Quantum Hamilton Equations: Derivation and Application

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Classical Analytical Mechanics

Hamilton Principle ⟷ Hamilton-Jacobi Theory

$$S[x]=\int_{t_0}^{t_1}[\frac{1}{2}m v^2(t)-V(x(t))]dt$$

$$\frac{\partial S}{\partial t}(x,t)-V(x)-\frac{1}{2\mathrm{m}}|\nabla S(x,t)|^2=0$$

Kinetic and Dynamic Equations

$$v(t)=\dot{x}(t) \qquad m a=F$$

Quantum Mechanics

Schrödinger equation

$$-i\hbar\frac{\partial}{\partial t}\psi(x,t)=\left(\frac{-\hbar^2}{2m}\Delta+V(x,t)\right)\psi(x,t)$$

Born postulate

$$p(x,t)=|\psi(x,t)|^2$$

Stochastic Mechanics

$$i\hbar\frac{\partial\psi}{\partial t}=\left(\frac{-\hbar^2}{2m}\Delta+V(x,t)\right)\psi$$

$$v=\frac{\hbar}{m}\nabla\Im\ln[\psi] \quad u=\frac{\hbar}{m}\nabla\Re\ln[\psi]$$

$$dx(t)=[v(x,t)+u(x,t)]dt+\sqrt{\frac{\hbar}{m}}dW_f(t)$$

$$dx(t)=[v(x,t)-u(x,t)]dt+\sqrt{\frac{\hbar}{m}}dW_b(t)$$

$$m\langle a\rangle=F$$

E. Nelson, Phys. Rev. **150**, 1079 (1966)

Variational Principle

$$i\hbar\frac{\partial\psi}{\partial t}=\left(\frac{-\hbar^2}{2m}\Delta+V(x,t)\right)\psi$$

$$v=\frac{\hbar}{m}\nabla\Im\ln[\psi] \quad u=\frac{\hbar}{m}\nabla\Re\ln[\psi]$$

$$J[u,v]=E\left[\int_{t_0}^{t_1}dt\left(\frac{1}{2}m(v(t)-iu(t))^2-V(x(t))\right)+\Phi_0(x)\right]$$

K. Yasue, J. Math. Phys. **22**, 1010 (1981)
F. Guerra, L. M. Morato, Phys. Rev. D **27**, 1774 (1983)
M. Pavon, J. Math. Phys. **36**, 6774 (1995)

$$dx(t)=[v(x,t)+u(x,t)]dt+\sqrt{\frac{\hbar}{m}}dW_f(t)$$

$$dx(t)=[v(x,t)-u(x,t)]dt+\sqrt{\frac{\hbar}{m}}dW_b(t)$$

$$m\langle a\rangle=F$$

Quantum Analytical Mechanics

Action Principle

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

Schrödinger Equation

$$i\hbar\frac{\partial\psi}{\partial t}=\frac{-\hbar^2}{2m}\Delta\psi+V(x)\psi$$

$$v=\frac{\hbar}{m}\nabla\,\Im\ln[\psi]\qquad u=\frac{\hbar}{m}\nabla\,\Re\ln[\psi]$$

Kinematic and Dynamic Equations

$$dx(t)=[v(x,t)+u(x,t)]\,dt+\sqrt{\frac{\hbar}{m}}\,dW_f(t)$$

$$dx(t)=[v(x,t)-u(x,t)]\,dt+\sqrt{\frac{\hbar}{m}}\,dW_b(t)$$

$$m\langle a\rangle=F$$

Stochastic Optimal Control

Quantum action principle M. Pavon, J. Math. Phys. **36**, 6774 (1995)

$$J(\hat{u},\hat{v}) = min_v \, max_u \, E\left[\int_{t_0}^{t_1} dt \left(\frac{1}{2} m \left(v(t) - iu(t)\right)^2 - V(x(t))\right) + \Phi_0(x)\right]$$

v-Player: $J_1[u,v] = -J[u,v]$

u-Player: $J_2[u,v] = \ \ J[u,v]$

} Nash-equilibrium for a Zero-sum game

Coupled forward-backward stochastic differential equations

$$dx(t) = [v(x,t) + u(x,t)]dt + \sqrt{\frac{\hbar}{m}} dW_f(t)$$

$$dx(t) = [v(x,t) - u(x,t)]dt + \sqrt{\frac{\hbar}{m}} dW_b(t)$$

Stochastic Optimal Control

$$J(\hat{u},\hat{v}) = min_v \, max_u \, E\left[\int_{t_0}^{t_1} dt \left(\frac{1}{2} m \left(v(t) - iu(t)\right)^2 - V(x(t))\right) + \Phi_0(x)\right]$$

Real part: saddle-point action principle

$$J_r(\hat{u},\hat{v}) = min_v \, max_u \, E\left[\int_{t_0}^{t_1} dt \left(\frac{1}{2} m \left(v^2(t) - u^2(t)\right) - V(x(t))\right) + S_0(x)\right]$$

Imaginary part: saddle point entropy production principle

$$J_i(\hat{u},\hat{v}) = min_v \, max_u \, E\left[\int_{t_0}^{t_1} dt \, v(t) u(t) + R_0(x)\right]$$

M. Pavon, J. Math. Phys. **36**, 6774 (1995)

Stationary case: v=0

$$J(\hat{u}) = max_u \, E\left[\int_{t_0}^{t_1} dt \left(-\frac{1}{2} m u^2(t) - V(x(t))\right) + S_0(x)\right]$$

Extremal principle for stochastic Hamiltonian

B. Oksendal, A. Sulem, J. Optim. Appl. **161**: 22-55, 2014

$$H = -\frac{1}{2} m u^2 - V(x) + p(t) u + q(t) \qquad \frac{\partial H}{\partial u} = 0 \;\Leftrightarrow\; -mu + p = 0$$

$$dx(t) \;=\; u(x,t)\,dt + \sqrt{\frac{\hbar}{m}}\,dW_f(t)$$ forward in time

$$du(x,t) \;=\; -\frac{1}{m}\frac{dV}{dx}\,dt + \frac{q(t)}{m}\,dW_b(t)$$ backward in time

Stationary problem

$$dx(t) = u(x,t)\,dt + \sqrt{\frac{\hbar}{m}}\,dW_f(t)$$ forward in time

$$du(x(t)) = -\frac{1}{m}\frac{dV}{dx}\,dt + \frac{q(t)}{m}\,dW_b(t)$$ backward in time

Itô-Formula for u(x(t)) and comparison

$$\frac{-\hbar^2}{m}u\frac{du}{dx} - \frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + \frac{1}{m}\frac{dV}{dx} = 0$$

Riccati equation for the stationary Schrödinger equation

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \qquad \psi = \mathrm{e}^{R(x)} \qquad \frac{dR}{dx} = u$$

1d harmonic oscillator

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

$$\frac{d\langle x\rangle(t)}{dt} = \langle u\rangle(t)$$

$$\frac{d\langle u\rangle(t)}{dt} = -\langle x\rangle(t)$$

Averages follow classical paths

$$(x_0(t), u_0(t)) \ \ solution \ \rightarrow \ \left(x_{cl}(t)+x_0(t), u_{cl}(t)+u_0(t)\right) \ \ also$$

Coherent States!

$(x_0(t),u_0(t))$ is the ground state process corresponding to the classical stationary solution(s)

1d harmonic oscillator

Dimensionless equations

$$dx(t) = u(x)dt + dW_f(t)$$
$$du(x) = -x\,dt + q(t)\,dW_b(t)$$

Iterative solution I

- integrate forward the SDE for x using last u
- determine next u from backward integration of Riccati equation

Problem: This standard way in the mathematical literature to solve the optimization problem is "equivalent" to solving the Schrödinger equation → **LITTLE GAIN**

1d harmonic oscillator

Iterative solution II

- integrate forward the SDE for x using last u
- integrate backward the SDE for u using last x

Problem: u(x(t)) has to be adapted to the filtration produced by x(t)

A. Bachouch, E. Gobet, A. Matoussi, Empirical Regression Method for Backward Doubly Stochastic Differential Equations 2015, URL: https://hal.archives-ouvertes.fr/hal-01152886

C. Bender, R. Denk, A forward scheme for backward SDE's Stochastic Process. Appl., 2007, 117, 1793

C. Bender, J. Steiner, *Least-Squares Monte Carlo for Backward SDEs*, in Springer Proceedings in Mathematics Vol. 12, R. A. Carmona, P. Del Moral, P. Hu, N. Oudjane (Eds.), Springer (2012)

1d harmonic oscillator

Discretized equations

$$x^{i+1}(t_{j+1}) = x^{i+1}(t_j) + u^i(t_j)\Delta t + \Delta W(t_j)$$
$$u^{i+1}(t_j) = u^{i+1}(t_{j+1}) - x^{i+1}(t_{j+1})\Delta t + q(t_j)\Delta W(t_j)$$

To eliminate $q(t_j)$ multiply with $\Delta W(t_j)$ and form conditional expectation

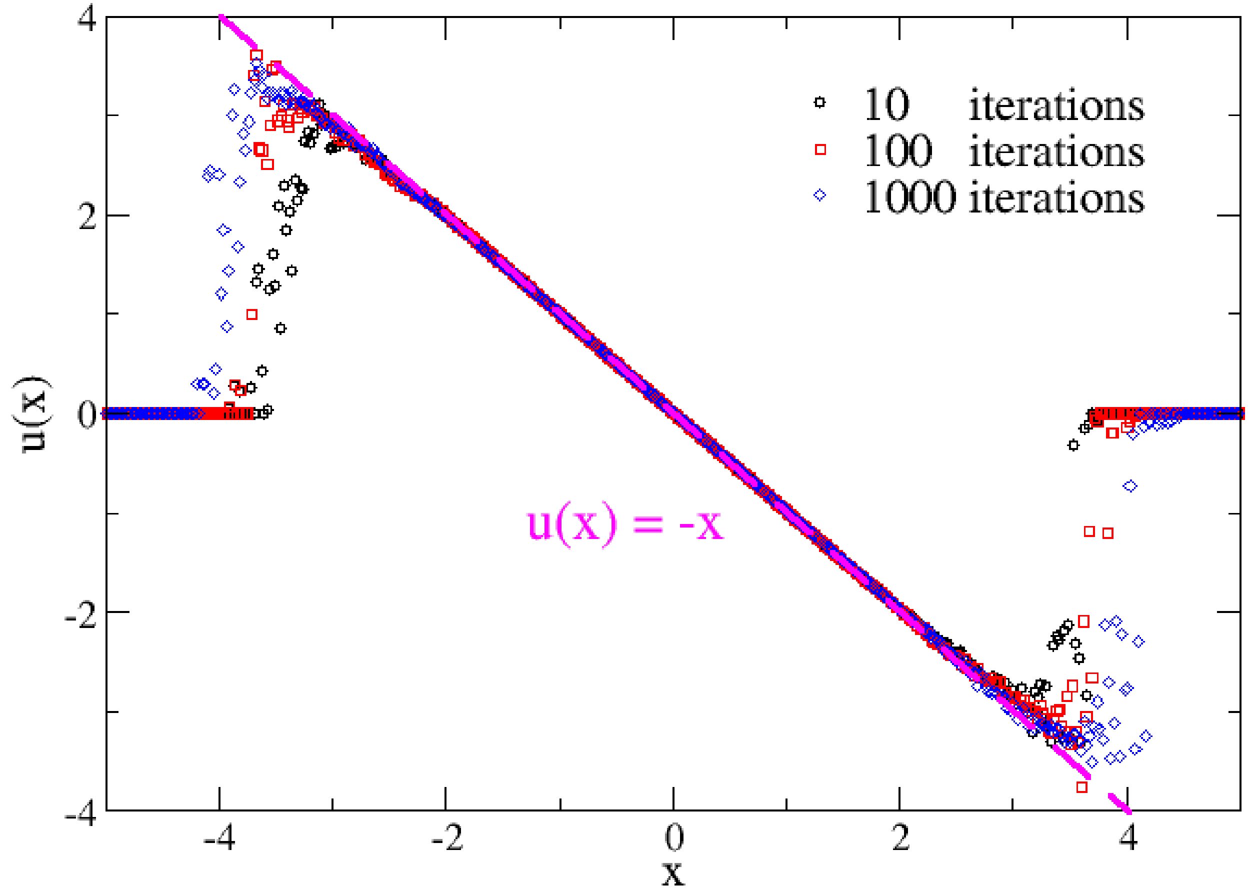
$$q(t_j) = \frac{1}{\Delta t} E\left[u^{i+1}(t_{j+1})\Delta W(t_j) \,\middle|\, F_{t_j}\right] = \frac{1}{\Delta t} E\left[u^{i+1}(t_{j+1})\Delta W(t_j) \,\middle|\, x(t_j)\right]$$

Numerical solution using least-squares Monte Carlo scheme

C. Bender, J. Steiner, *Least-Squares Monte Carlo for Backward SDEs*, in Springer Proceedings in Mathematics Vol. 12, R. A. Carmona, P. Del Moral, P. Hu, N. Oudjane (Eds.), Springer (2012)

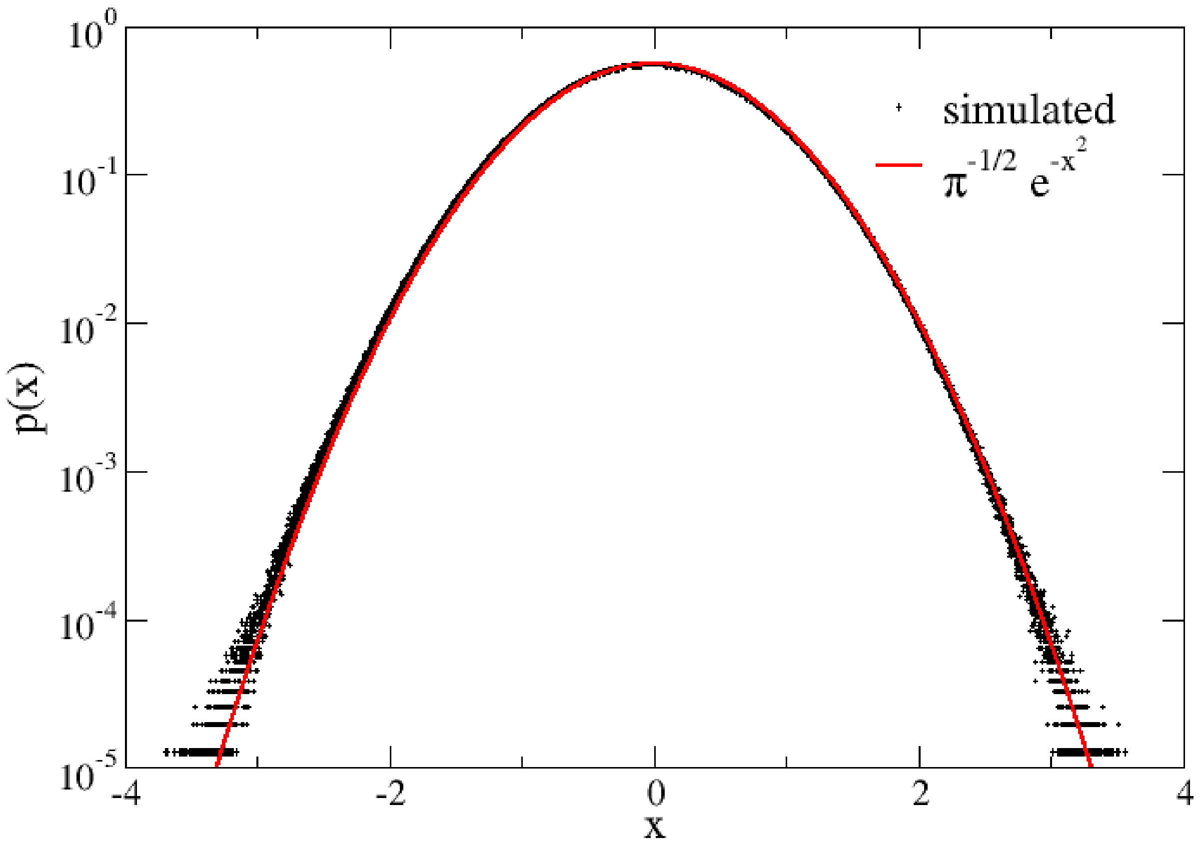
1d harmonic oscillator

Iteration result for the osmotic velocity



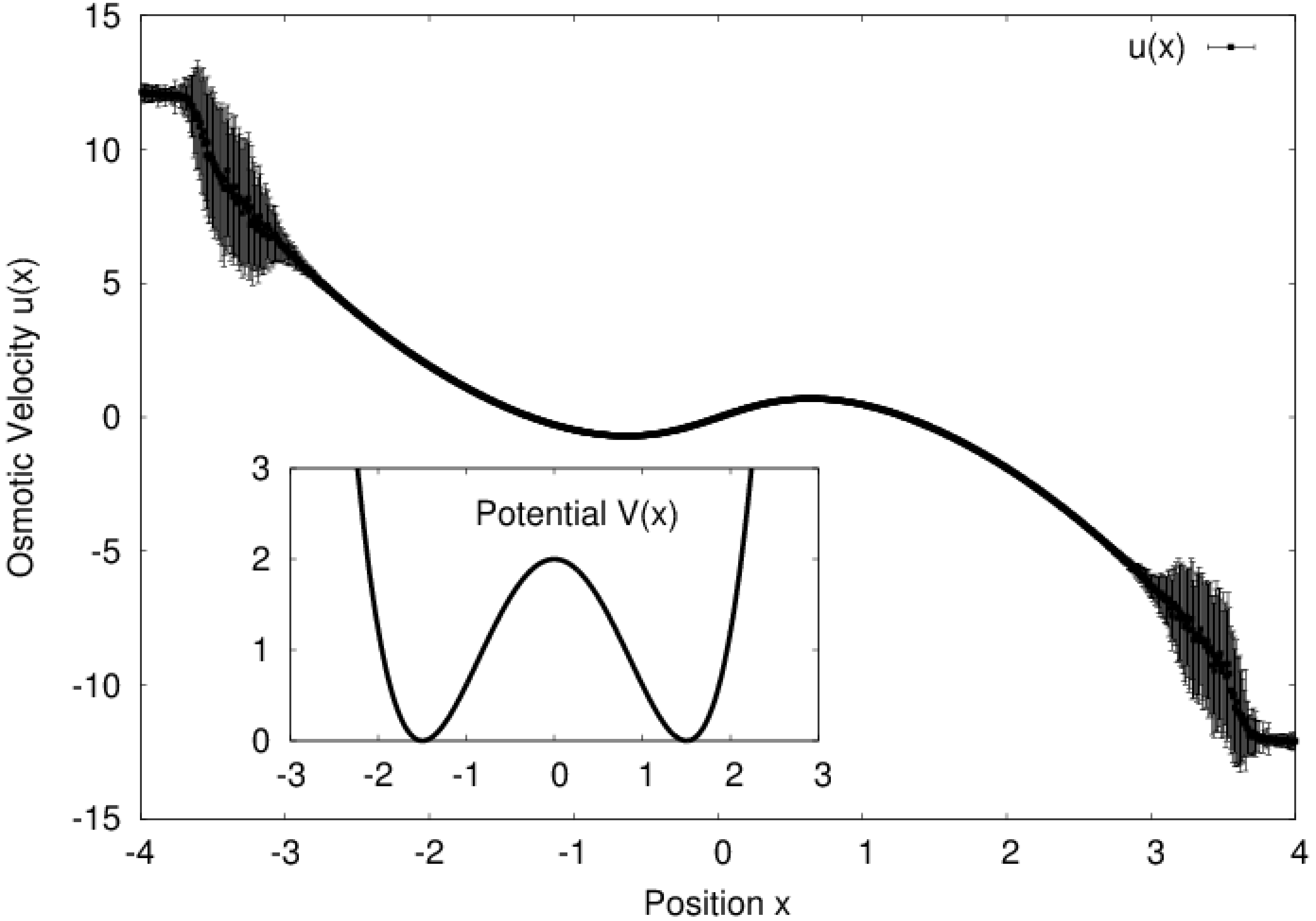
1d harmonic oscillator

Probability density obtained by using the resulting osmotic velocity



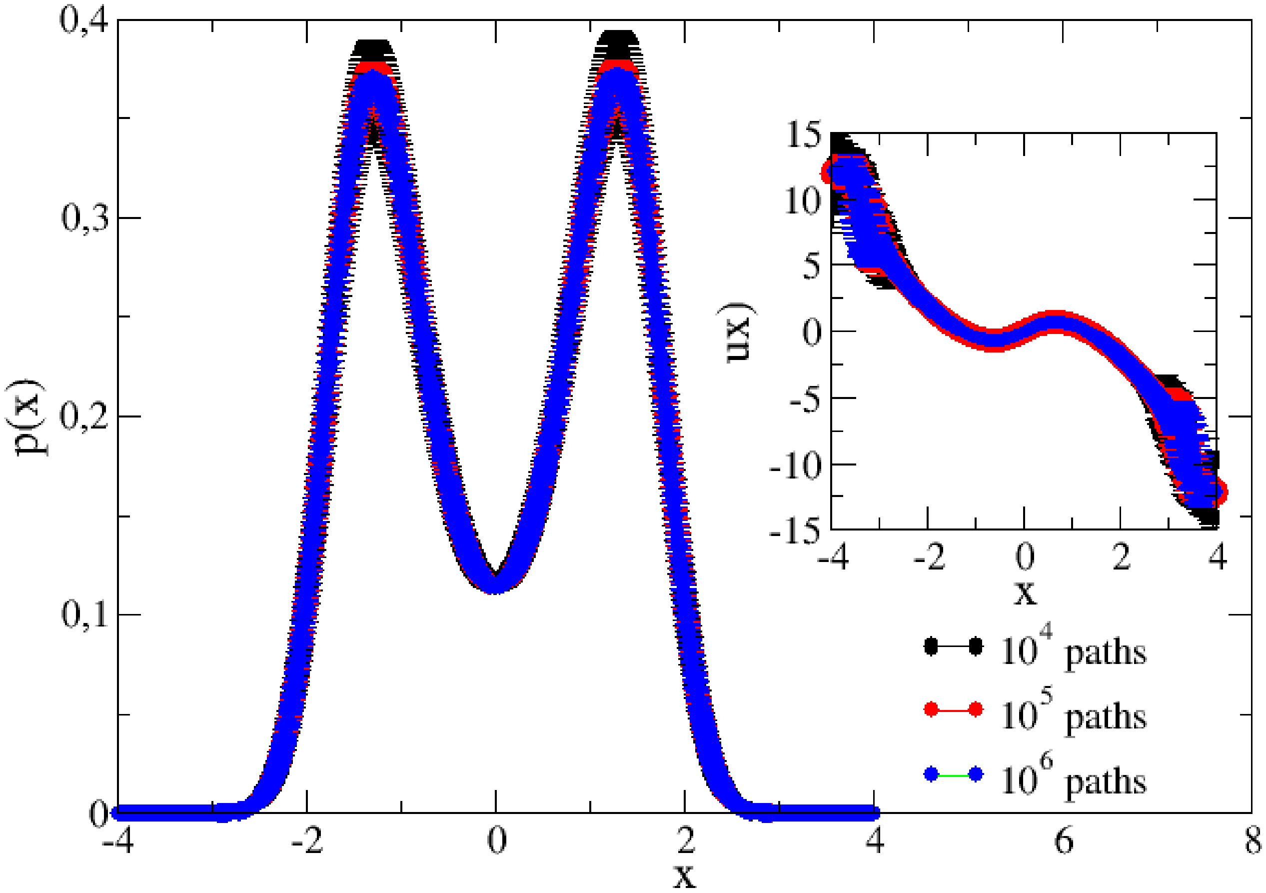
1d double-well potential

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



1d double-well potential

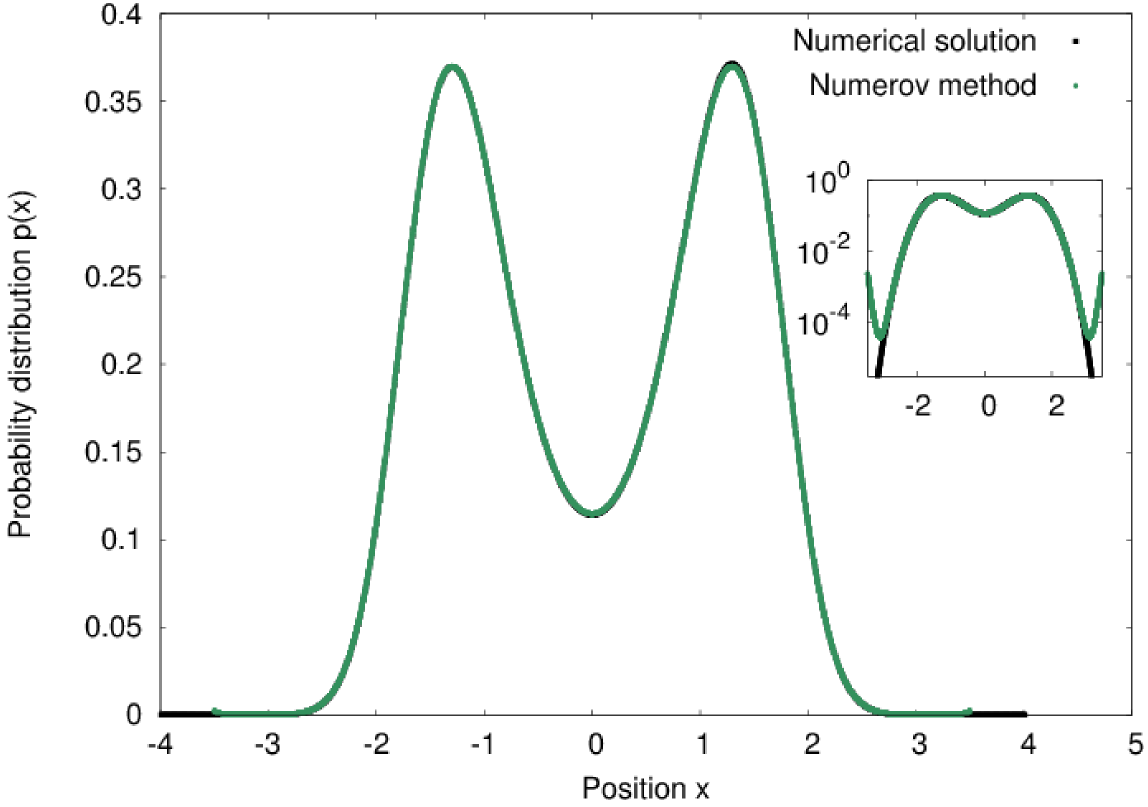
Systematic reduction of numerical uncertainty



1d double-well potential

Ground state energy $$E_0 = \int_{-\infty}^{\infty} \left(\frac{1}{2} u(x)^2 + V(x) \right) p(x)\, dx = 1.1033$$

Estimate: ground state in one well – WKB splitting $$E_0 = 1.0633$$



Numerov Method

J. M. Blatt, J. Comp. Phys. 1, 382 (1967)

Conclusions

Successful derivation and application of quantum Hamilton Equations of motion

N spinless particles can be done

Numerics for n-dimensional case needs to be developed

Numerics for non-stationary case needs to be developed

Spin incorporation?

J. Köppe, W. Grecksch, W. Paul, Annalen der Physik, accepted

Funding: State Saxony-Anhalt through its base funding of MLU