

```
In [16]: # 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, TrialWF, Walker, DMCPParams, DMCSim, Importance
```

System: 1D Harmonic Oscillator with Importance Sampling

Potential

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

Trial wavefunction (Gaussian)

$$\psi_T(x) = e^{-\alpha x^2/2}$$

This cell defines the Hamiltonian and trial wavefunction, initializes walkers, and runs importance-sampled DMC.

```
In [17]: # System: 1D harmonic oscillator with importance sampling
V(R) = 0.5 * R[1]^2
H = Hamiltonian(1, 0.5, V)

alpha = 1.0
logpsi(R) = -0.5 * alpha * R[1]^2
gradlogpsi(R) = [-alpha * R[1]]
lapllogpsi(R) = -alpha

trial = TrialWF(logpsi, gradlogpsi, lapllogpsi)
guiding = ImportanceGuiding(trial, H)

# 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; guiding=guiding)
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 [ ]: # 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 (IS) energy (post-eq, nequil=$nequil): E = $(Ebar_str) +/- $SEM")
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)")
println("Reference energy: $(format_sigfig(E_ref; sigfigs=2))")

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="Walker density")
        display(p2)

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

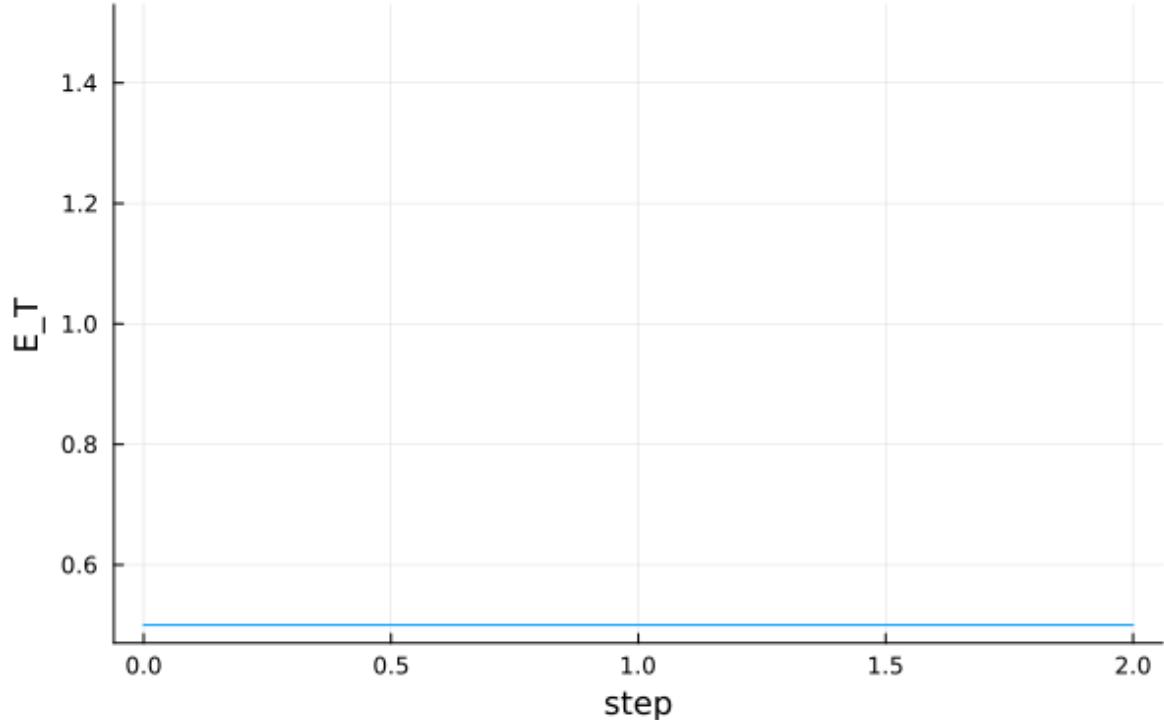
        p4 = plot(t, energy_variance_history, xlabel="step", ylabel="Var(E_L)", title="Local energy variance")
        display(p4)

        if !isempty(sim.walker_positions_history)

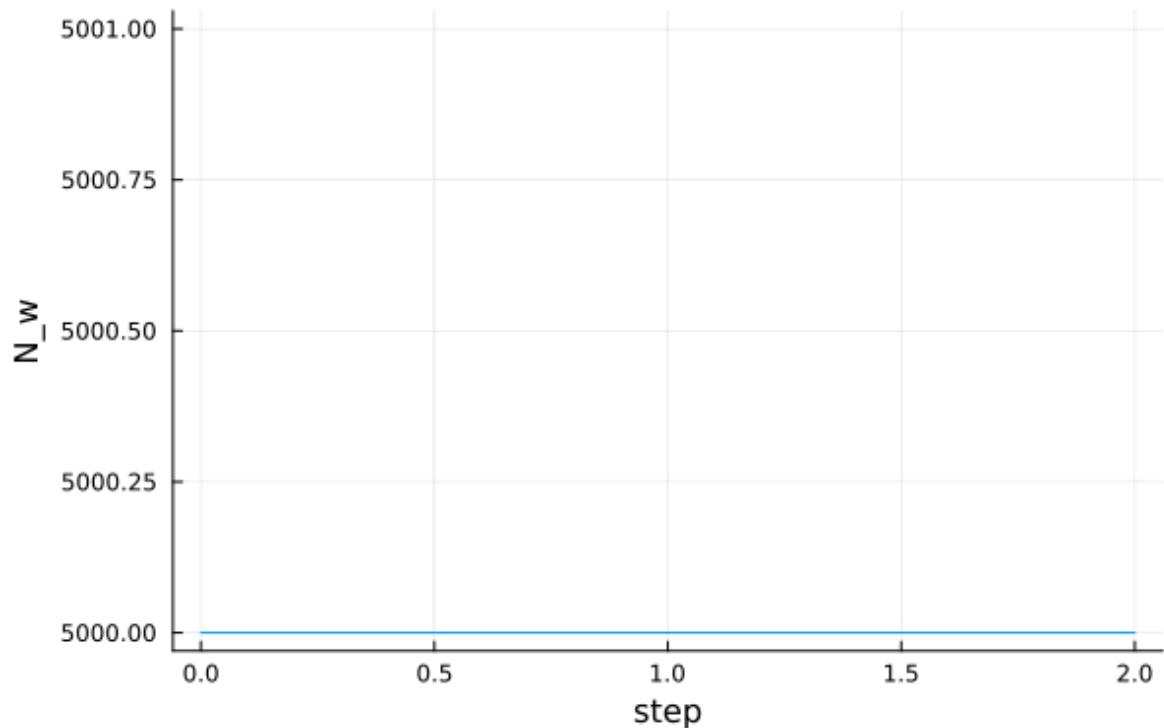
```

```
    snap = sim.walker_positions_history[end]
    p5 = plot_snapshot_1d_density(snap; nbins=120, title="Final walk
display(p5)
end
end
```

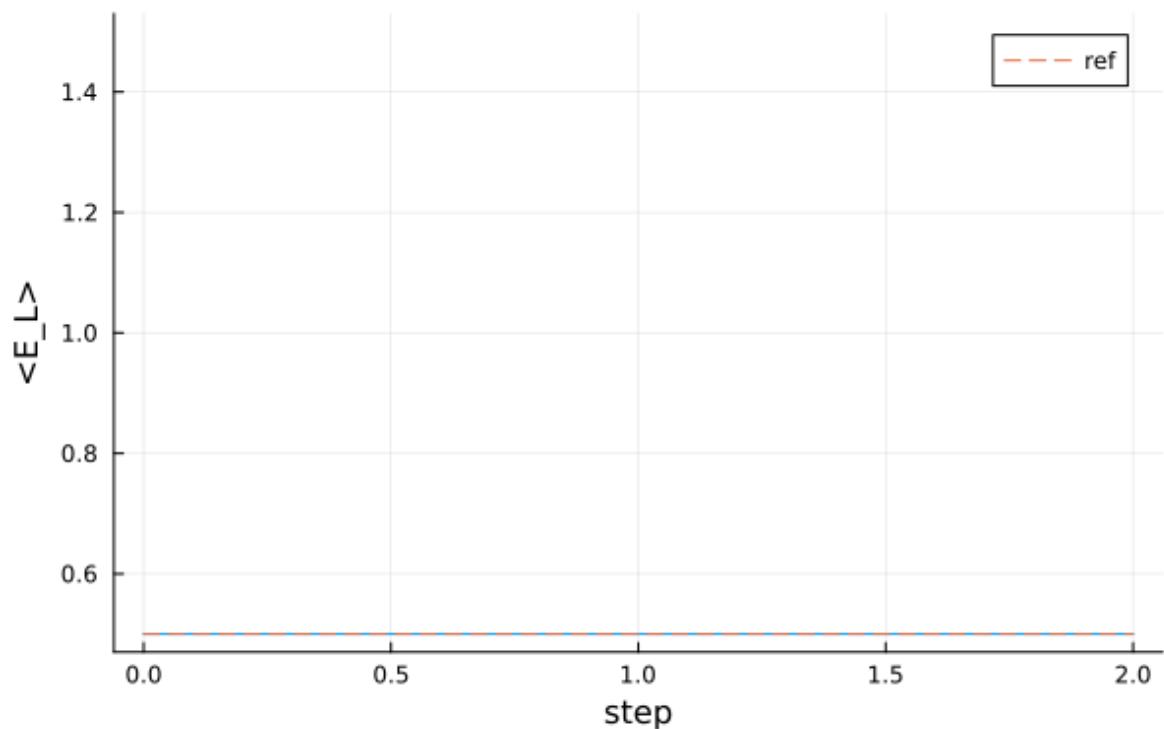
Reference energy



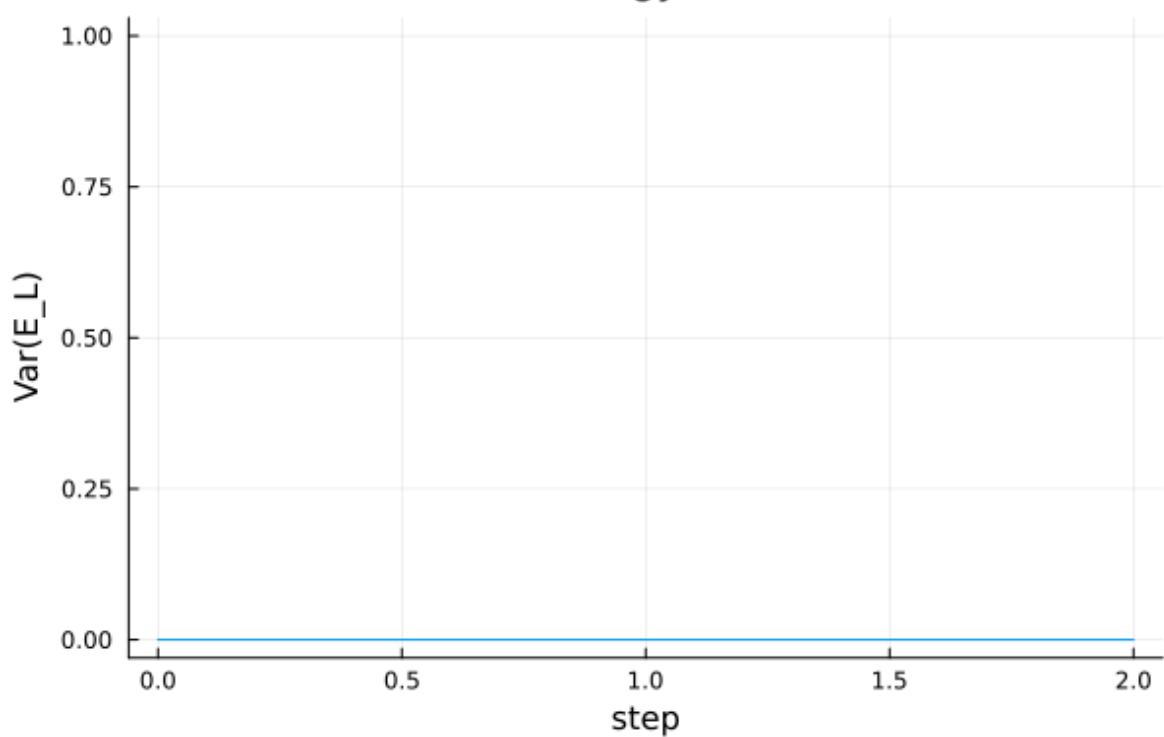
Walker population



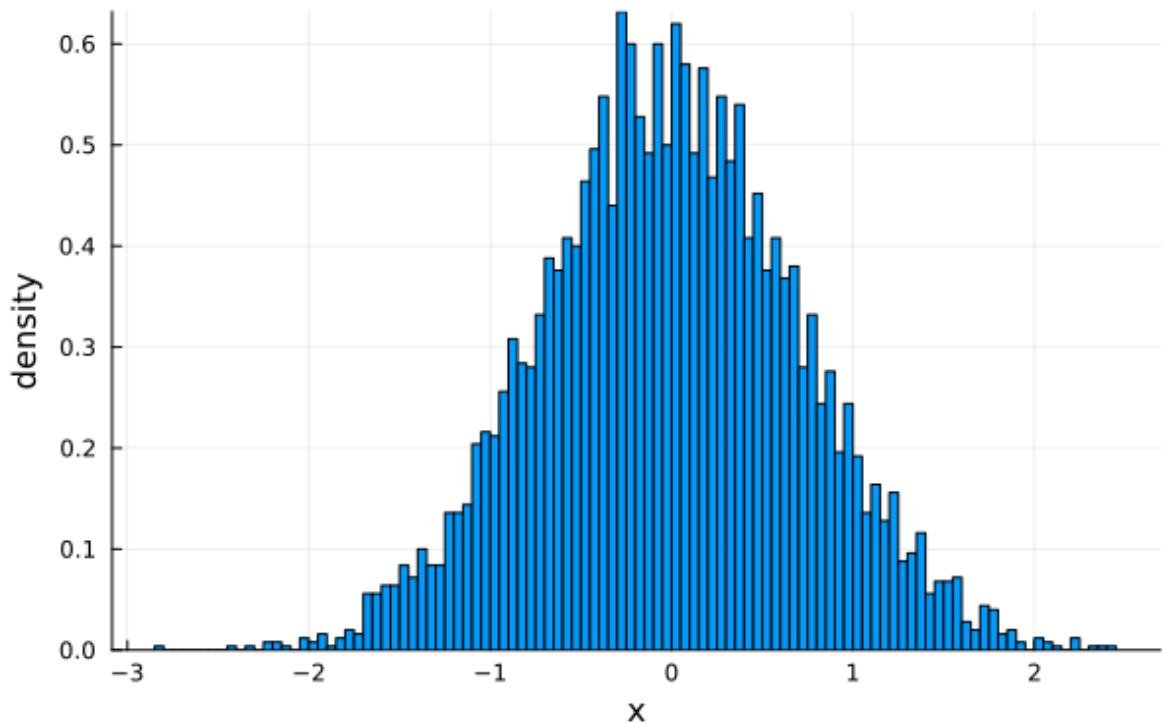
Mean local energy



Local energy variance



Final walker density



H0 DMC (IS) energy (post-eq, nequil=50): $E = 0.500000 \pm 0.000000$

Final step: $E = 0.50$, $\text{Var}(E_L) = 0.00$

Reference energy: 0.50000