Variational methods for finding ground states of quantum systems

Jonathan Schümann

Dezember 12, 2024

Outline

1. Physical task

2. Numerical task
   2.1. Simple sampling
   2.2. Importance sampling

3. Examples

Physical task

[Pottorf et al.; Eur. J. Phys. 20 (1999) 205]

[Gould et al.; An Introduction to Computer Simulation Methods (Addition Wesley, 2006); Chapt. 16.7]

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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- we're not interested in the wavefunctions $\psi_i(\mathbf{x})$
- no physical intuition is used

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

Numerical task

[Jeckelmann; Lecture 07: Monte-Carlo Integration (Lecture on Computerphysik, 2022)]

[Gould et al.; An Introduction to Computer Simulation Methods (Addition Wesley, 2006); Chapt. 11]

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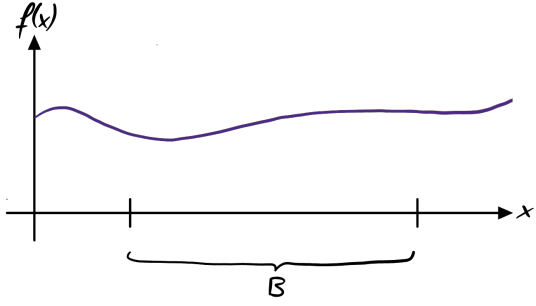

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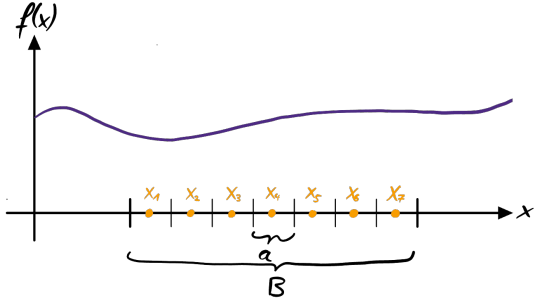

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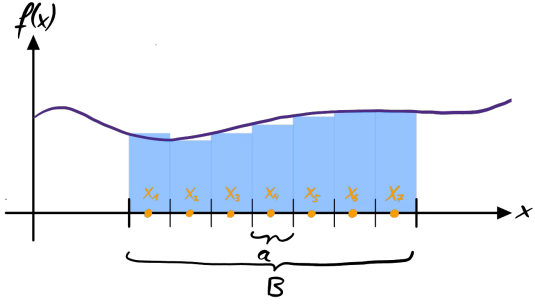

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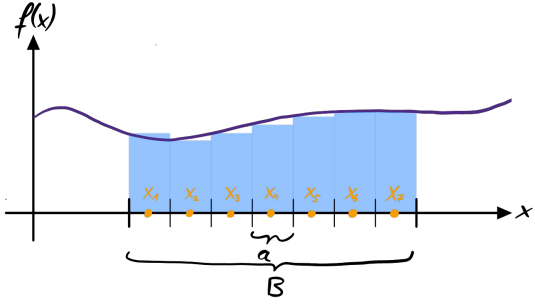

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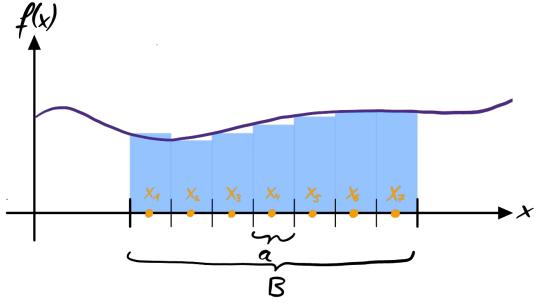

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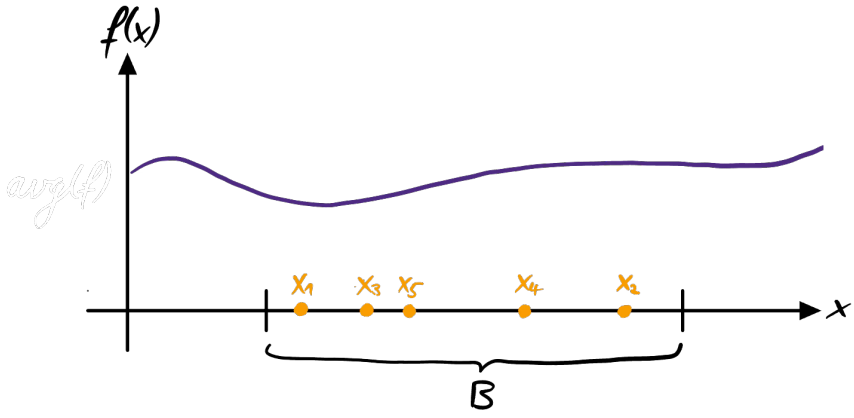

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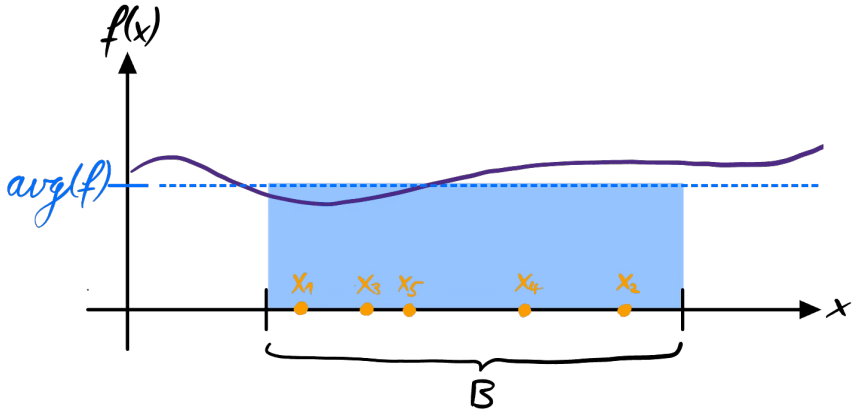

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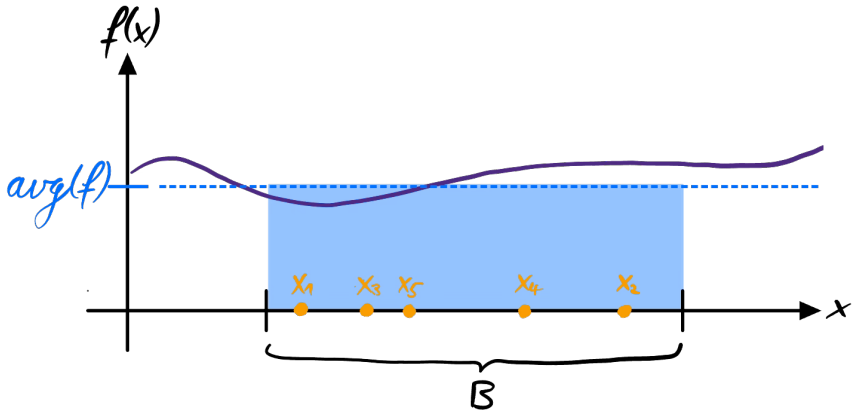

- error: $|I - S_M^{MC}| \propto M^{-\frac{1}{2}}$

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

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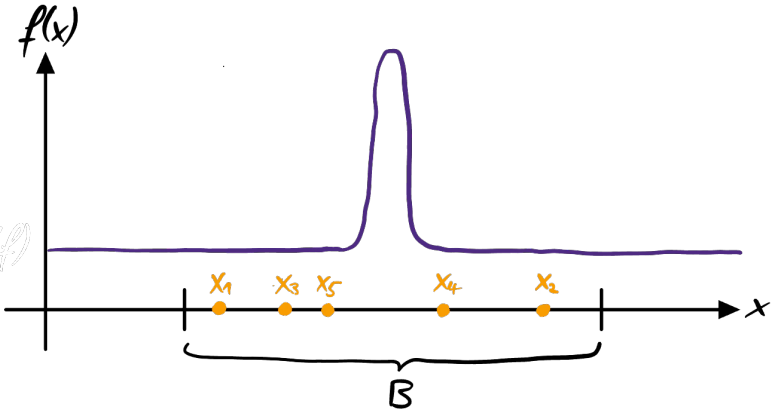

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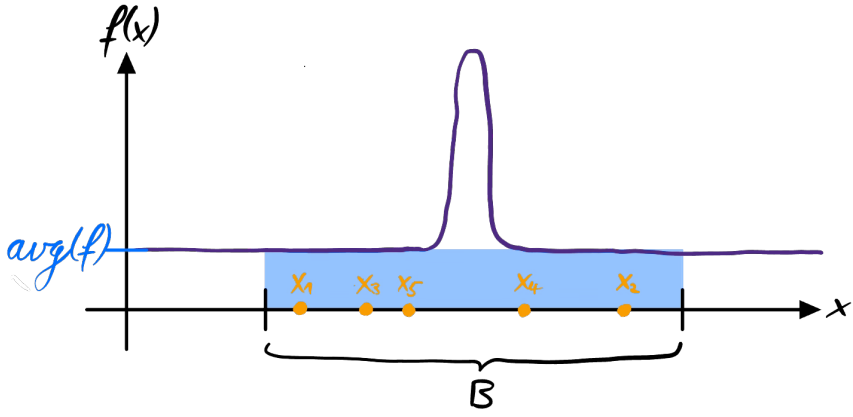

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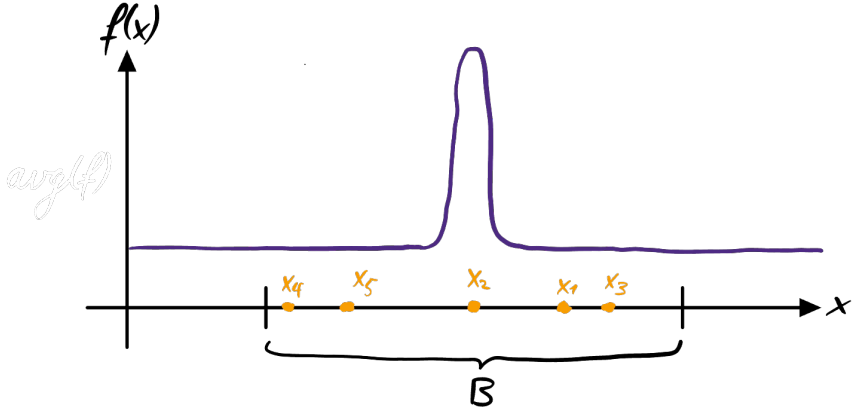

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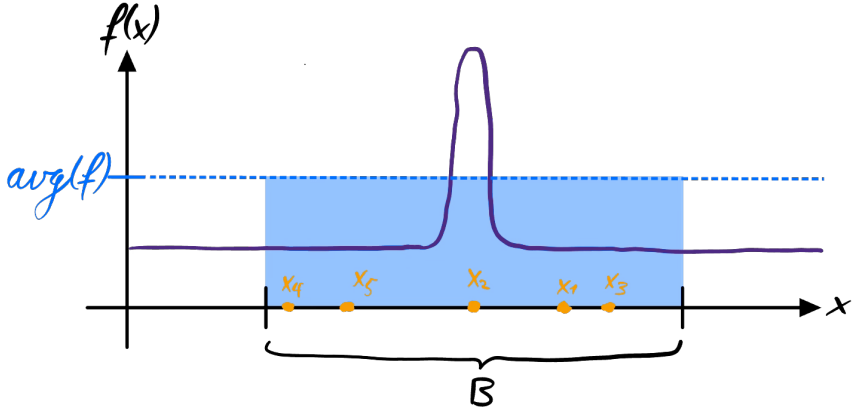

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- our goal is to calculate the variational energy $E(\lambda)$:

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- using importance sampling we find:

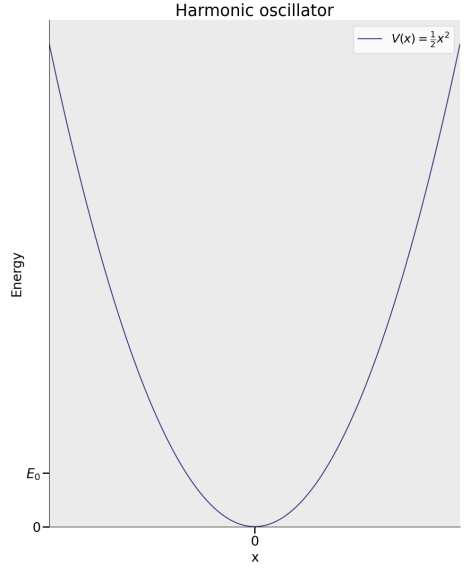
$$E(\lambda) = \int_{-\infty}^{\infty} dx \rho(x;\lambda) E_{local}(x;\lambda) \approx \frac{1}{N}\frac{1}{M} \sum_{i=1}^{N} \sum_{j=1}^{M} E_{local}(x_j^{(i)};\lambda)$$

Examples

[https://github.com/JSchuemann-physics/VariationalMethods]

Harmonic oscillator

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



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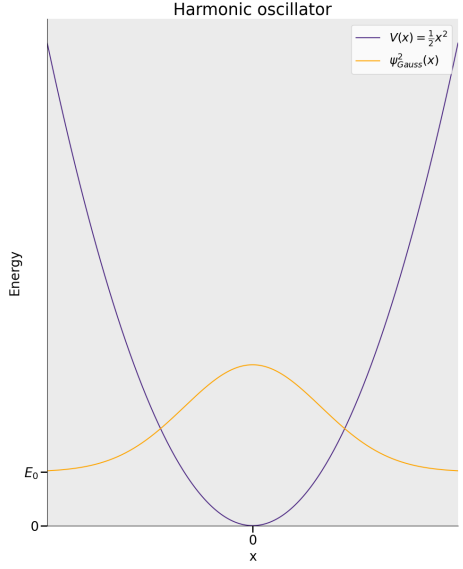

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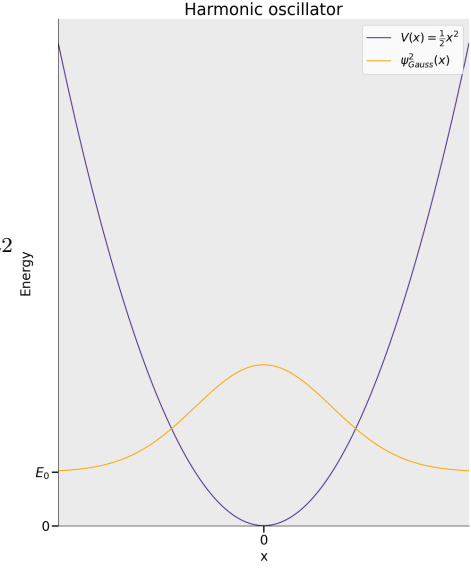

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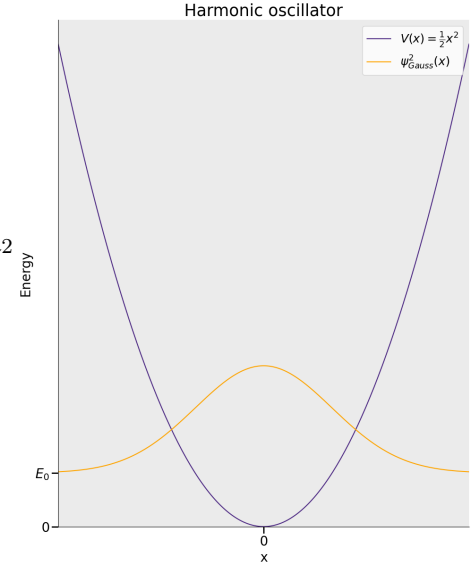
- exact solution: $E_0 = \frac{1}{2}$



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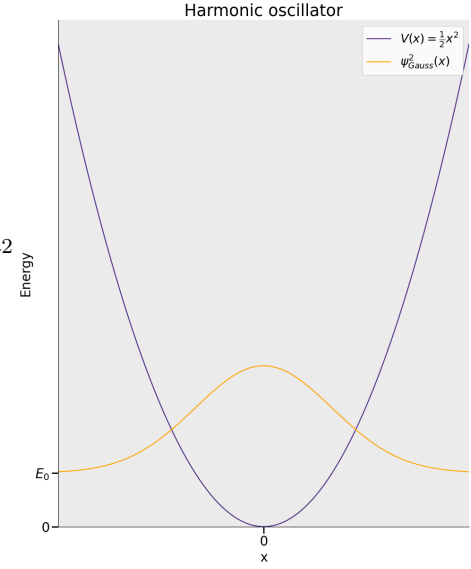
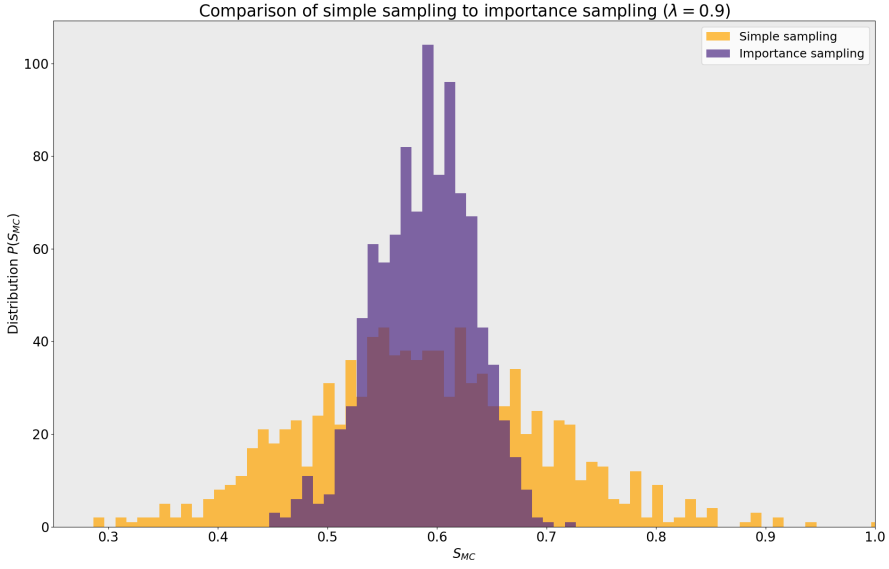
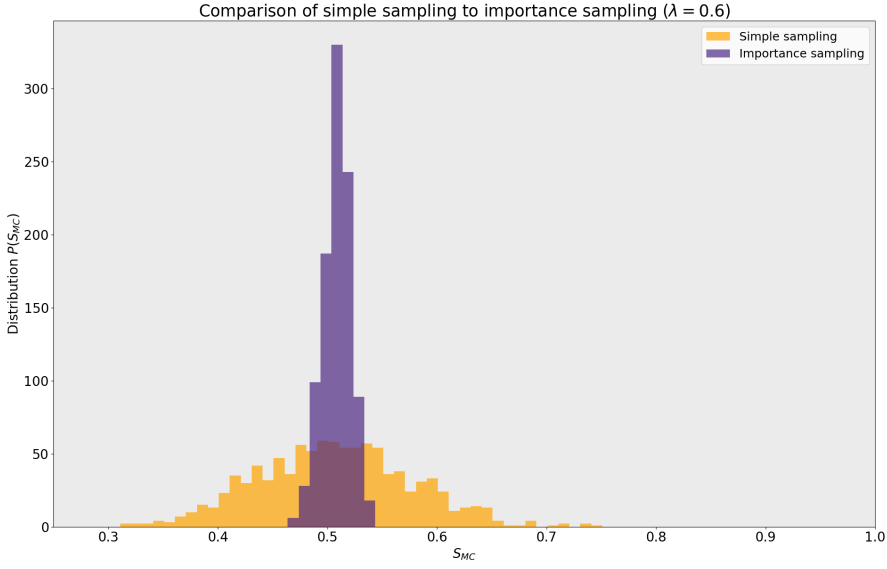


Simple sampling vs. importance sampling



Simple sampling vs. importance sampling



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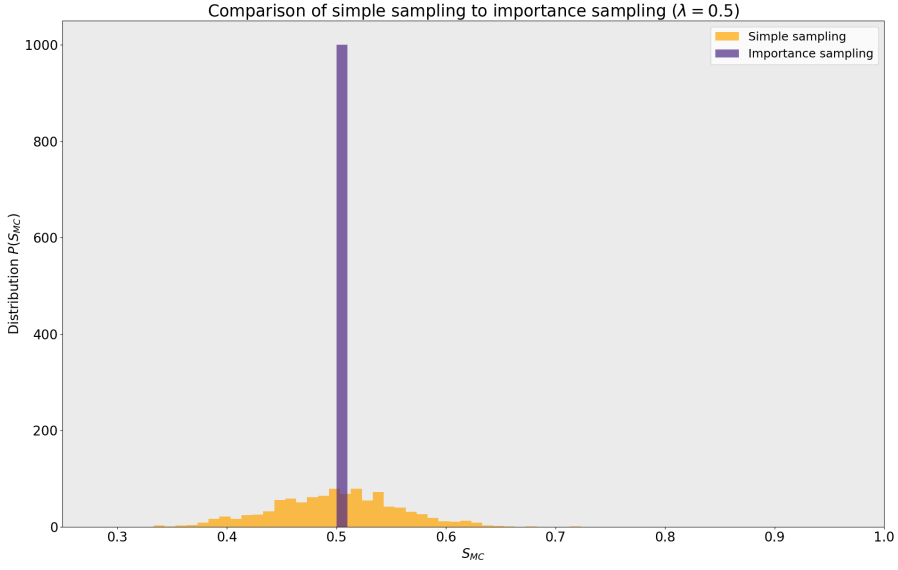
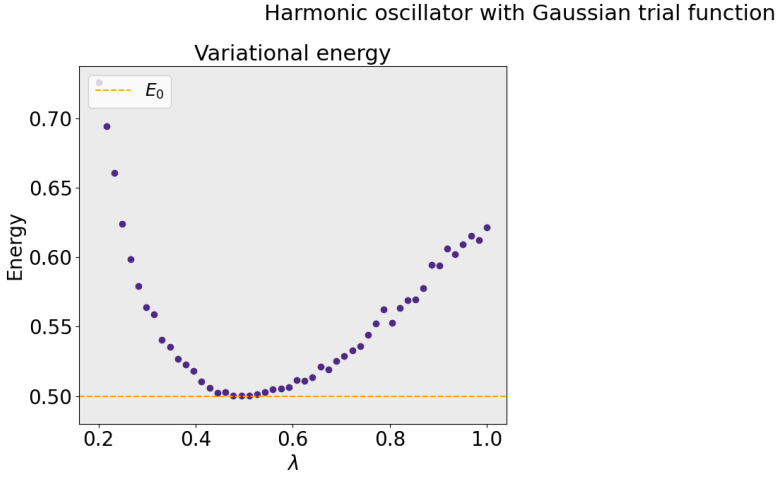


Harmonic Oscillator - Groundstate



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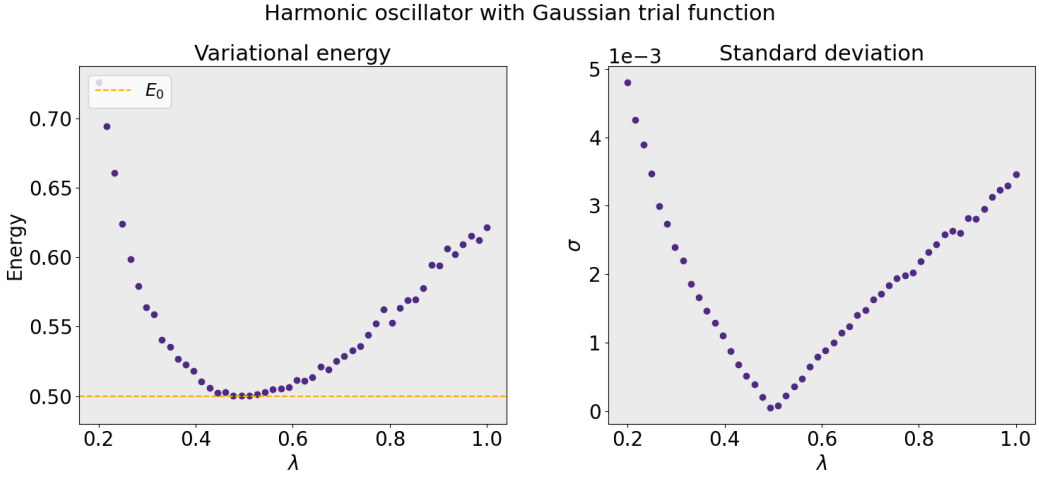
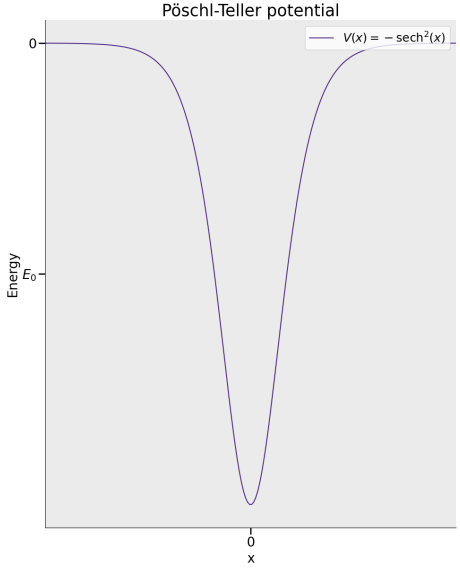


Pöschl-Teller potential

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



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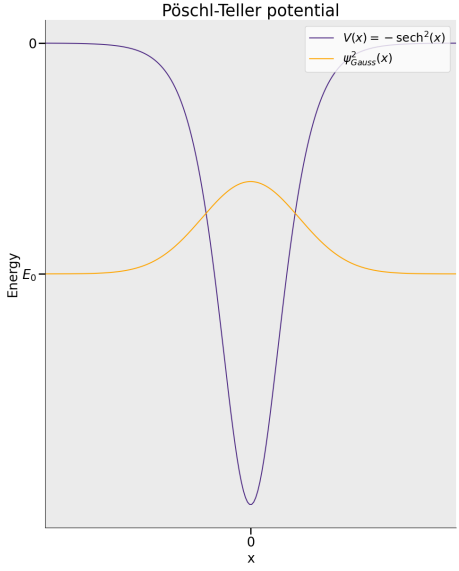

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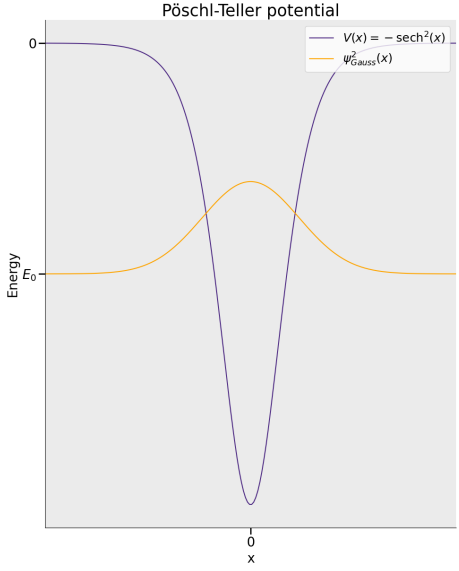

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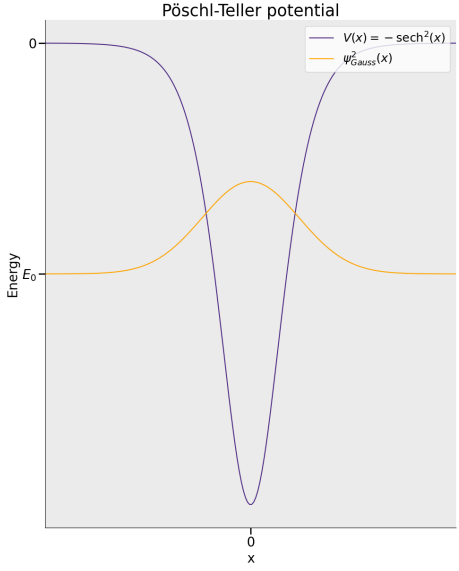

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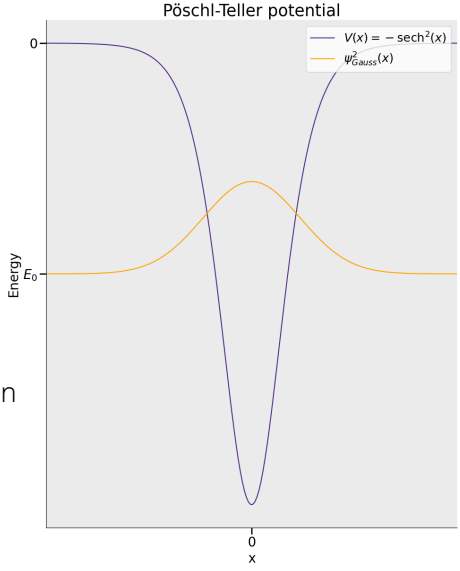
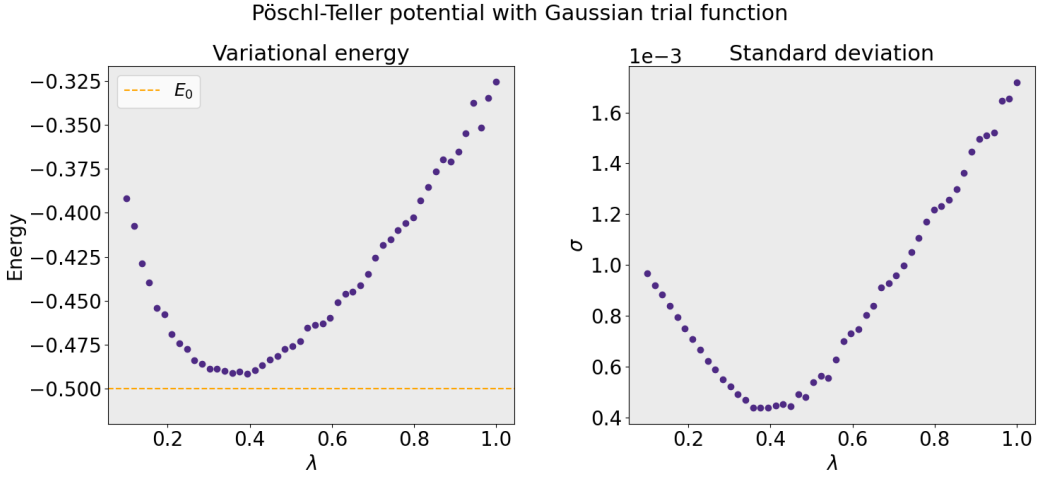


Pöschl-Teller-Potential - Groundstate



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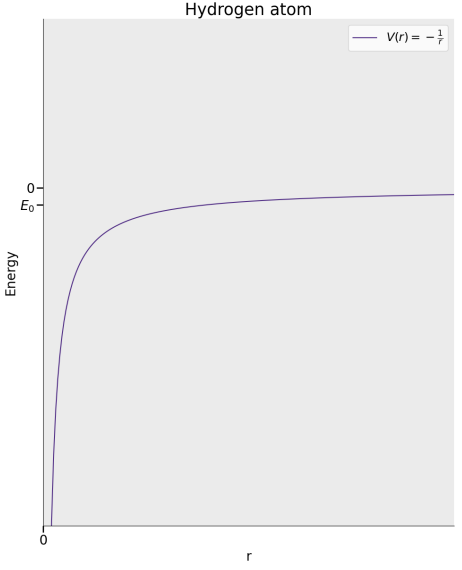

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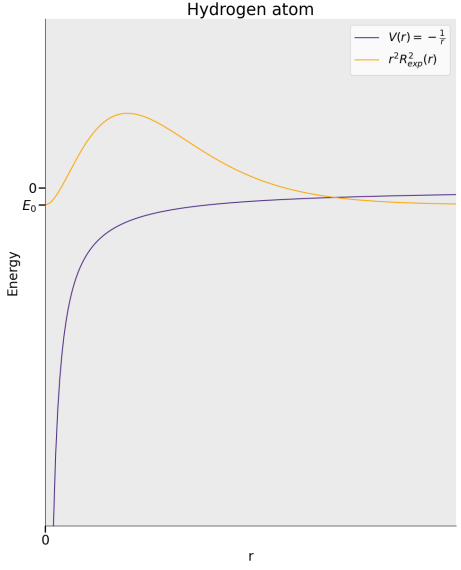

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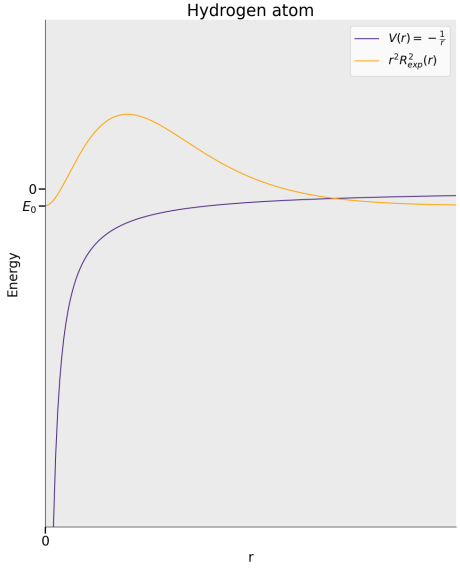

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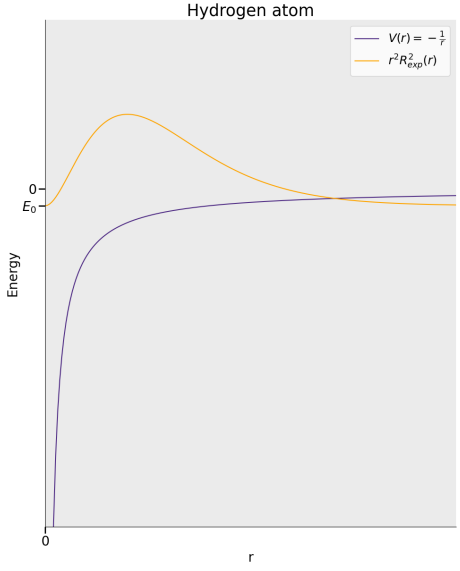

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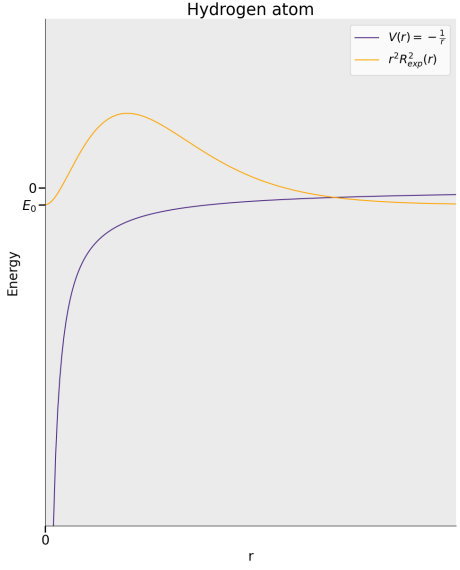
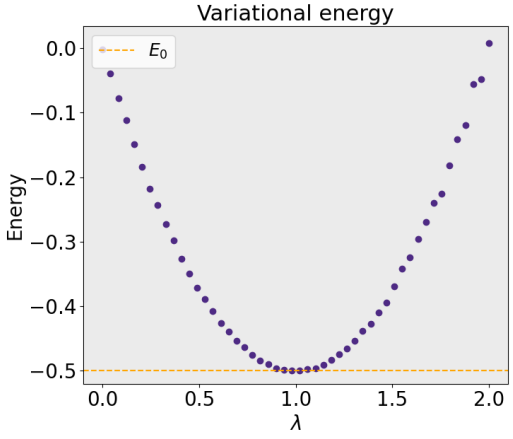
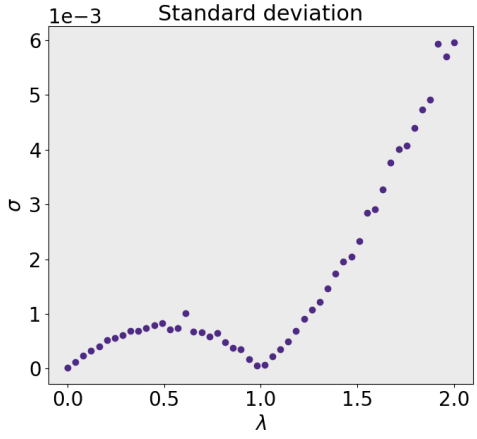


Hydrogen atom - Groundstate

Hydrogen atom with exponentially decaying trial function.





Conclusion

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Conclusion

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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