Homework 2

Yusheng Zhao

March 31, 2023

Contents

1 Problem 1

1.1 A

$F(x) = -\frac{\partial U(x)}{\partial x} = -(x-1)$, at $t=0$, $x=0$ so $F=1$.

1.2 B

According to the velocity Verlet algorithm, we know

$$\vec{x}(t+\delta t) = \vec{x}(t) + \delta t \vec{v}(t) + \frac{1}{2}\delta t^2 \vec{a}(t)$$

and

$$\vec{v}(t+\delta t) = \vec{v}(t) + \frac{1}{2}\delta t[\vec{a}(t) + \vec{a}(t+\delta t)]$$

with $x(0) = 0, v(0) = 0, a(0) = F(0)/m = 1$,

$$\vec{x}(\Delta t = 0.5) = 1/8$$

then, $a(\Delta t = 0.5) = -(1/8 - 1) = 7/8$

$$\vec{v}(\Delta t = 0.5) = 15/32$$

1.3 C

We know $E = \frac{1}{2}mv^2 + \frac{1}{2}(x-1)^2$, for $t = 0$, $E = 0.5$. For $t = 0.5$, $E = 225/2048 + 49/128 = 1009/2048 \approx 0.492675$

1.4 D

It was not conserved. This is because the time-step is not truly infinitesimal, the updated velocity position are not truly accurate. Therefore, there will be error in the energy calculated according to those values.

2 Problem 2

2.1 A

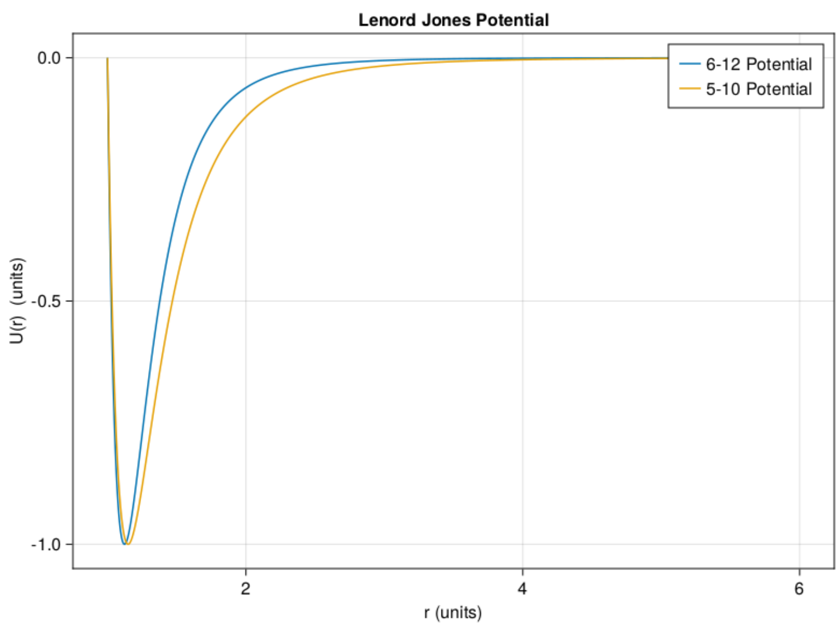
```
using CairoMakie
u612(x) = 4 * ((1/x^12) - (1/x^6))
u510(x) = 4 * ((1/x^10) - (1/x^5))
f = Figure()
ax = Axis(f[1, 1],
    title = "Lenord Jones Potential",
    xlabel = "r (units)",
    ylabel = "U(r)  (units)"
)
x = 1.0:0.001:6
u1 = u612.(x)
u2 = u510.(x)
lin612 = lines!(ax, x, u1,label="6-12 Potential")
lin510 = lines!(ax, x, u2,label="5-10 Potential")
axislegend()
save("p2.png",f)
```

2.2 B

According to the plot, the potential energy mainly dies out around $r = 2.5$. Therefore, I would assign $r_u = 2.5$ and $r_l = 0.9 * r_u = 2.25$. Then the cutoff function $S(r)$ will be introduced as

$$\begin{cases} S(r) = 1; r < r_l \\ S(r) = \frac{(r_u - r)^2 (r_u + 2r - 3r_l)}{(r_u - r_l)^3}; r_l < r < r_u \\ S(r) = 0; r > r_u \end{cases} \tag{1}$$

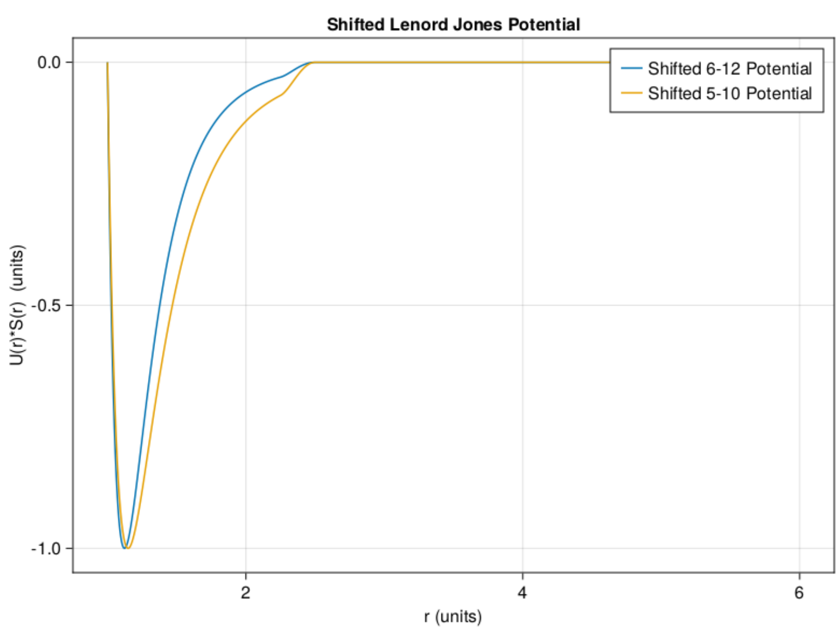
There was a typo in the slides.



2.3 C

```
using CairoMakie
function sr(r::T,rl::T,ru::T) where T
    if r < rl
        return one(r)
    elseif r > ru
        return zero(r)
    else
        return (ru-r)^2 * (ru + 2*r - 3*rl) / (ru-rl)^3
```

```
    end
end
u612(x) = 4 * ((1/x^12) - (1/x^6))
u510(x) = 4 * ((1/x^10) - (1/x^5))
f = Figure()
ax = Axis(f[1, 1],
    title = "Shifted Lenord Jones Potential",
    xlabel = "r (units)",
    ylabel = "U(r)*S(r)  (units)"
)
x = 1.0:0.001:6
ru = 2.5
u1 = u612.(x) .* sr.(x, 0.9*ru, ru)
u2 = u510.(x) .* sr.(x, 0.9*ru, ru)
lin612 = lines!(ax, x, u1,label="Shifted 6-12 Potential")
lin510 = lines!(ax, x, u2,label="Shifted 5-10 Potential")
axislegend()
save("p2_shifted.png",f)
```



There should not be any efficiency difference since both functions are turned off at the same position r. In terms of accuracy, I guess $5-10$ L-J potential will win.

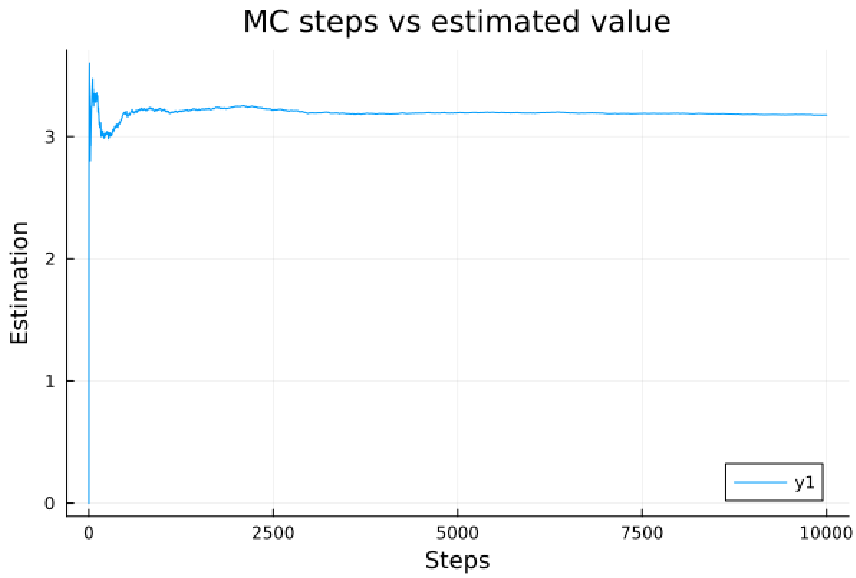
3 Problem 3

In partition function, the probability of a state is proportional to e^{KE/k_BT}. If you want the probability to stay the same, you need $KE_{inst}/(k_BT_{inst}) = KE_{target}/k_BT_{Target}$ therefore, $v_{inst}/v_{target} = \sqrt{\frac{T_{inst}}{T_{target}}}$

4 Problem 4

```
begin
    using Random, Distributions, Plots
    n_trials = 10000
    samples = rand(Uniform(-1,1),(2,n_trials))
    sums = zeros(Float64,n_trials+1)
    for ctr in 1:n_trials
        x,y = samples[:,ctr]
        if x^2 + y^2 <= 1
            sums[ctr+1] = sums[ctr] + 1.0
        else
            sums[ctr+1] = sums[ctr]
        end
    end
    #we are essentially estimating the area
    sums ./= 1:n_trials+1
    sums .*= 4
    plot(1:length(sums), sums,xlabel="Steps",ylabel="Estimation",title="MC steps vs est
    savefig("mc.png")
    println("Estimation of pi is: $(sums[end])")
end
```

I esimated π to be 3.12888711128887. Please see the plot below.


MC steps vs estimated value
Estimation
Steps
0
1
2
3
0
2500
5000
7500
10000
y1