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In [7]: # 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, DMCParams, DMCSim, Importance
```

System: Fixed-Node DMC for 1D Harmonic Oscillator (Odd Parity)

Potential

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

Trial wavefunction (odd parity)

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

The fixed node at $x = 0$ enforces odd parity. This cell defines the Hamiltonian and trial wavefunction, initializes walkers, and runs fixed-node DMC.

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In [8]: # System: fixed-node DMC for a single particle in a 1D HO (odd parity)
omega = 1.0
V(R) = 0.5 * omega^2 * R[1]^2
H = Hamiltonian(1, 0.5, V)

alpha = omega
logpsi(R) = begin
    x = R[1]
    ax = abs(x)
    return ax == 0 ? -Inf : log(ax) - 0.5 * alpha * x^2
end

gradlogpsi(R) = begin
    x = R[1]
    ax = abs(x)
    s = sign(x)
    return ax == 0 ? [0.0] : [(s / ax) - alpha * x]
end

lapllogpsi(R) = begin
    x = R[1]
    ax = abs(x)
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    return ax == 0 ? -Inf : -1.0 / ax^2 - alpha
end

signpsi(R; tol=1e-12) = abs(R[1]) < tol ? 0.0 : sign(R[1])

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

# Walkers and params
targetN = 1000
walkers = [Walker([randn()]) for _ in 1:targetN]

E_ref = 1.5 * omega
params = DMCParams(0.005, 400, 50, targetN, E_ref, 0.1, 10, 50)

# Run
rng_sim = MersenneTwister(7)
sim = DMCSim(H, params, walkers, rng_sim; guiding=guiding, nodepolicy=FixedNodePolicy())
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 odd-parity (first excited) energy

$$E_1 = \frac{3}{2}\omega$$

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.

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In [10]: # Results and plots
t = (0:params.nsteps) .* params.dt

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("Fixed-node H0 (odd parity) DMC energy (post-eq, nequil=$nequil): $Ebar")
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=5))")
```

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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 history")
        display(p2)

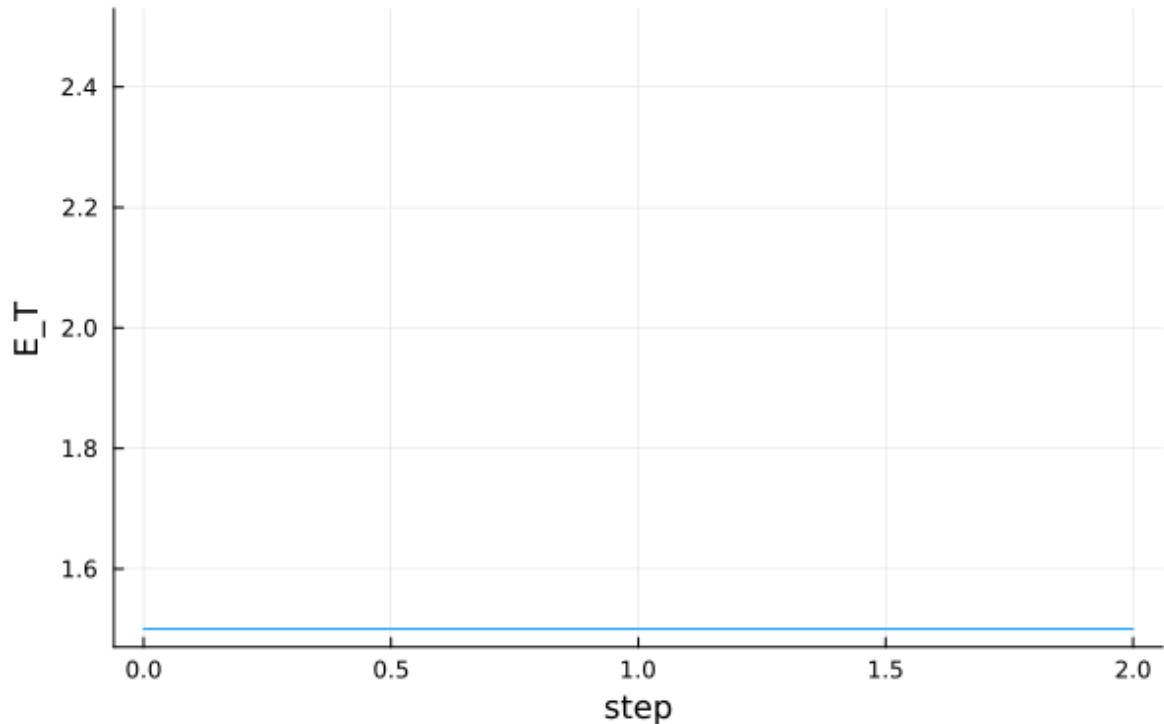
        p3 = plot(t, energy_mean_history, xlabel="step", ylabel="⟨E_L⟩", title="Mean energy history")
        plot!(p3, [t[1], t[end]], [E_ref, E_ref], ls=:dash, label="ref")
        display(p3)

        p4 = plot(t, energy_variance_history, xlabel="step", ylabel="Var(E_L)", title="Variance of energy history")
        display(p4)

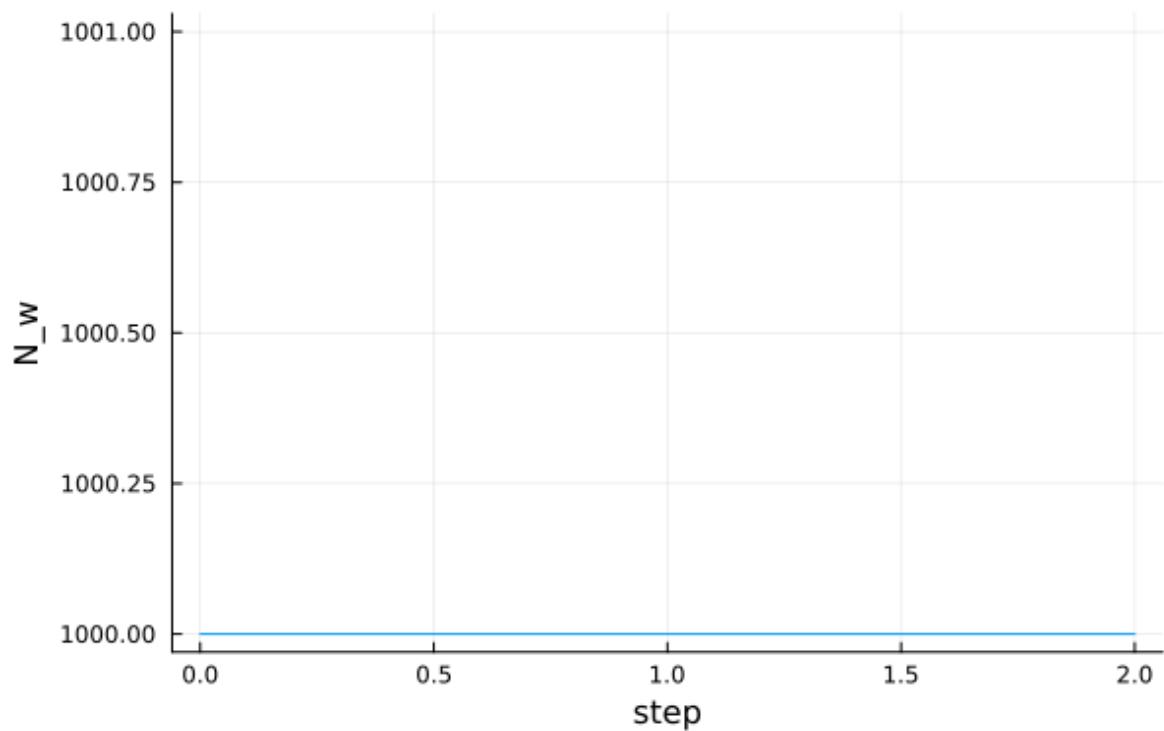
        if !isempty(sim.walker_positions_history)
            snap = sim.walker_positions_history[end]
            p5 = plot_snapshot_1d_density(snap; nbins=120, title="Final walker positions distribution")
            display(p5)
        end
    end
end

```

Reference energy



Walker population



Mean local energy

