GROUND STATE ENERGY SIMULATIONS USING MONTE CARLO RANDOM WALK

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Abstract. Placeholder for abstract.

Contents

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1. Introduction

Overview of the challenges in solving the Schrödinger equation numerically The connection between the imaginary-time Schrödinger equation and diffusion processes Historical development of Monte Carlo methods in quantum mechanics Brief comparison with alternative numerical approaches (matrix diagonalization, variational methods) Motivation: why random walks are particularly well-suited for ground state energy calculations

2. Method

2.1. Theoretical Foundation. While the usage of Monte Carlo methods to simulate quantum mechanics may seem strange at first, looking at the time-dependent Schrödinger equation as a diffusion equation in imaginary time reveals the connection that makes it possible. Here is the time-dependent Schrödinger equation for a particle of mass m in a potential $V(x)$:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = \hat{H}\psi(x,t) \tag{2.1}$$

By using $\tau = it$, it becomes:

$$\frac{\partial}{\partial \tau}\psi(x,\tau) = \frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi(x,\tau) - \frac{V(x)}{\hbar}\psi(x,\tau) = -\frac{\hat{H}}{\hbar}\psi(x,\tau) \tag{2.2}$$

This is a diffusion equation with a growth/decay term with a diffusion constant $D = \hbar/2m$ where the growth/decay term determines whether the population density of walkers at a given position increases or decreases.

The general solution to equation 2.2 can be written using the eigenstates and eigenvalues of the Hamiltonian:

$$\psi(x,\tau) = \sum_n c_n\phi_n(x)e^{-E_n\tau/\hbar} \tag{2.3}$$

where $\phi_n(x)$ are the eigenfunctions of the Hamiltonian with corresponding energies E_n, and c_n represents the projection of the initial wavefunction onto each eigenstate. If we consider the case where $\tau \to \infty$, all terms decay exponentially, but the ground state decays the slowest:

$$\lim_{\tau\to\infty}\psi(x,\tau) = c_0\phi_0(x)e^{-E_0\tau/\hbar} \tag{2.4}$$

If we then were able to simulate the diffusion process for a sufficiently long time, then the distribution of our random walkers would approach the ground state wavefunction $\phi_0(x)$, so the decay rate of the walker population would be the ground state energy E_0.

2.2. Implementation Details. To implement this approach computationally, we discretize both space and time. For simplicity, we describe the one-dimensional case, though the method extends naturally to higher dimensions.

We introduce a spatial lattice with spacing h_x and temporal steps of size h_τ. The probability $p(j,n)$ for a walker to be at lattice site j after n time steps satisfies:

$$p(j,n+1) = \frac{1}{2}[1-a(j)][p(j-1,n) + p(j+1,n)] \tag{2.5}$$

Here, $a(j)$ represents the probability of a walker being absorbed at site j, which is related to the potential by:

$$a(j) = h_\tau \frac{V(x_j)}{\hbar} \tag{2.6}$$

In the continuum limit with small h_x and h_τ, we obtain:

$$\frac{\partial p}{\partial \tau} = \frac{1}{2}\frac{\partial^2 p}{\partial x^2} - \frac{V(x)}{\hbar}p \tag{2.7}$$

which matches our imaginary-time Schrödinger equation when we identify $p(x, \tau)$ with $\psi(x, \tau)$ (up to normalization).

The ground state energy can be extracted by measuring the rate at which the walker population decays:

$$E_0 = -\frac{\hbar}{\Delta\tau} \ln\left\{\frac{p(\tau + \Delta\tau)}{p(\tau)}\right\} \tag{2.8}$$

where $p(\tau)$ represents the total number of walkers surviving at time τ. In practical implementations, we determine E_0 by plotting $\ln(p(\tau))$ against τ and measuring the slope after initial transients have decayed.

For bounded potentials like the infinite square well, it is convenient to relate the energy to a dimensionless quantity. If we set $x = aj/J$ where a is the well width and J is an integer boundary parameter, the ground state energy is related to the decay rate λ by:

$$E_0 = \frac{\hbar^2}{ma^2}\lambda J^2 \tag{2.9}$$

For the infinite square well, the exact ground state energy is $E_0 = \pi^2\hbar^2/8ma^2$, so we expect $\lambda J^2 = \pi^2/8 \approx 1.234$.

A practical issue with the absorption-only algorithm is that the walker population inevitably decays to zero. To maintain statistical accuracy, we implement a branching mechanism. By introducing a reference energy E_s, we modify the absorption probability to:

$$a(j) = h_\tau \frac{V(x_j) - E_s}{\hbar} \tag{2.10}$$

When $a(j) < 0$ (i.e., when $V(x_j) < E_s$), instead of absorption, we create a new walker with probability $|a(j)|$. By dynamically adjusting E_s to maintain a steady walker population, we obtain an estimate of E_0.

2.3. Algorithm Variants.

Several variants of the random walk method have been developed to address different challenges:

2.3.1. *Simple Absorption Method.*

The basic method uses random walks with position-dependent absorption probabilities and is suitable for simple one-dimensional problems. Walkers start at an initial position and perform unbiased random steps until they are either absorbed or reach a specified maximum time.

2.3.2. *Diffusion Monte Carlo (DMC) with Branching.* To improve statistical efficiency, DMC introduces a branching mechanism where walkers can both die and replicate. The reference energy E_s is adjusted dynamically to maintain a roughly constant population:

$$E_s(\tau + \Delta\tau) = \langle V \rangle - \frac{N(\tau + \Delta\tau) - N(\tau)}{N(\tau)\Delta\tau}\hbar \tag{2.11}$$

where $\langle V \rangle$ is the average potential energy of the current walker distribution, and $N(\tau)$ is the number of walkers at time τ.

2.3.3. *Importance Sampling Methods.* For many potentials, efficiency can be improved by using importance sampling. In guided random walk (GRW) methods, walkers are guided by a trial wavefunction $\psi_T(x)$ that approximates the ground state. This modifies the diffusion process to concentrate walkers in important regions of the potential.

2.3.4. *Computing Expectation Values.* To calculate observables other than energy, we need to sample from the probability distribution $|\psi_0(x)|^2$ rather than $\psi_0(x)$. This can be achieved through a procedure where walkers evolve for time τ, their positions are recorded, and then they continue for another period τ. Only positions of walkers that survive both periods are included in the average:

$$q(x, \tau) = \int G(0, 0; x, \tau)G(x, \tau; y, 2\tau)dy \propto |\psi_0(x)|^2 \tag{2.12}$$

where $G(x_1, \tau_1; x_2, \tau_2)$ is the Green's function of the imaginary-time Schrödinger equation.

For the harmonic oscillator potential $V(x) = \frac{1}{2}x^2$, the exact ground state wavefunction is $\psi_0(x) = \pi^{-1/4}e^{-x^2/2}$, leading to $|\psi_0(x)|^2 = \pi^{-1/2}e^{-x^2}$. This provides a benchmark for testing the accuracy of our sampling procedure.

For field theory applications, the method extends naturally to random walks in function space, where the probability of absorption/creation becomes:

$$a[\phi] = h_\tau \left(v \sum_{j=1}^{N} V(\phi)_j - E_s \right) \tag{2.13}$$

where v is the unit cell volume in the discretized space.

The optimal runtime parameter τ_{opt} and initial walker count N_0 to achieve a desired accuracy δE_0 can be estimated from:

$$\tau_{opt} \approx \frac{\ln(N_0)}{2E_m - E_0} \approx \frac{\ln(E_0/\delta E_0)}{E_m - E_0} \tag{2.14}$$

$$N_0 \approx \left(\frac{E_0}{\delta E_0} \right)^{[2+E_0/(E_m - E_0)]} \tag{2.15}$$

where E_m is the energy of the first excited state not excluded by symmetry considerations.

3. Results

3.1. One-Dimensional Test Cases. Infinite square well potential (analytical $E_0 = \pi^2\hbar^2/8ma^2$) Harmonic oscillator potential ($E_0 = \hbar\omega/2 = 0.5$ in natural units)

$$V(x) = \frac{1}{2}x^2 \quad \text{with ground state} \quad \psi_0(x) = \pi^{-1/4}e^{-x^2/2} \tag{3.1}$$

Convergence analysis and parameter optimization

3.2. Higher-Dimensional Applications. Two-dimensional circular well with energy ratios $1.44 : 3.61 : 6.50$ Excited state energies using nodal constraints Statistical uncertainty and error analysis

$$\sigma_{E_0} \approx \frac{E_0}{\sqrt{N_\tau}} \approx N_0^{-1/2}e^{E_0\tau/2} \tag{3.2}$$

3.3. Performance Considerations. Scaling with system dimensionality Efficiency comparison with other methods Error estimation and confidence intervals

$$\tau_{opt} \approx \frac{\ln(N_0)}{2E_mE_0} \approx \frac{\ln(E_0/\delta E_0)}{E_m - E_0} \tag{3.3}$$

4. Discussion

4.1. Parameter Optimization. Effects of lattice spacing, time step, and walker population Balancing computational cost and accuracy Handling statistical fluctuations through averaging techniques

4.2. Method Strengths and Limitations. Robust performance in higher dimensions Challenges with excited states and nodal surfaces Comparison with traditional numerical methods Applicability to different potential types

4.3. Advanced Applications. Extensions to field theory with probability

$$a[\phi] = h_\tau \left(v \sum_{j=1}^{N} V(\phi)_j E_s \right) \tag{4.1}$$

Many-body quantum systems Handling sign problems for fermions

5. Conclusion

Summary of key findings and method effectiveness Practical recommendations for implementation Future directions for method improvement Potential applications to more complex quantum systems

Appendix

Detailed derivations of key equations Pseudocode for the main algorithms Benchmark data and supplementary results

Appendix A. Additional Citations

18 Examples
6 for each: random walk, Monte Carlo, random numbers
3 in academia, 3 outside academia

References