.

Thank you for your attention!

Nelson's stochastic mechanics

E. Nelson, *Derivation of the Schrödinger equation from Newtonian mechanics. Phys. Rev.* **150**, *1079 (1966)*

Forward backward stochastic differential equations (FBSDE)

$$\mathrm{d}x(t) = \big[v(t, x(t)) + u(t, x(t))\big]\mathrm{d}t + \sigma \mathrm{d}W(t) \ , \quad x(t_0) = x_0$$
$$\mathrm{d}x(t) = \big[v(t, x(t)) - u(t, x(t))\big]\mathrm{d}t + \sigma \mathrm{d}W_*(t) \, , \quad x(T) = x_T$$

where:

- $x(t) = x(t, \omega)$ is a stochastic process in $\mathbb{R}^{n \cdot d}$
- $x(t)$ is connected to a probability distribution ρ satisfying a forward and backward Fokker–Planck equation
- $W(t)$ is a $n \cdot d$ dimensional Wiener processes
- current velocity $v = \sigma^2 \nabla S(t, x(t))$
- $\mathbb{E}[v] = \langle \hat{p} \rangle_\Psi$
- osmotic velocity $u = \sigma^2 \nabla R(t, x(t)) = \sigma^2 \nabla \ln \rho(t, x(t))$
- $\mathbb{E}[u] = 0$ and $\mathbb{E}\big[v^2 + u^2\big] = \Big\langle \left({}^{\Delta \hat{p}}/_{m}\right)^2 \Big\rangle_\Psi$