Assignment 3

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Handin: Oct. 6th. 12am

I made two PDFs for this assignment:

1. (assignment3_WMC.pdf) A PDF including all of the functions desribed in the exercises along with all plots, markdown and printouts.

2. (assignment3.pdf) A PDF where most of the code is hidden including the functions mentioned in the assignment text. Printouts, markdown and figures as left as the only answer for the exercises.

Please note in the assignent comments which one is the best for you to correct.

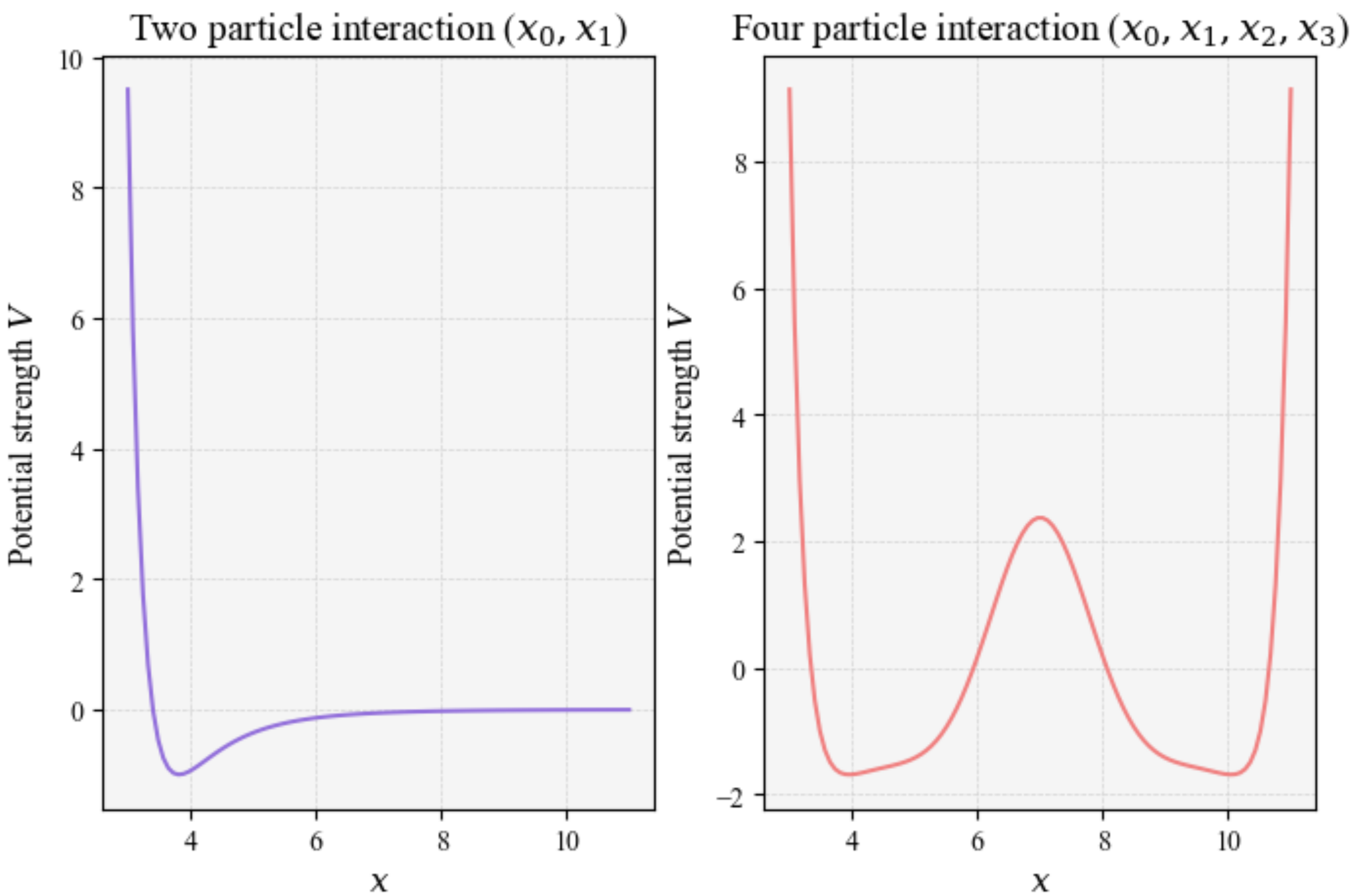
Questions for Week 4: Solving Nonlinear equations

(A1) + (A2) Potenials for N=2 and N=4 particals

In [28]:

```
def V_two(x):
    x0 = np.array([x, 0, 0])
    x1 = np.array([0, 0, 0])
    points = np.vstack((x0, x1))

    strength = LJhelp.V(points)
    return strength

def V_four(x):

    x0 = np.array([x, 0, 0])
    x1 = np.array([0, 0, 0])
    x2 = np.array([14, 0, 0])
```

```
    x3 = np.array([7, 3.2, 0])
    points = np.vstack((x0, x1, x2, x3))

    strength = LJhelp.V(points)
    return strength
```



The two plots shown above are plots of the LJ-potential for a two particle system and a four particle system. The only variable in the system is the x-position of particle x_0 hence the x-axis.

The convergence test described in the assignment is implicit in all the functions, and all printouts show the root obtained from the specific algortihm along with the number of function-calls it took to converge towards that solution.

(B) Bisection root function

In [4]:
```
def bisection_root(f, a, b, tol=1e-13):
    fa, fb = f(a), f(b)
    if fa * fb > 0:
        raise ValueError("f(a) and f(b) must have different signs")
    counter = 2
    while (b - a) > tol:
        c = (a + b) / 2
        fc = f(c)
        counter += 1
        if fc == 0:
            return c, counter
        if fa * fc > 0:
            a, fa = c, fc
        else:
            b, fb = c, fc
    return (a + b) / 2, counter

EPSILON=0.997; # kJ/mol
SIGMA=  3.401; # Ångstrom
a_bound, b_bound = [2, 6]
x, n_calls = bisection_root(V_two, a_bound, b_bound)
print(f"Root found at x={x:.3f}" + r" in the space x = [2, 6]" + f" with n={n_calls} function calls")
print("Is root of x similar to σ (3.401)?", np.isclose(x, SIGMA, atol=1e-2))
```

```
Root found at x=3.401 in the space x = [2, 6] with n=48 function calls
Is root of x similar to σ (3.401)? True
```

(C) Newton Rhapson solver

In [5]:
```
def newton_root(f, df, x0, tol=1e-12, max_iterations=100):
    x = x0
    func_calls = 0
    for _ in range(max_iterations):
        fx = f(x)
        dfx = df(x)
        x_new = x - fx / dfx
```

```
        func_calls += 2
        if np.linalg.norm(x_new - x) < tol:
            return x_new, func_calls
        x = x_new
    raise ValueError("Maximum iterations reached. No solution found.")

def func(x):
    return 4*EPSILON* ( (SIGMA / x) **12 - (SIGMA / x)**6)

def dfunc(x):
    return 4*EPSILON* ( 6 * (SIGMA**6) / (x**7) -12 * (SIGMA**12) / (x**13) )


x0 = 2
x, n_calls = newton_root(func, dfunc, x0)
print(f"Root found at x={x:.3f}" + r" starting from x0=2" + f" with n={n_calls} function calls")
print("Is root of x similar to σ (3.401)?", np.isclose(x, SIGMA, atol=1e-2))
```

```
Root found at x=3.401 starting from x0=2 with n=26 function calls
Is root of x similar to σ (3.401)? True
```

(D) NR solver and bisection root function combination

In [6]:

```
def NR_bi_comb(a, b, x0, f, df, tol=1e-13, max_iterations=1000, dev_tol=1e-2):
    func_calls = 0
    x = x0
    fa, fb = f(a), f(b)
    func_calls += 2
    if fa * fb > 0:
        raise ValueError("f(a) and f(b) must have different signs")
    for _ in range(max_iterations):
        fx, dfx = f(x), df(x)
        func_calls += 2
        if abs(dfx) > dev_tol:
            x_new = x - fx / dfx
        else:
            x_new = (a + b) / 2
        if not (a < x_new < b):
            x_new = (a + b) / 2
        if abs(x_new - x) < tol:
            return x_new, func_calls
```

```
        fx_new = f(x_new)
        func_calls += 1
        if fa * fx_new < 0:
            b, fb = x_new, fx_new
        else:
            a, fa = x_new, fx_new
        x = x_new
    raise ValueError("Maximum iterations reached. No solution found.")

a_bound, b_bound = [2, 6]
x0 = 2
x_NR, n_calls_NR = NR_bi_comb(a_bound, b_bound, x0, func, dfunc)


print(f"Root found at x={x_NR:.3f}" + f" with n={n_calls_NR} function calls")
print("Is root of x similar to σ (3.401)?", np.isclose(x_NR, SIGMA, atol=1e-2))
```

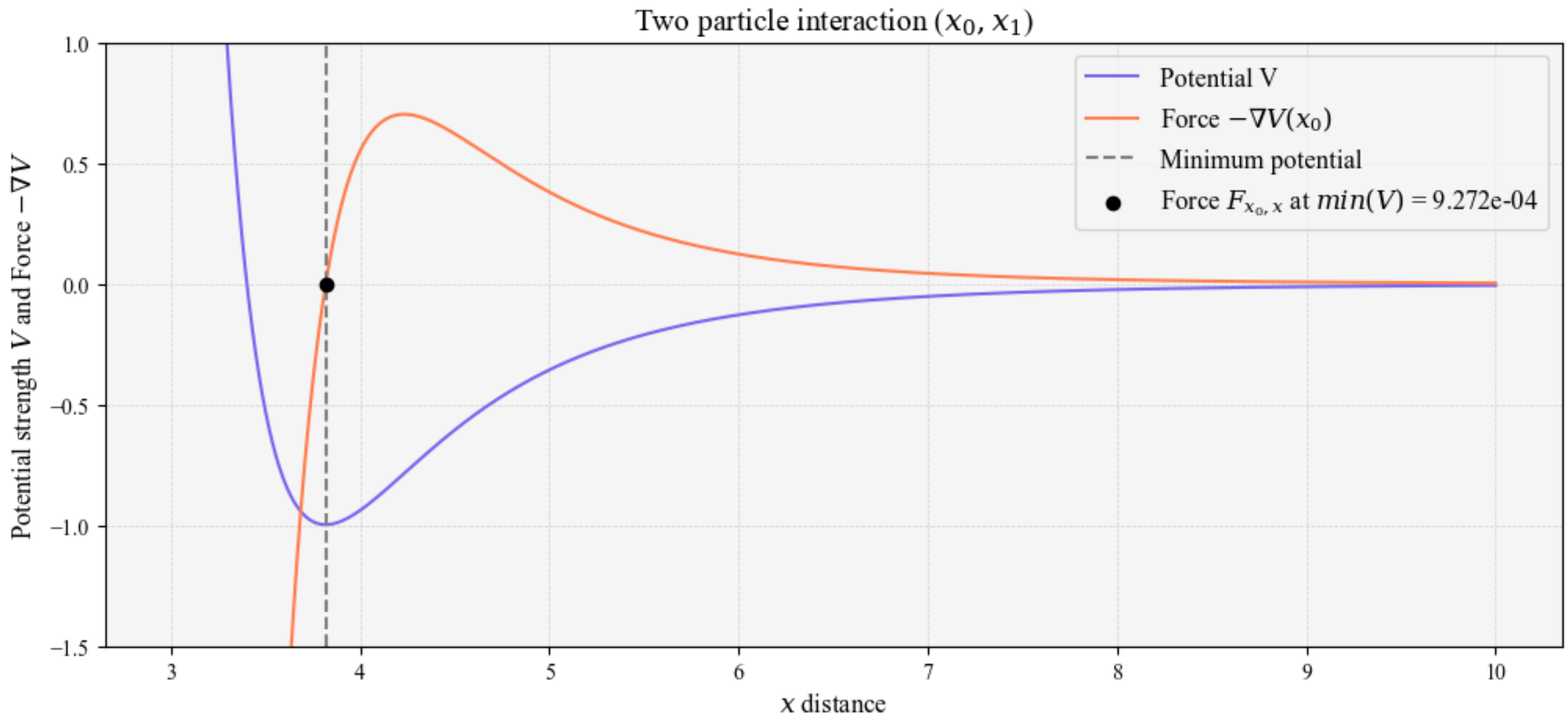
```
Root found at x=3.401 with n=40 function calls
Is root of x similar to σ (3.401)? True
```

(E)

```
Force working on particle x0 at x = 3.0: [-54.9536532   0.           0.        ]
Force working on particle x1 at x = 3.0: [54.9536532  0.          0.        ]
```

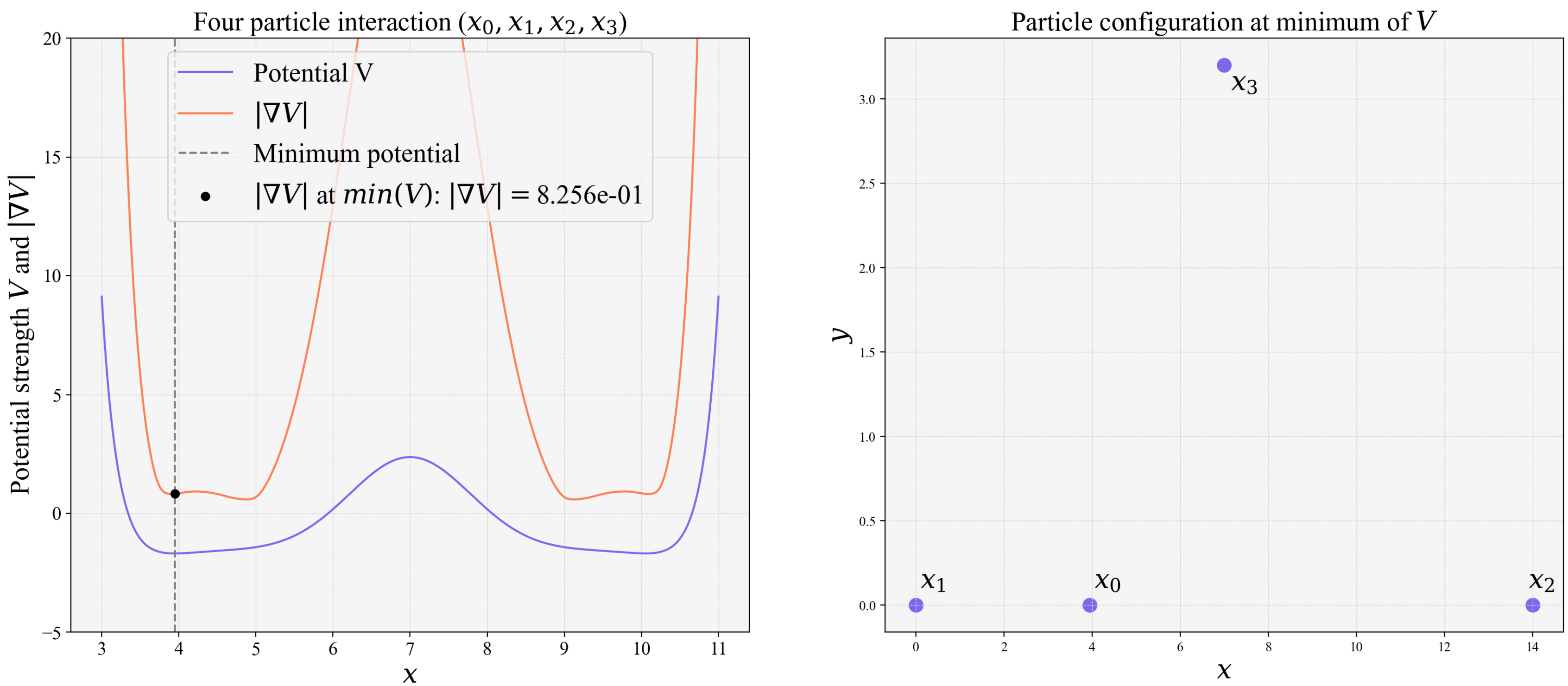
The negative gradient of the potential is the force acting on the system, and the direction of the force. So each element of the gradient tells us the force working on each particle in x, y and z. As we are working with two particles laying in the x plane the only force component between them is in the x direction. According to newtons third law, an object x_0 acting with a force on x_1 experience an equal and opposite force on itself. This is why the two quantities are equal and opposite and only have components in the x direction.

```
Out[8]: (-1.5, 1.0)
```



At the minimum of the potential, the force on the two particles is exactly zero, so the particles are in an a rest position (equilibrium).

```
Force working on particle x0 at x = 3.950: [-55.21445712  -0.20712564   0.        ]
Force working on particle x1 at x = 3.950: [ 5.49325687e+01 -9.47811027e-03  0.00000000e+00]
Force working on particle x2 at x = 3.950: [ 0.02298137 -0.00947811  0.        ]
Force working on particle x3 at x = 3.950: [0.25890705 0.22608186 0.        ]
```



In the four particle system, the magnitude of the force is never zero (yellow line in the plot). If the force is split up into x and y components (the force in z is 0), the force in one direction might be zero for a certain x, but is is never zero in both directions at the same time. I believe this is due to the assymetry of the system shown i the second plot above.

(F)

In [ ]:

```
def linesearch(F, X0, d, alpha_max, tolerance=1e-8):
    # Define the 1D function phi(α) = d · F(X0 + α d)
    def phi(alpha):
        return np.sum(d * F(X0 + alpha * d))

    # Using bisection to find root of phi in [0, alpha_max]
    a, b = 0.0, alpha_max
    fa, fb = phi(a), phi(b)
    ncalls = 2
```

```
    if fa * fb > 0:
        raise ValueError("No sign change: try larger alpha_max or different direction")

    alpha, extra_calls = bisection_root(phi, a, b, tol=tolerance)
    ncalls += extra_calls

    return alpha, ncalls

X0 = np.array([[4, 0, 0], [0, 0, 0 ], [14, 0, 0], [7, 3.2, 0]])
d = -dV_four(4)
alpha_max = 1.0

alpha, n_calls = linesearch(LJhelp.gradV, X0, d, alpha_max)
print(f"Optimal step length α: {alpha:.3f} with n={n_calls} function calls")
print(f"Gradient at (X0 + α * d) in direction d: {np.dot(LJhelp.gradV(X0 + alpha * d).ravel(), d.ravel())}'
```

```
Optimal step length alpha: 0.452 with n=31 function calls
Gradient at (X0 + alpha * d) in direction d: 1.1624196055081193e-08
```

Questions for week 5: Nonlinear Optimization

(G) Golden section minimum

In [ ]:
```
def golden_section_min(f, a, b, tol=1e-7):
    tau = (np.sqrt(5) - 1) / 2
    x1 = a + (1 - tau) * (b - a)
    x2 = a + tau * (b - a)
    f1 = f(x1)
    f2 = f(x2)
    n_calls = 2

    while np.abs(b - a) > tol:
        if f1 > f2:
            a = x1
            x1, f1 = x2, f2
            x2 = a + tau * (b - a)
            f2 = f(x2)
```

```
        else:
            b = x2
            x2, f2 = x1, f1
            x1 = a + (1 - tau) * (b - a)
            f1 = f(x1)
        n_calls += 1

    if f1 < f2:
        return x1, n_calls
    else:
        return x2, n_calls

def line_V(f, X0, d):
    def phi(alpha):
        return f(X0 + alpha * d)
    return phi

a, b = 0, 1
X0 = np.array([[4, 0, 0], [0, 0, 0 ], [14, 0, 0], [7, 3.2, 0]])
x_opt, n_calls = golden_section_min(line_V(LJhelp.V, X0, d), a, b)
```

```
Optimal x: 0.452 with n=36 function calls
Is x similar to alpha from linesearch (0.452)? True
```

Below the optimal distance r_0 is found for the two particle portential using the Golden-Section-minimizer

```
r0 for two particle system: 3.817 with n=39 function calls
```

(H) BFGS minimizer

In [ ]:

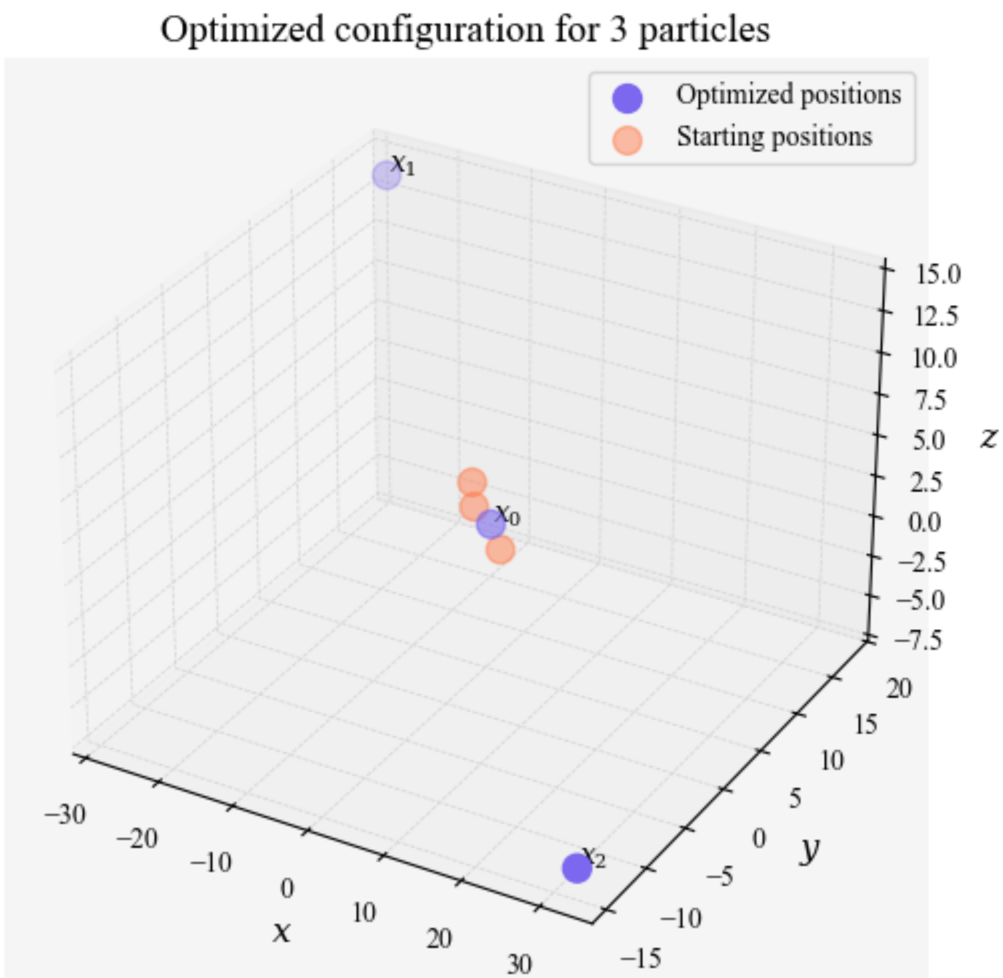
```
def BFGS(f, grad, X, tolerance=1e-6, max_iterations=10000, verbose=False):
    converged = False
    X = X.copy()
    B = np.eye(len(X))  # Initial inverse Hessian approximation
    n_calls = 0
    g = grad(X)

    for i in range(max_iterations):

        n_calls += 1
```

```
        if np.linalg.norm(g) < tolerance:
            converged = True
            if verbose:
                print(f"Converged after {i} iterations and {n_calls} function calls.")
            break

        s = np.linalg.solve(B, -g)
        x_new = X + s
        g_new = grad(x_new)
        n_calls += 1

        y = g_new - g

        ys = np.dot(y, s)
        Bs = B @ s
        sBs = np.dot(s, Bs)


        B = B + np.outer(y, y) / ys - np.outer(Bs, Bs) / sBs
        X, g = x_new, g_new

        if i == max_iterations - 1 and verbose:
                print(f"Reached maximum iterations ({max_iterations}) with {n_calls} function calls.")

    return X, n_calls, converged
```

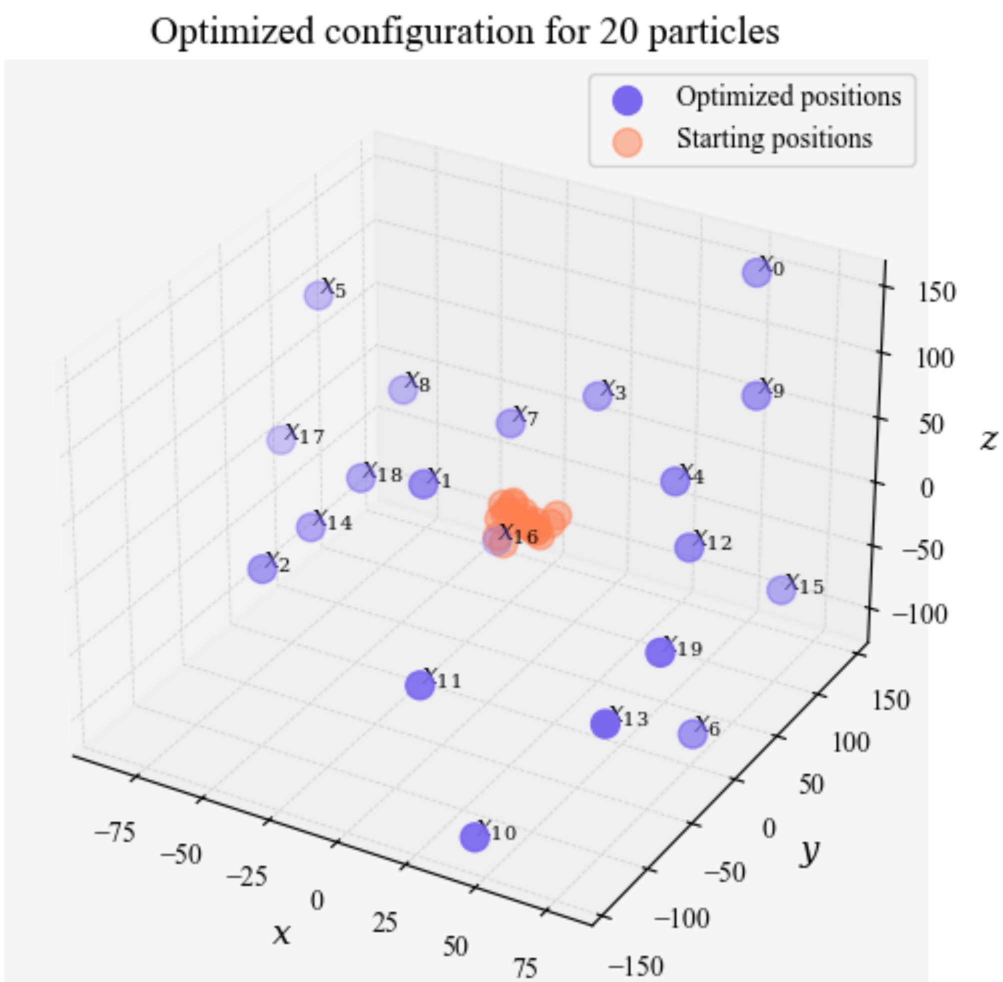
```
Converged after 6 iterations and 13 function calls.

Optimized configuration:
[[3.68186699 3.93837516 1.48584684]
 [3.00028518 0.30055214 0.55046137]]
for N=2 particles

Inter-particle distances:
[[0.         3.81749343]
 [3.81749343 0.        ]]

The inter-particle distance is equivalent to the result from (g): True
```

(I) BFGS minimizer for different N

Figure



Figure




```
Highest N with convergence: 20
BFGS optimization results:
```

N	Function calls	Total # of bonds	Bonds within 1% of r0	Converged
2	13	1	1	True
3	33	3	0	True
4	39	6	0	True
5	101	10	0	True
6	59	15	0	True
7	87	21	0	True
8	51	28	0	True
9	7	36	0	True
20	61	190	0	True

From the table and the plots, it is evident, that even though all configurations converged, all of them (except for $N = 2$) failed to have any Van der Waals bonds or even form the disired lattice structure.

(G) Line-search BFGS algorithm

In [21]:

```
def linesearch_wrapper(f, X, s, alpha_max=1.0, tol=1e-7):
    def phi(alpha):
        return f(X + alpha * s)
    alpha, n_calls = golden_section_min(phi, 0, alpha_max, tol=tol)
    return alpha, n_calls


def BFGS_linesearch(f, gradf, X, tolerance=1e-6, max_iterations=10000, verbose=False):
    converged = False
    X = X.copy()
    B = np.eye(len(X))  # Initial inverse Hessian approximation
    n_calls = 0
    g = gradf(X)

    for i in range(max_iterations):
```

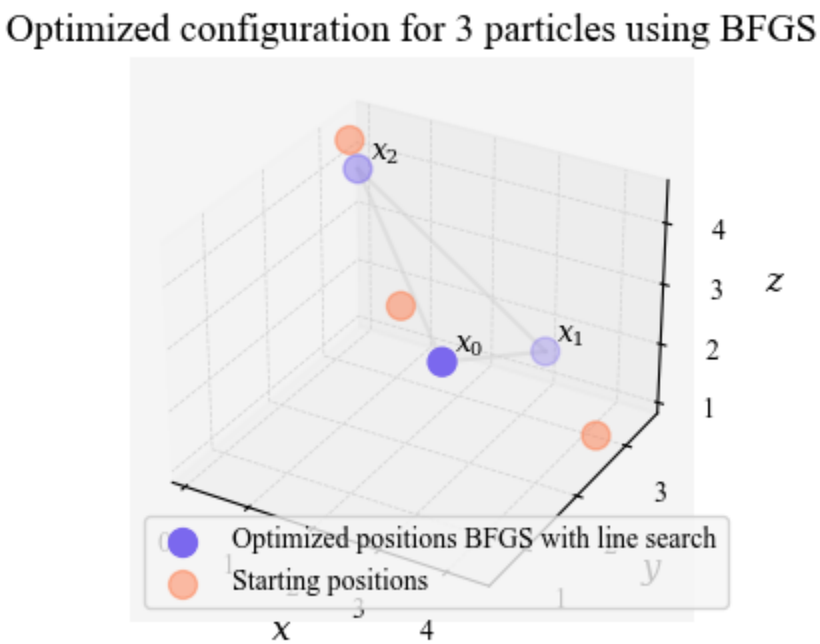
```
        n_calls += 1

        if np.linalg.norm(g) < tolerance:
            converged = True
            if verbose:
                print(f"Converged after {i} iterations and {n_calls} function calls.")
            break

        s = np.linalg.solve(B, -g)

        # Line search to find optimal step length alpha
        alpha, ls_calls = linesearch_wrapper(f, X, s)
        n_calls += ls_calls

        s = alpha * s.copy()
        x_new = X + s
        g_new = gradf(x_new.copy())
        n_calls += 1

        y = g_new - g

        ys = np.dot(y, s)
        Bs = B @ s
        sBs = np.dot(s, Bs)
        if ys > 1e-12:  # Ensure non-zero division
            B = B + np.outer(y, y) / ys - np.outer(Bs, Bs) / sBs

        X, g = x_new, g_new

        if i == max_iterations - 1 and verbose:
                print(f"Reached maximum iterations ({max_iterations}) with {n_calls} function calls.")

    return X, n_calls, converged
```

```
Highest N with convergence: 20
Summary of line-search BFGS results:
```

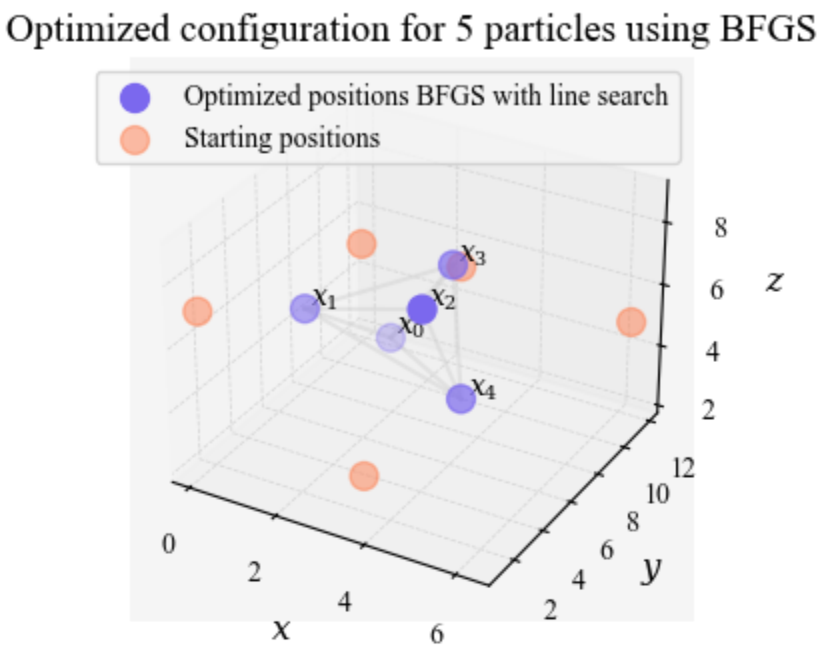
N	Function calls	Total # Bonds	Bonds within 1% of r0	converged
2	39	1	1	True
3	647	3	3	True
4	761	6	6	True
5	24321	10	9	True
6	8741	15	12	True
7	6613	21	15	True
8	5169	28	18	True
9	2965	36	19	True
20	66957	190	23	True

As seen from the table, many more Van der Waals bonds are achieved between the particles. This is also visible in the plots below, where most configurations form nice lattice-like structures. This came at the cost of a lot more function calls, but the algorithms are generally fast to run.

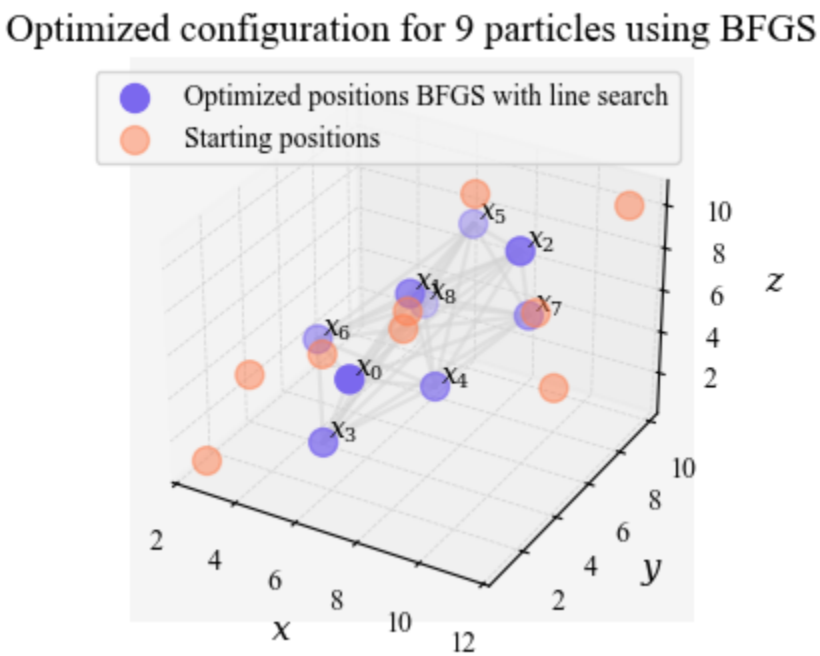
Figure


Optimized configuration for 3 particles using BFGS
x_2
x_0
x_1
4
3
2
1
z
3
y
x
4
Optimized positions BFGS with line search
Starting positions

Figure


Optimized configuration for 5 particles using BFGS
Optimized positions BFGS with line search
Starting positions
x
y
z
0
2
4
6
2
4
6
8
10
12
2
4
6
8
x0
x1
x2
x3
x4

Figure



Optimized configuration for 9 particles using BFGS
Optimized positions BFGS with line search
Starting positions
x
y
z

The plots above show the optimized particle positions from the BFGS algorithm with implemented line searching. For the three chosen $N \in [3, 5, 9]$ the particles behave as expected forming a lattice in 3D where most of the bonds are within 1% of r_0. For the $N = 20$ configuration, all except one particle behaves well - one is placed very far from all other particles.