**Question** **Fall 2023**

# Transition Path Extraction

You are provided with a file called PES.txt consisting of 40 × 40 density grid data. In each grid, there is a corresponding energy value. The file look like Fig. 0.1 if you execute the following python script.

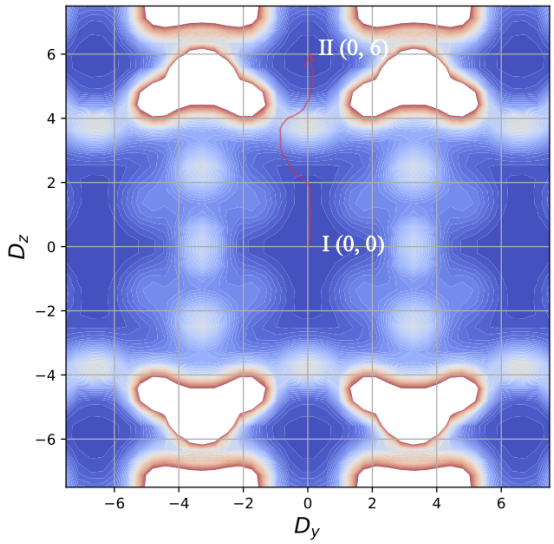


Figure 0.1: An 40 × 40 potential energy surface.

```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import cm

cut = 25*8
fig = plt.figure(figsize=(6, 6))
levels = np.linspace(0, cut, 50)

data = np.loadtxt('PES.txt')
x, y, z = data[:, 0], data[:, 1], data[:, 2]
N = int(np.sqrt(len(data)))
x = x.reshape(N, N); y = y.reshape(N, N); z = z.reshape(N, N)
z -= z.min(); print(x.max(), y.max(), z.max())
plt.contourf(x, y, z, levels=levels, cmap=cm.coolwarm)
plt.xlabel('$D_y$', fontsize=15)
plt.ylabel('$D_z$', fontsize=15)
plt.grid()

plt.savefig('PES-example.pdf')
```

In Fig. 0.1, I also highlighted two energy minima at I (0, 0) and II (0, 6.5). Now your job is to find the minimum cost transition path (represented by 20 consecutive grid points) to connect I and II from the given data. The expected output should look like the following

```
Minimum Path from I to II
coordinate [0, 0] with the energy of **
...
...
coordinate [0, 6] with the energy of ***
```

You should produce another plot which show the path (similar to the red arrow in Fig. 0.1) on the PES as well.

## 0.1 How to submit your solution?

You are strongly recommended to create a jupyter notebook and then share it via Google Colab. An example can be found at `https://colab.research.google.com/drive/1yAQ1pbTYWDjIpnncQXI92HC7LOlqo_-p?usp=sharing`