```
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

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

Trial wavefunction (odd parity)

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

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

```
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)
```

```
        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=FixedN
    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.

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 HO (odd parity) DMC energy (post-eq, nequil=$(nequil)):
E_final_str, var_str = format_pair_sigfig(energy_mean_history[end], energy_v
println("Final step: E = $(E_final_str), Var(E_L) = $(var_str)")
println("Reference energy: $(format_sigfig(E_ref; sigfigs=5))")
```

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

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

        p3 = plot(t, energy_mean_history, xlabel="step", ylabel="<E_L>", tit
        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
        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
end
```
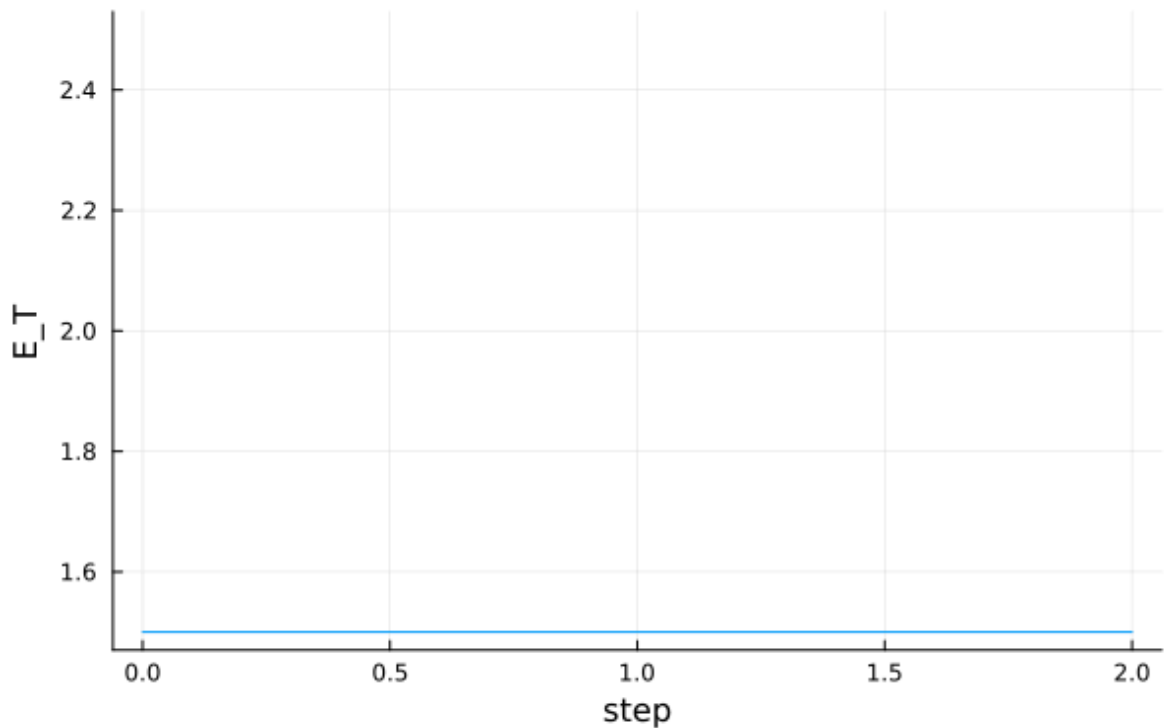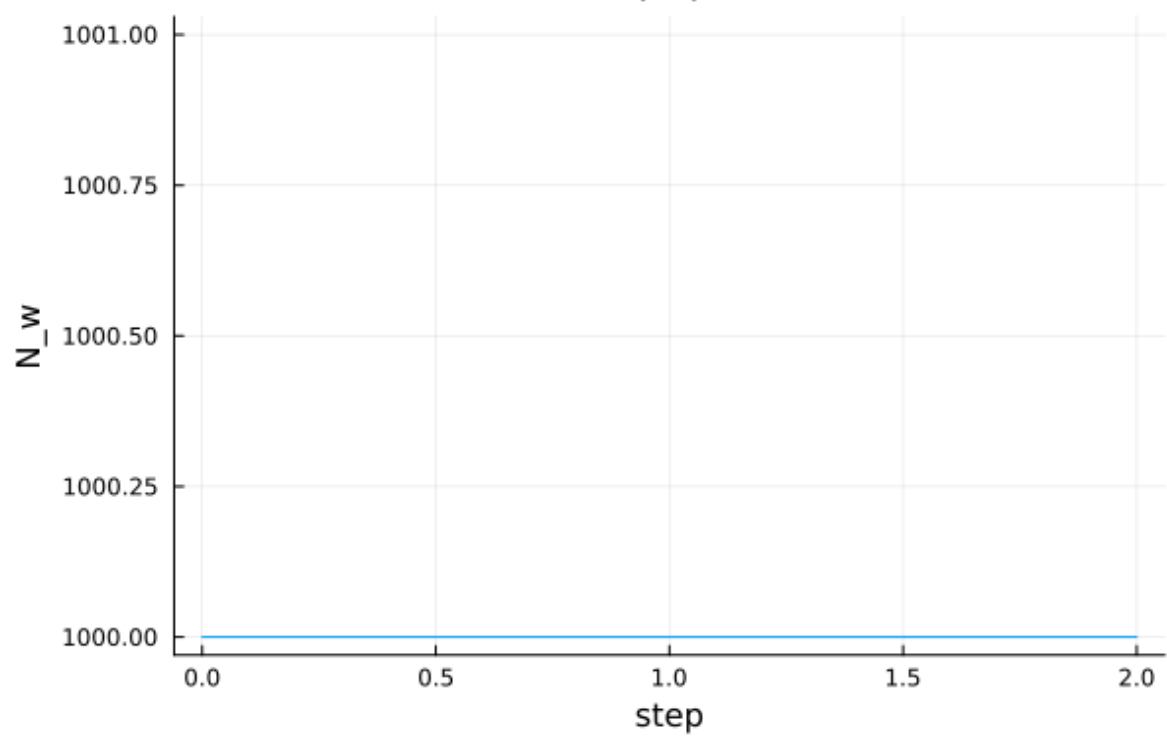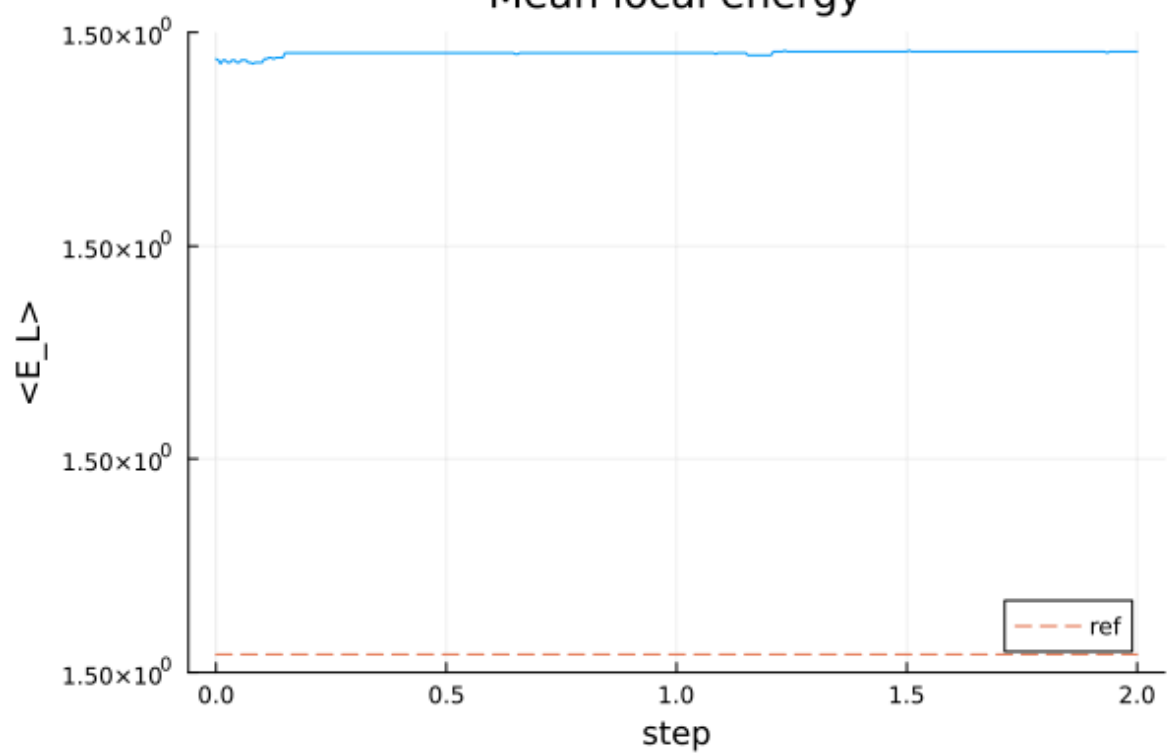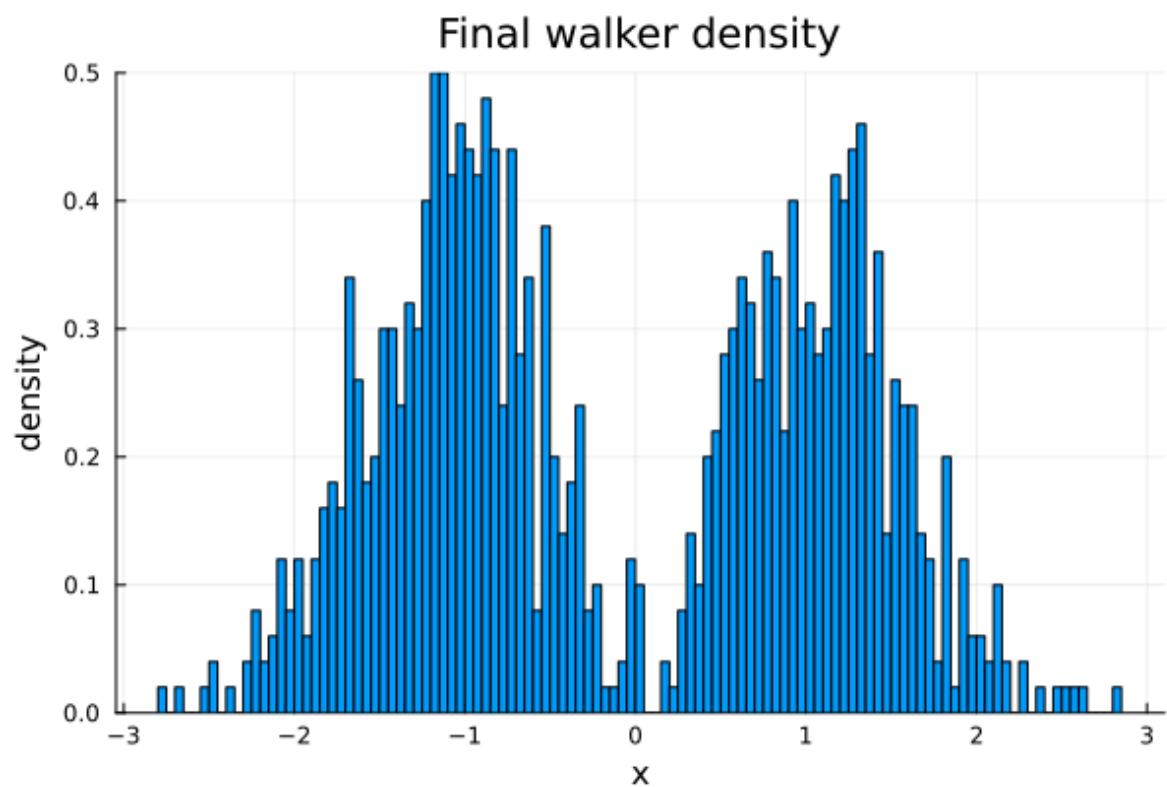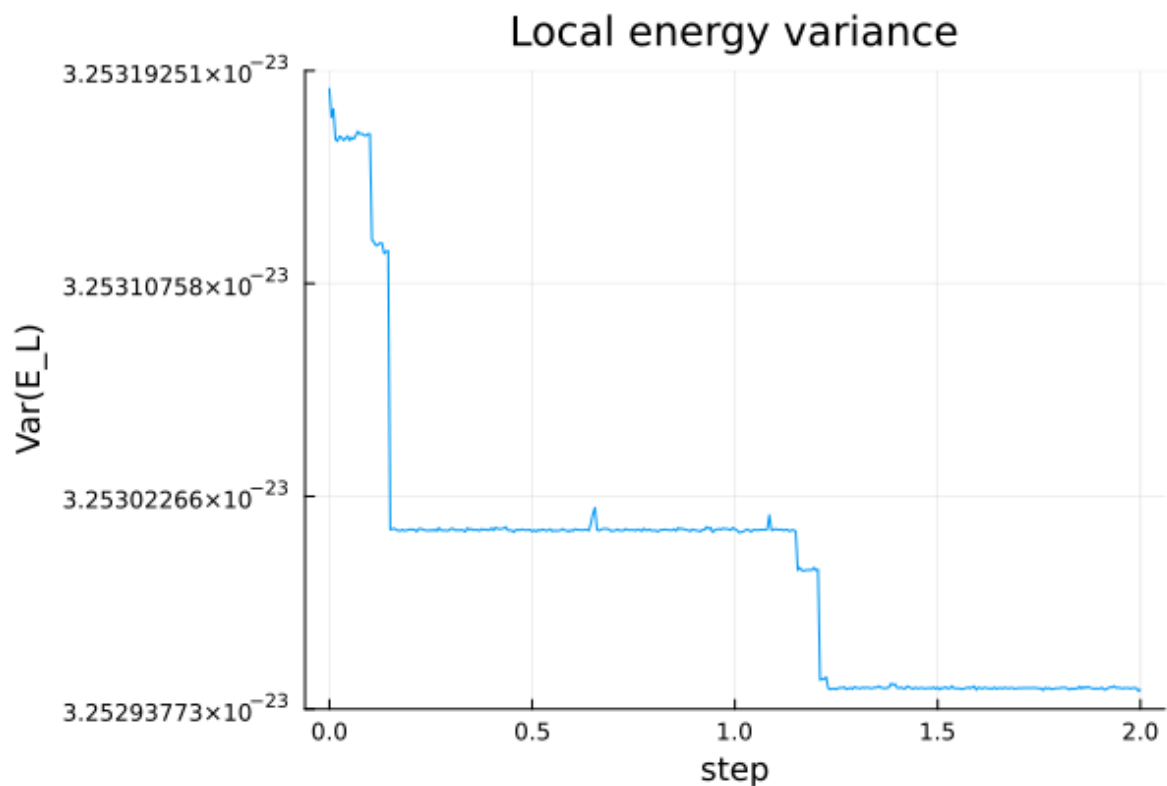

Reference energy

Walker population

Mean local energy

Local energy variance

Final walker density

Fixed-node HO (odd parity) DMC energy (post-eq, nequil=50): E = 1.5000000000
0011191 +/- 0.00000000000000008
Final step: E = 1.50000000000110800257858, Var(E_L) = 0.0000000000000000000
00033
Reference energy: 1.5000