

```
In [10]: # Preamble: minimal imports + local include
using Random
using Statistics
using Printf
using Plots
using Logging

include("formatting.jl")

if !isdefined(Main, :System1D)
    include("../src/System1D.jl")
end
using .System1D: Hamiltonian, Walker, DMCPParams, DMCSim, run_simulation!, pl
```

## System: 1D Harmonic Oscillator (No Importance Sampling)

### Potential

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

**Trial wavefunction** No importance sampling is used in this notebook (effectively  $\psi_T(x) = 1$ ).

This cell defines the Hamiltonian, initializes walkers, and runs the simulation.

```
In [11]: # System: 1D harmonic oscillator
V(R) = 0.5 * R[1]^2
H = Hamiltonian(1, 0.5, V)

# Walkers and params
targetN = 5000
walkers = [Walker([2 * rand() - 1]) for _ in 1:targetN]

params = DMCPParams(0.005, 400, 50, targetN, 0.5, 0.1, 10, 50)

# Run
rng_sim = MersenneTwister(42)
sim = DMCSim(H, params, walkers, rng_sim)
run_simulation!(sim; snapshot_steps=[params.nsteps])

ET_history = sim.ET_history
population_history = sim.population_history
energy_mean_history = sim.energy_mean_history
energy_variance_history = sim.energy_variance_history

nothing
```

## Results

## Exact ground-state energy

$$E_0 = \frac{1}{2} \text{ (a.u.)}$$

This cell reports the post-equilibration energy and plots the reference energy, population, mean local energy, and local-energy variance over time, plus the final walker density.

```
In [12]: # Results and plots
t = (0:params.nsteps) .* params.dt
E_ref = 0.5

nequil = params.nequil
start_idx = min(nequil + 1, length(energy_mean_history))
postE = energy_mean_history[start_idx:end]

Ebar = mean(postE)
SEM = (length(postE) > 1) ? std(postE) / sqrt(length(postE)) : NaN

Ebar_str, SEM_str = format_with_uncertainty(Ebar, SEM)
println("HO DMC energy (post-eq, nequil=$(nequil)): E = $(Ebar_str) +/- $(SEM_str) eV")
E_final_str, var_str = format_pair_sigfig(energy_mean_history[end], energy_variance_history[end])
println("Final step: E = $(E_final_str), Var(E_L) = $(var_str) eV")
println("Reference energy: $(format_sigfig(E_ref; sigfigs=2)) eV")

Logging.with_logger(Logging.NullLogger()) do
    redirect_stderr(devnull) do
        p1 = plot(t, ET_history, xlabel="step", ylabel="E_T", title="Reference energy")
        display(p1)

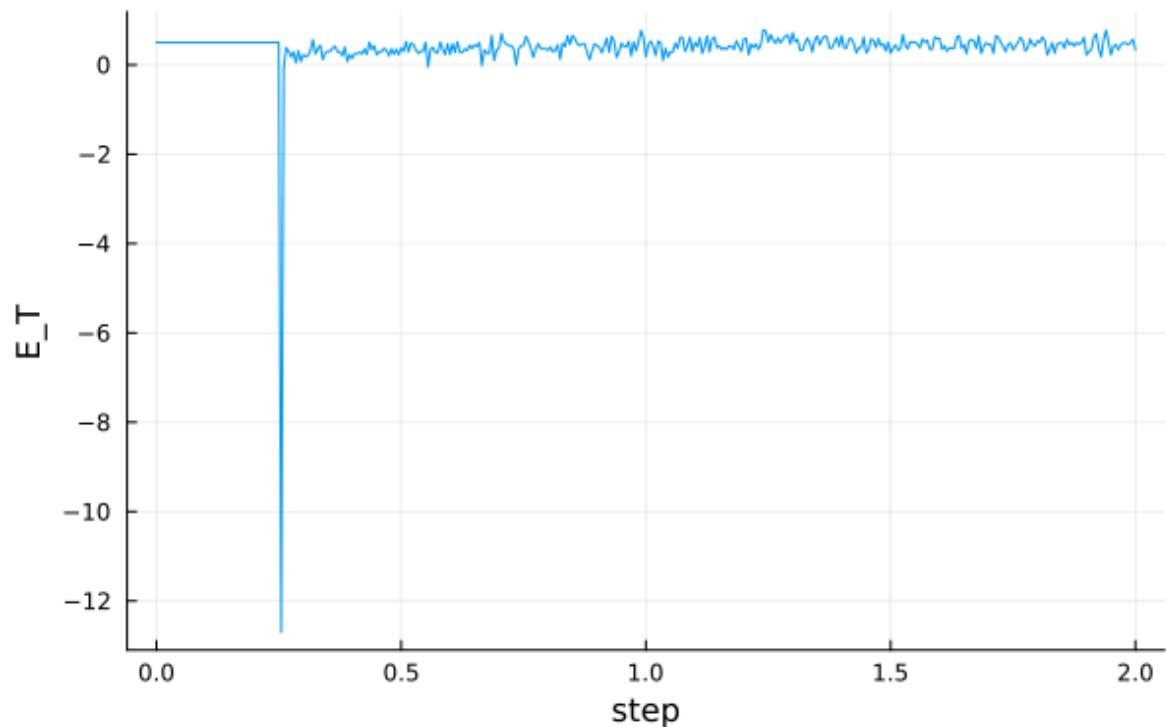
        p2 = plot(t, population_history, xlabel="step", ylabel="N_w", title="Population")
        display(p2)

        p3 = plot(t, energy_mean_history, xlabel="step", ylabel="<E_L>", title="Mean energy")
        plot!(p3, [t[1], t[end]], [E_ref, E_ref], ls=:dash, label="ref")
        display(p3)

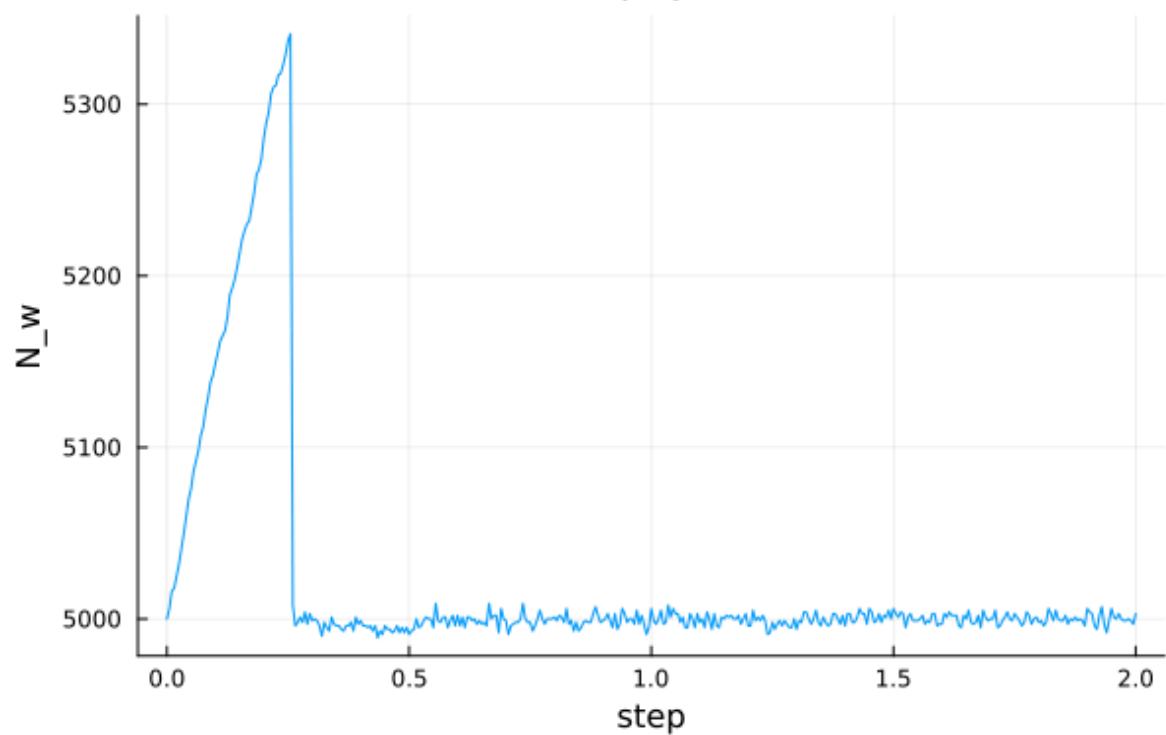
        p4 = plot(t, energy_variance_history, xlabel="step", ylabel="Var(E_L)", title="Energy variance")
        display(p4)

        if !isempty(sim.walker_positions_history)
            snap = sim.walker_positions_history[end]
            p5 = plot_snapshot_1d_density(snap; nbins=120, title="Final walker density")
            display(p5)
        end
    end
end
```

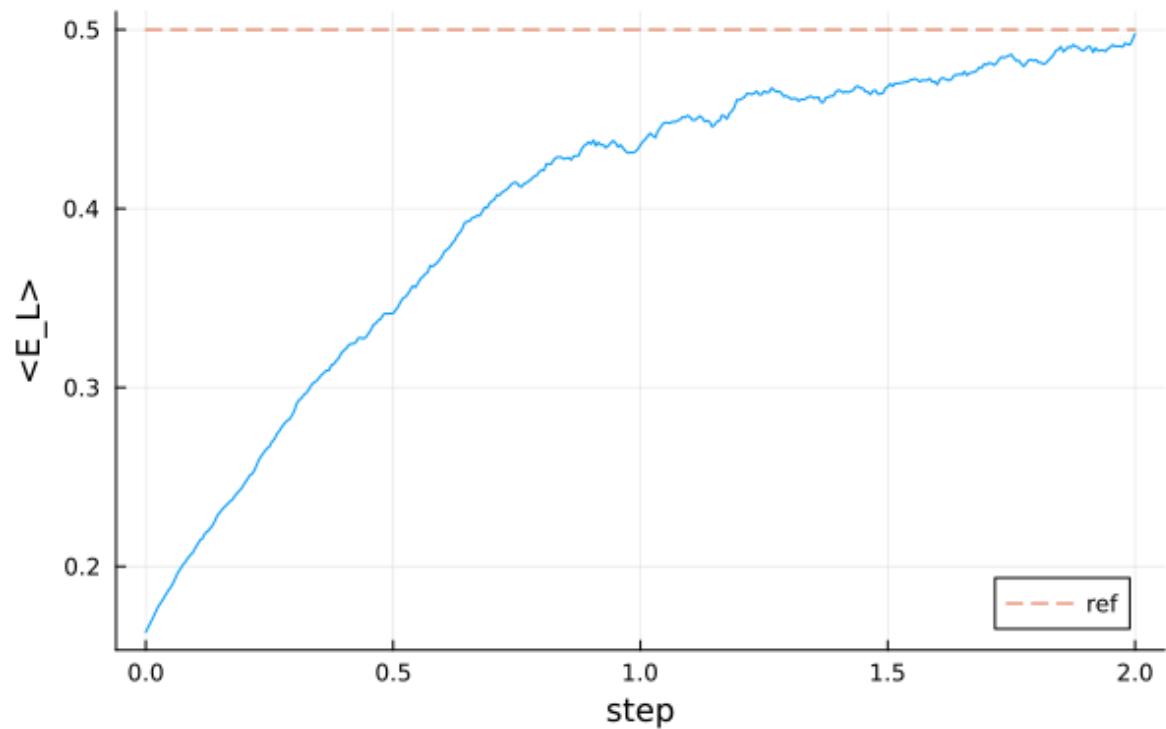
Reference energy



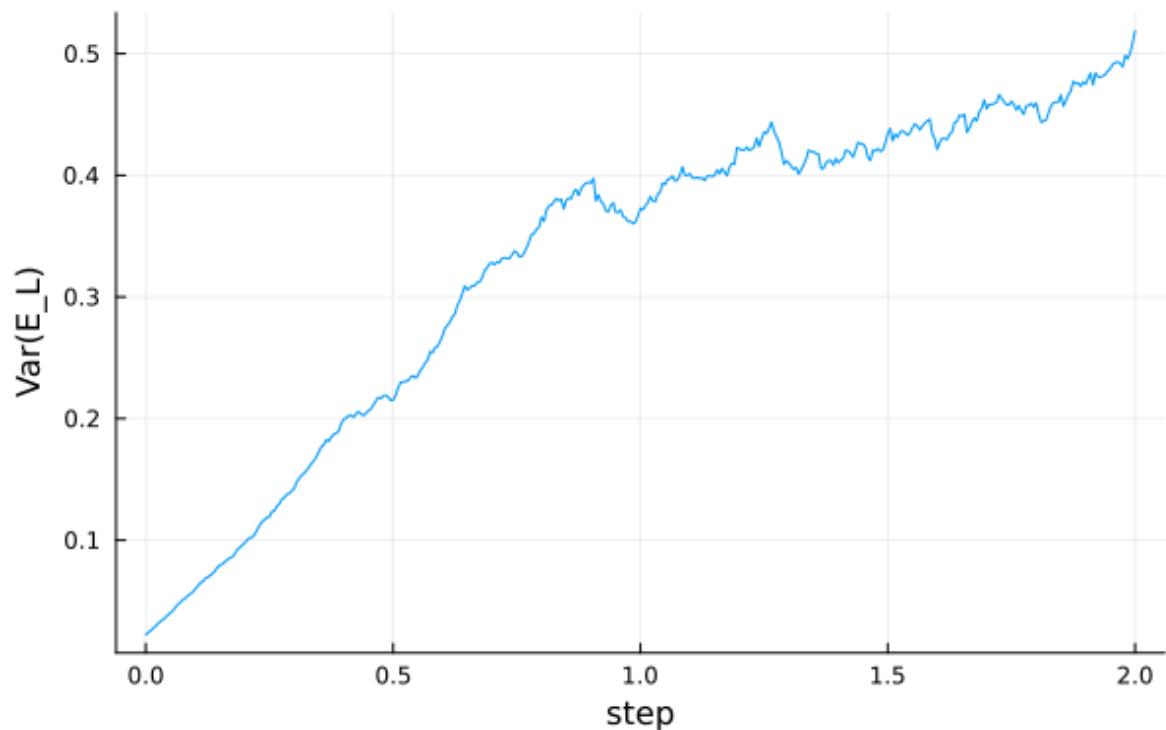
Walker population



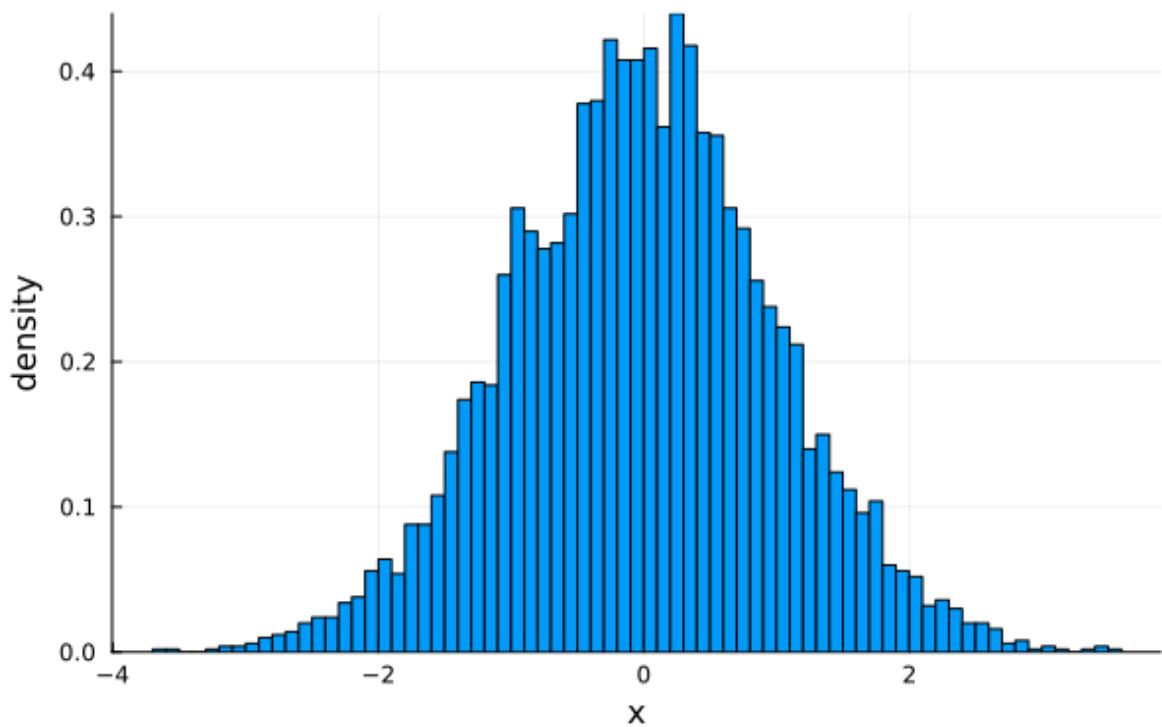
### Mean local energy



### Local energy variance



## Final walker density



H0 DMC energy (post-eq, nequil=50):  $E = 0.428 \pm 0.003$

Final step:  $E = 0.50$ ,  $\text{Var}(E_L) = 0.52$

Reference energy: 0.50