Variational methods for finding ground states of quantum systems

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Outline

Physical task

Stationary Schrödinger equation

- given a Hilbert space $\mathcal{H}$ and a Hamiltonian H the stationary Schrödinger equation reads:

$$H\psi_{i,\alpha}(\mathbf{x}) = E_i\psi_{i,\alpha}(\mathbf{x}),\ \psi_{i,\alpha} \in \mathcal{H}, E_i \in \mathbb{R}$$

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- rarely analytically solvable

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- no physical intuition is used

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- solve the integral and find the minimizing variational parameter λ_{min}

Numerical task

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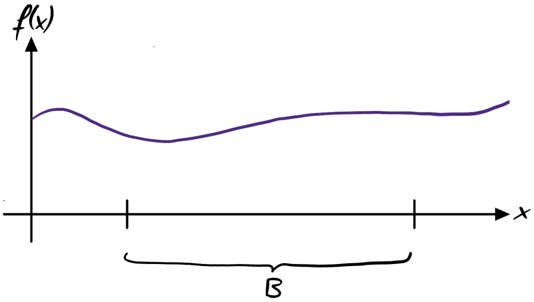

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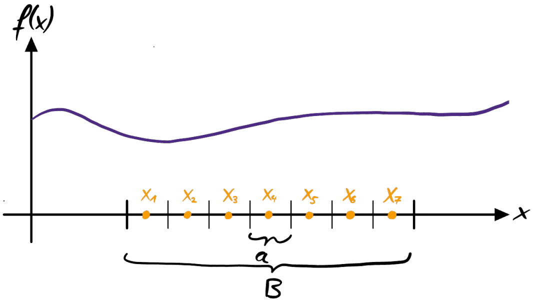

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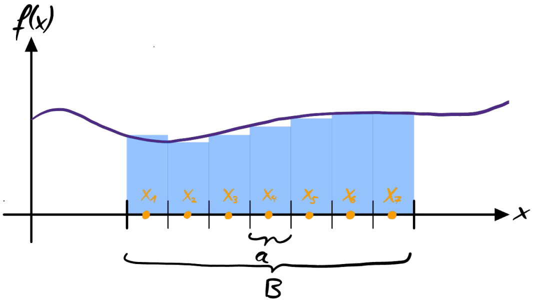

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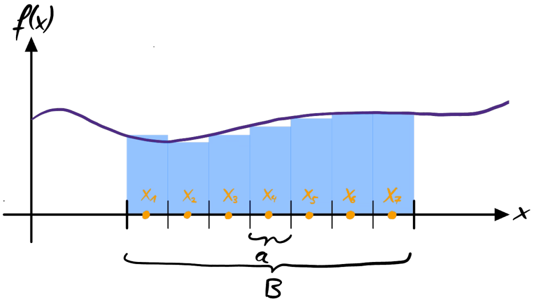

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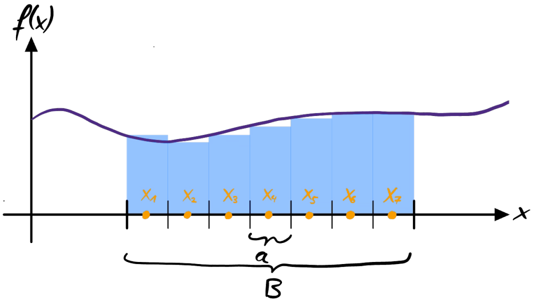

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- problem: slow convergence for high dimension D

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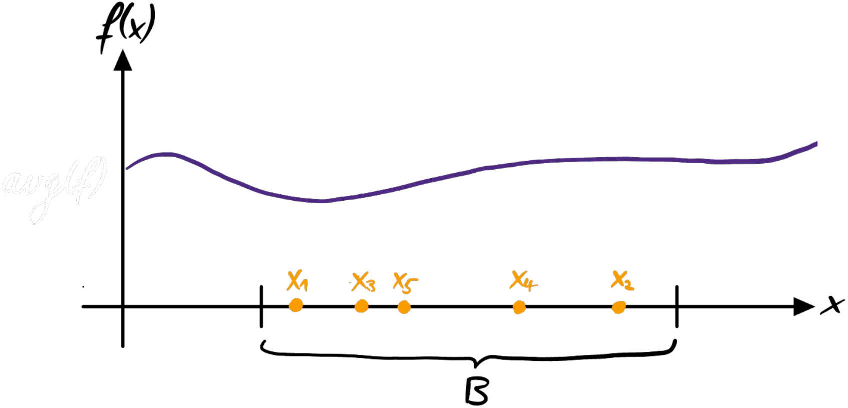

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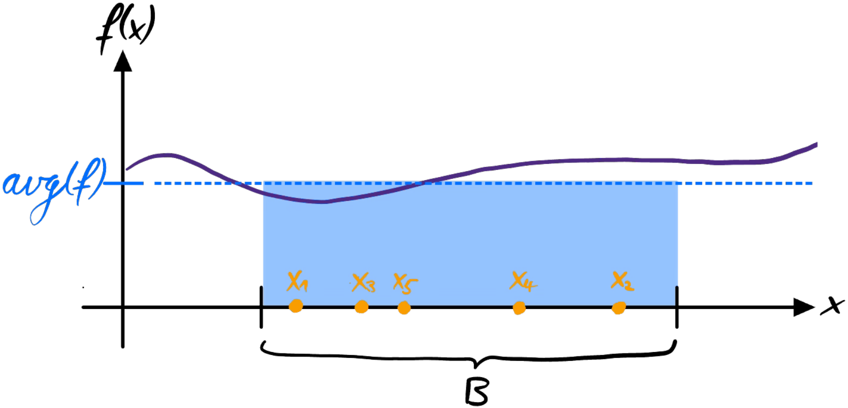

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- problem: $\mathrm{vol}(B)$ might be unknown and σ_M might be very large

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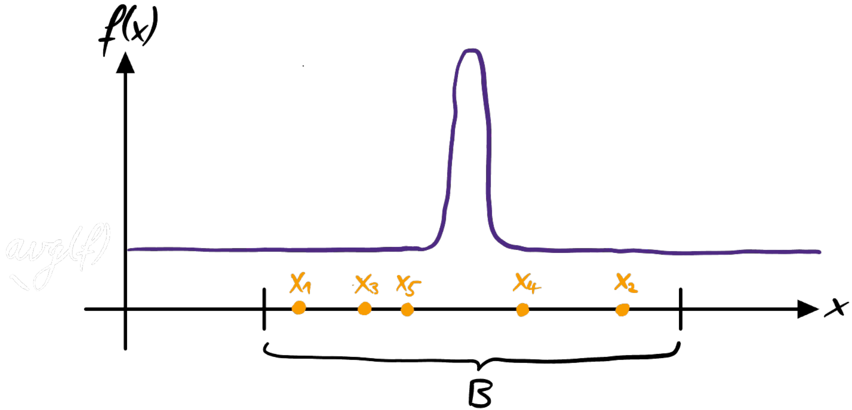

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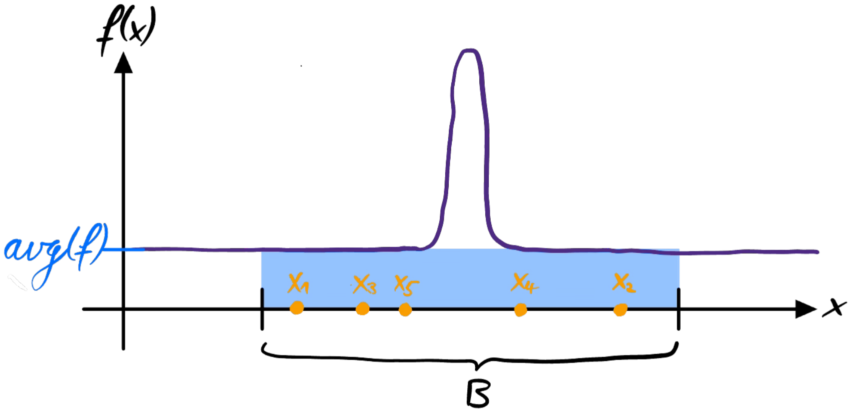

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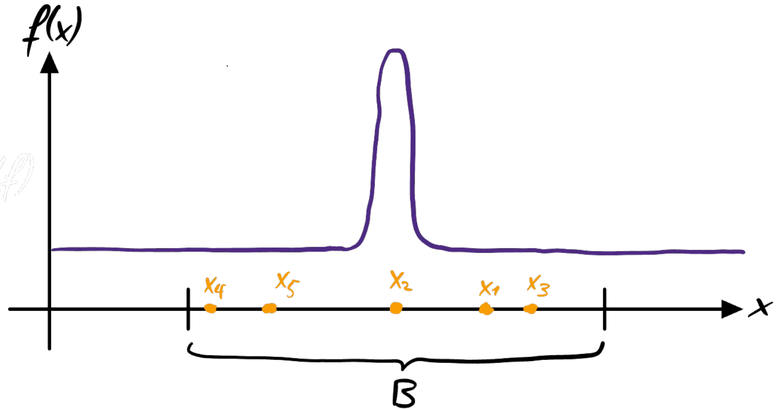

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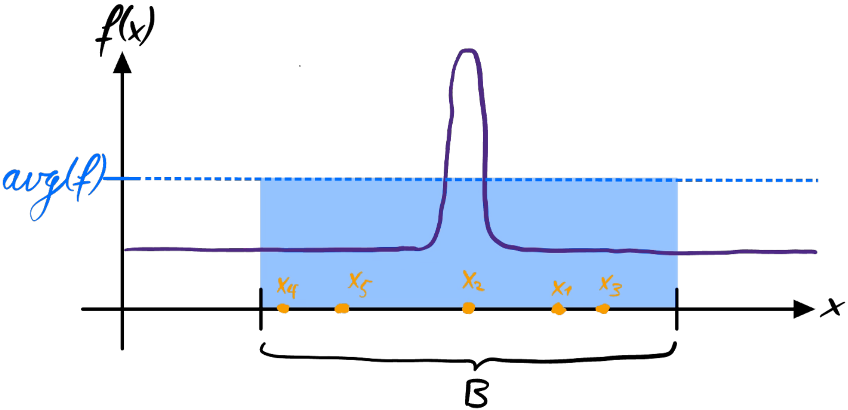

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- our goal is to calculate the variational energy $E(\lambda)$:

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- using importance sampling we find:

$$E(\lambda) = \int_{-\infty}^{\infty} dx \rho(x;\lambda) E_{local}(x;\lambda) \approx \frac{1}{N}\frac{1}{M}\sum_{i=1}^{N}\sum_{j=1}^{M} E_{local}(x;\lambda)(x_j^{(i)};\lambda)$$

Examples

Harmonic oscillator

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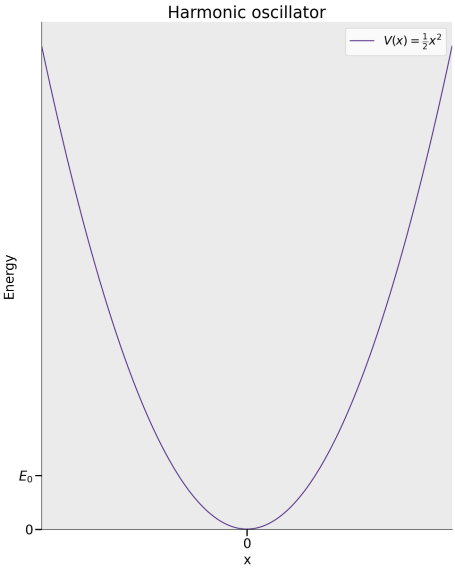

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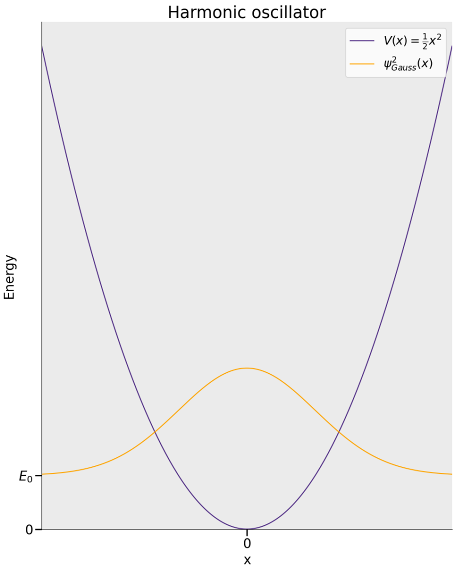

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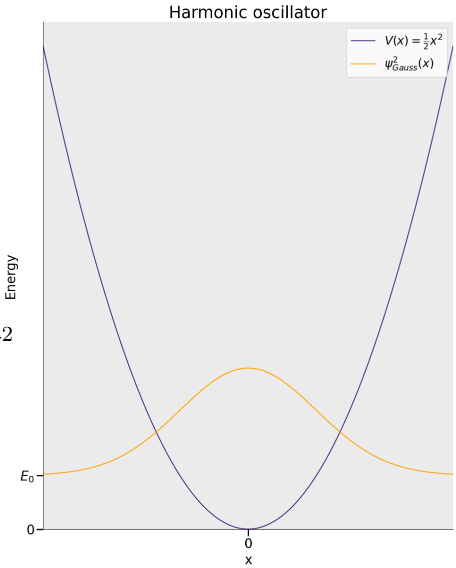

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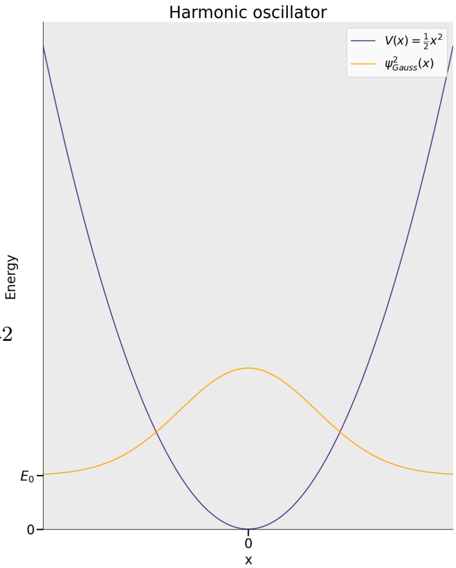

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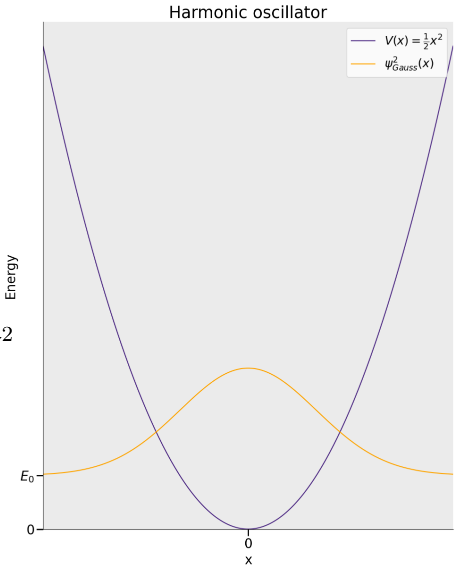
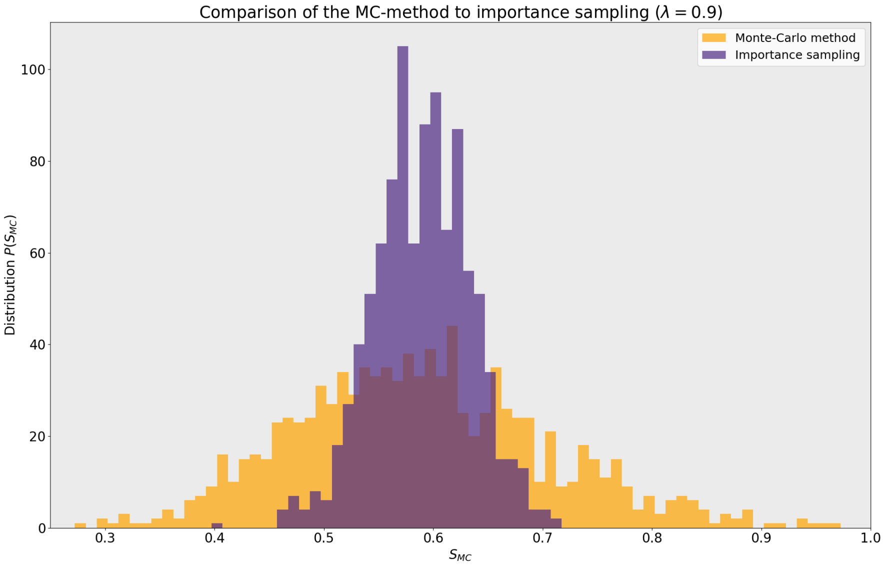
- for $\lambda = \frac{1}{2}$ the variational ansatz is the exact solution
  $\Rightarrow E(x;\lambda = \frac{1}{2}) \equiv E_0 = \frac{1}{2}$



Monte-Carlo method vs. Importance Sampling



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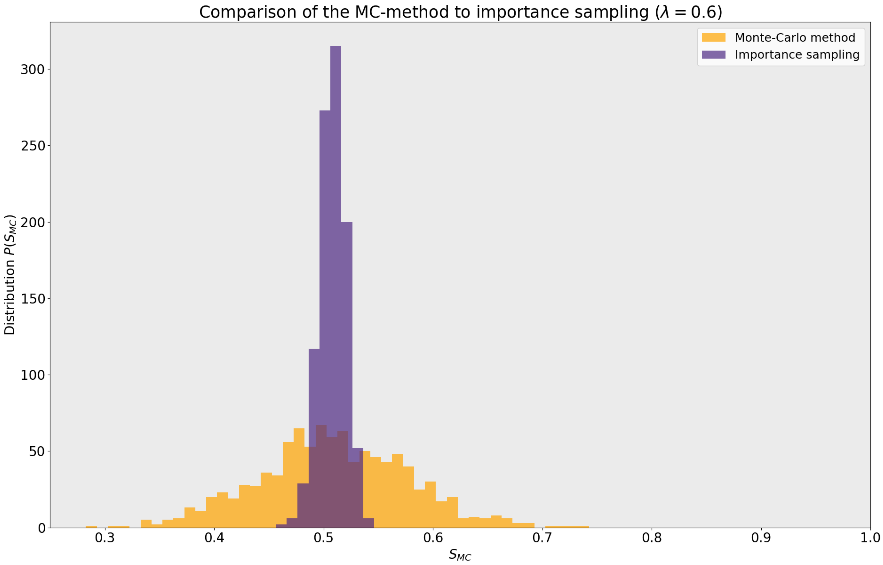

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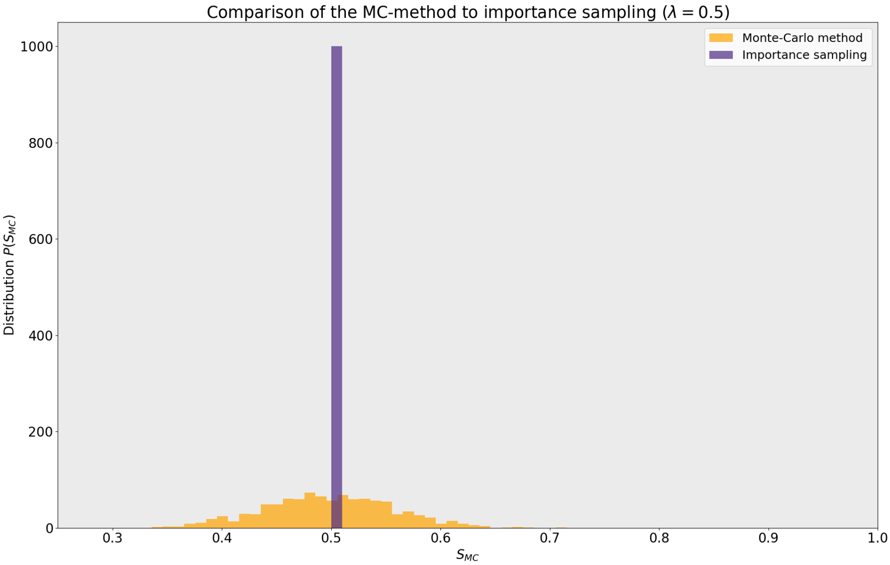
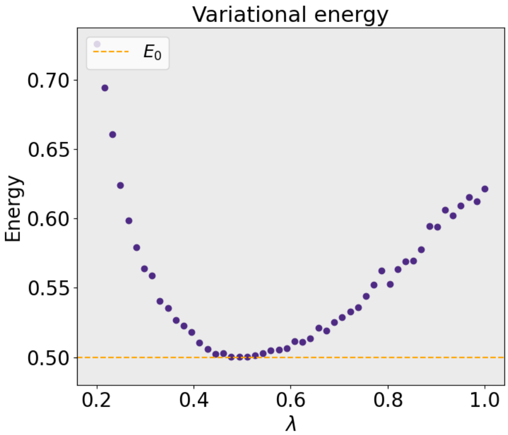


Harmonic Oscillator – Groundstate

Harmonic oscillator with Gaussian trial function



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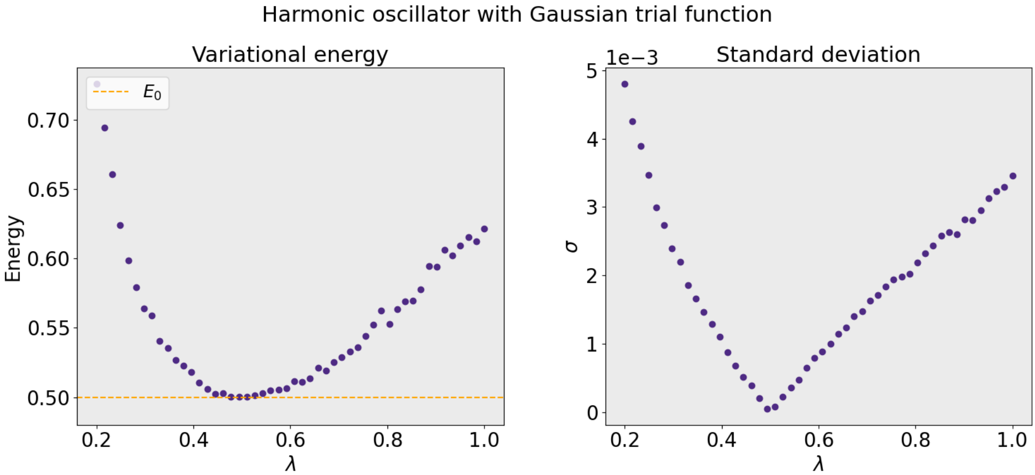
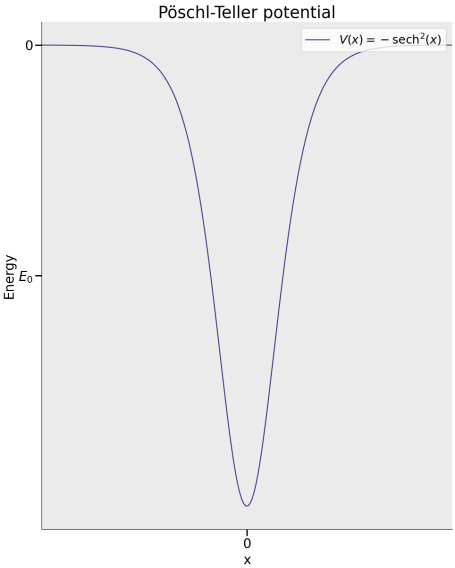


Pöschl-Teller potential

- Hamiltonian: $H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \mathrm{sech}^2(x)$ $(\hbar = m = 1)$



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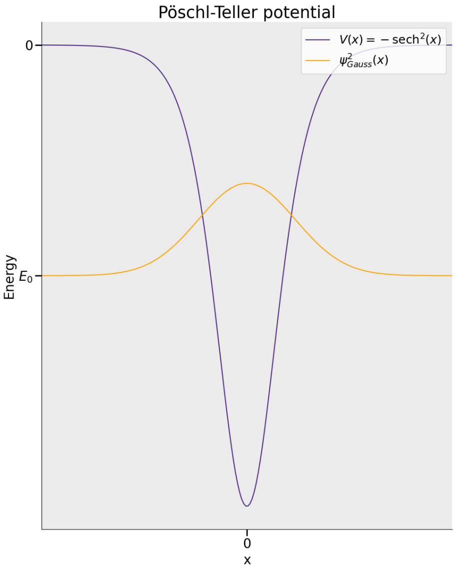

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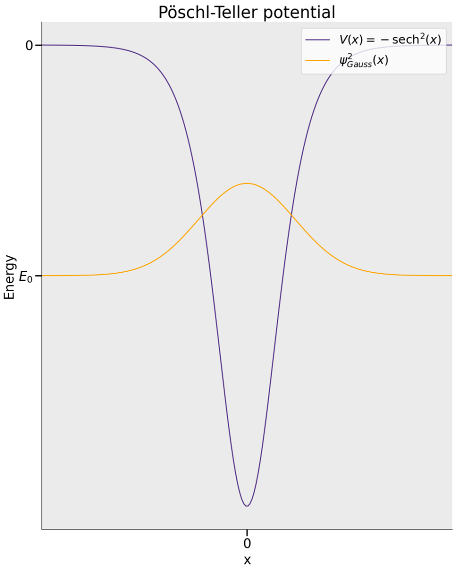

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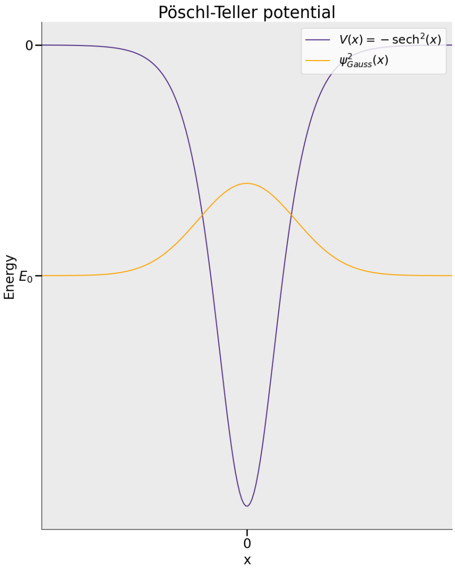

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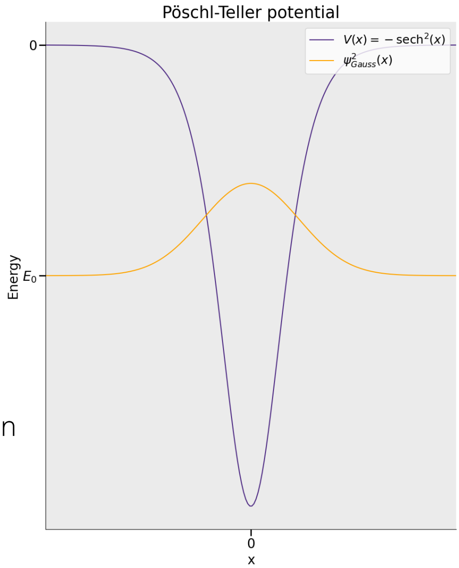
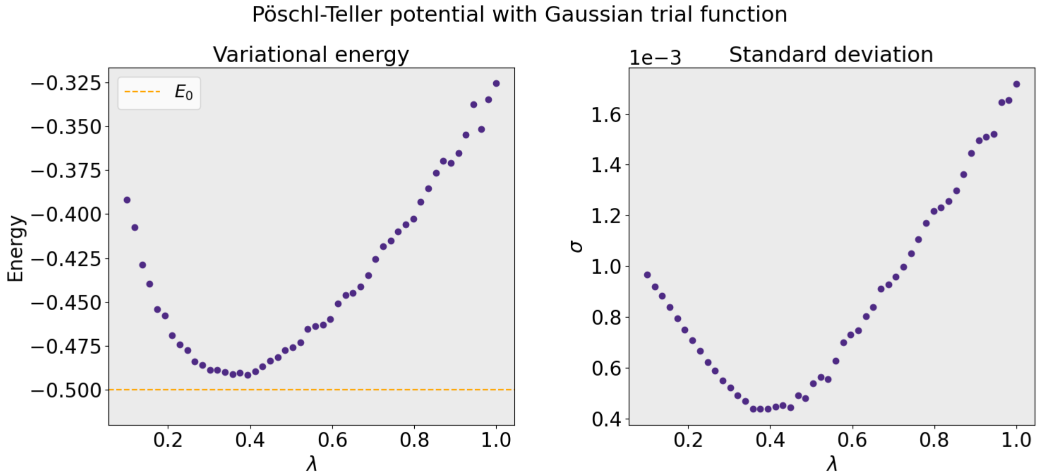
- the variational ansatz is not the exact solution $\Rightarrow E_0 < E(x; \lambda_{min})$



Pöschl-Teller-Potential - Groundstate



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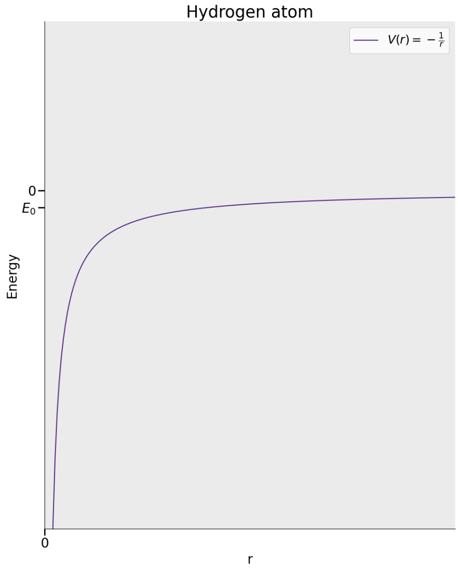

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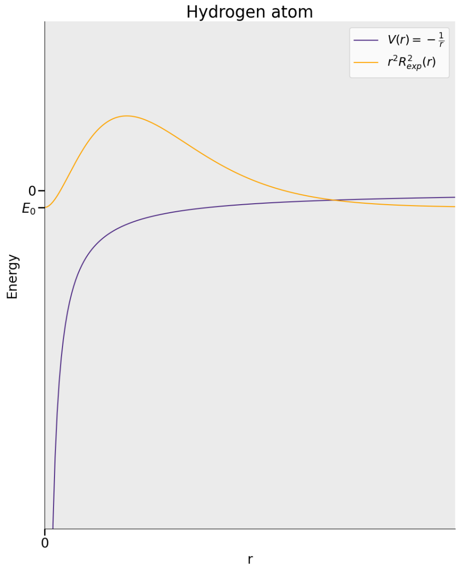

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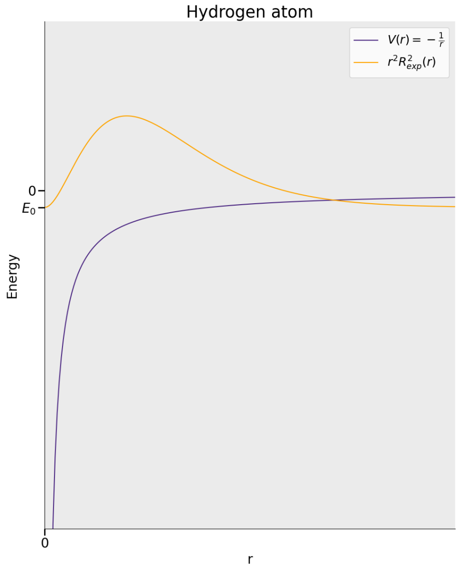

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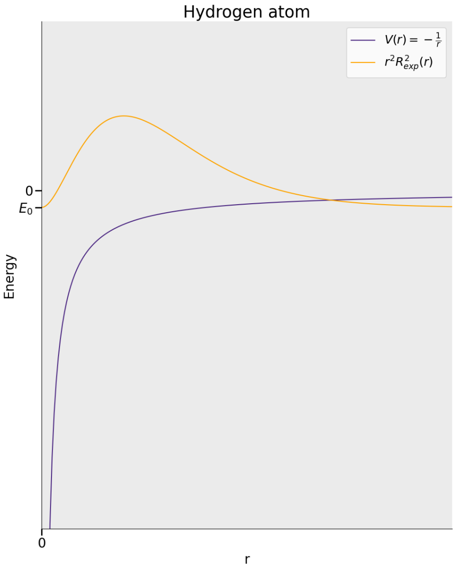

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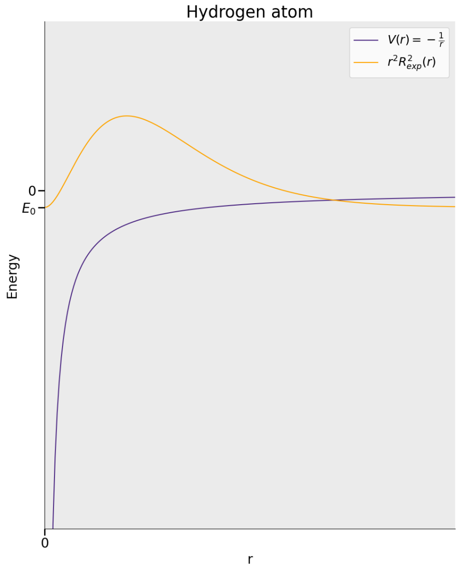
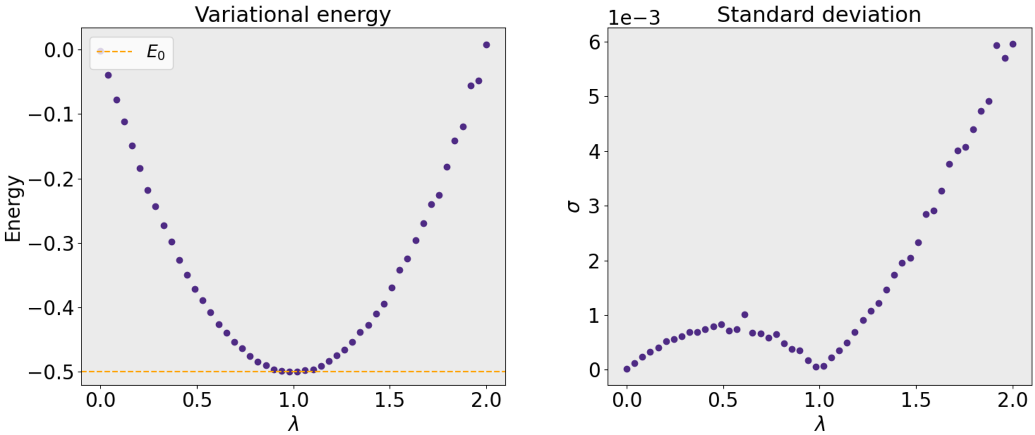
- exact solution: $E_0 = -\frac{1}{2}$
- for $\lambda = 1$ the variational ansatz is the exact solution
  $\Rightarrow E(x;\lambda = 1) \equiv E_0 = -\frac{1}{2}$



Hydrogen atom - Groundstate

Hydrogen atom with exponentially decaying trial function.



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2. for many particles this involves solving high dimensional integrals for which stochastical integration methods are superior to quadrature rules
3. using importance sampling rather than simple sampling reduces the error and therefore the needed computation time significantly