

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

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

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In [ ]: # 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
```

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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 = DMCPParams(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.

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In [ ]: # 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

println(@sprintf("Fixed-node H0 (odd parity) DMC energy (post-eq, nequil=%d)
println(@sprintf("Final step: E = %.6f, Var(E_L) = %.6f", energy_mean_histor
println(@sprintf("Reference energy: %.6f", E_ref))

Logging.with_logger(Logging.NullLogger()) do
    redirect_stderr(devnull) do

```

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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

```