Mark Wei Dawids

s225098

Assignment F

Part 1

1.)

From the assignment, for T4-DNA:

Contour length: $L = 71.8\ \mu m$

Persistence length: $P \approx 64\ nm$

Effective width: $\omega_{eff} = 9\ nm$

$$R_F \approx \left(\omega_{eff} P\right)^{\frac{1}{5}} L^{\frac{3}{5}} = (9 * 10^{-9} * 64 * 10^{-9})^{\frac{1}{5}} * (71.8 * 10^{-6})^{\frac{3}{5}} = 2.92 * 10^{-6}\ m$$
$$= 2.92\ \mu m$$

$$R_G = \sqrt{\frac{< R_F >^2}{6}} = \sqrt{\frac{(2.92 * 10^{-6})^2}{6}} = 1.21 * 10^{-3}\ m = 1.21\ mm$$

2.)

We are given that microchannel has dimensions of $1\ \mu m$ high and $50\ \mu m$ wide.

From this we know that $D = 1\ \mu m$, as it is the smallest dimension of the microchannel, and hence is the dimension that causes the "squeezing" / confinement of the DNA.

Therefore, we know that this microchannel is in the de Gennes regime as: $R_G > D > P$.

From equation 3.3 in the lecture notes, we know that the confinement free energy in the de Gennes regime is: $F_{con} \approx k_B T \frac{(\omega_{eff} P)^{\frac{1}{3}}}{D^{\frac{5}{3}}} L$

$$F_{micro} = k_B T \frac{(9 * 10^{-9} * 64 * 10^{-9})^{\frac{1}{3}}}{(1 * 10^{-6})^{\frac{5}{3}}} * 71.8 * 10^{-6} = 5.97\ k_B T$$

Considering that this process of confinement of the T4-DNA molecule essentially increases the free energy by $5.97\ k_B T$ from the reference energy of zero, this process is energetically unfavourable. Therefore, the DNA molecules would not spontaneously enter the microchannel.

3.)

We are given that the nano-slits have dimensions of $h = 100\ nm$ high and $50\ \mu m$ wide.

Using equation 2: $\frac{F_{slit}}{k_B T} = A_S L$, where $A_S = \frac{(\omega_{eff} P)^{\frac{1}{3}}}{D^{\frac{5}{3}}}$

We set $D = 100\ nm$, as it is the smallest dimension:

$$F_{slit} = k_B T \frac{(9 * 10^{-9} * 64 * 10^{-9})^{\frac{1}{3}}}{(100 * 10^{-9})^{\frac{5}{3}}} * 71.8 * 10^{-6} = 277\ k_B T$$

$$\Delta F = F_{slit} - F_{micro} = 277 - 5.97 = 271\ k_B T$$

4.)

Considering that there is such a large difference between free energies between the nano-slit and microchannel, where $F_{slit} \gg F_{micro}$, a DNA molecule left in the slit would spontaneously migrate to the microchannel, as it is energetically favourable.

Part 2

5.)

The dimensions of the nanopit are given as: $d = 100\ nm$ deep and with $a = 300\ nm$ square wide holes.

From the paper, Equation 4 states that the confinement free energy of contour L is equal to: $\frac{F_p}{k_B T} = A_p L + B L^2$

Where Equation 5 states: $A_p \sim P\left(\frac{1}{(h+d)^2} + \frac{2}{a^2}\right) = 64 * 10^{-9} * \left(\frac{1}{(200*10^{-9})^2} + \frac{2}{(300*10^{-9})^2}\right) = 3.02 * 10^6\ m^{-1}$

And Equation 6 states: $B \sim \frac{w}{V_{pit}} = \frac{w_{eff}}{(h+d)a^2} = \frac{9*10^{-9}}{(200*10^{-9})(300*10^{-9})^2} = 5 * 10^{11}\ m^{-2}$

The paper states that the term B arises from the excluded-volume interactions experienced by the DNA in the pit. In other words, this term accounts for the fact that the DNA molecules take up physical space and therefore cannot overlap over itself.

Self-exclusion is neglected ($B = 0$):

$$F_p = (A_p L) k_B T = (3.02 * 10^6 * 71.8 * 10^{-6}) k_B T = 217\ k_B T$$

Self-exclusion is accounted for ($B \neq 0$):

$$F_p = (A_p L + B L^2) k_B T = (3.02 * 10^6 * 71.8 * 10^{-6} + 5 * 10^{11} * (71.8 * 10^{-6})^2) k_B T$$
$$= 2790\ k_B T$$

Part 3

6.)

Equation 7: $F_{spring} = \frac{L^2}{2PL_{spring}}\left(1 + \frac{1}{2\left(1-\frac{L}{L_{spring}}\right)}\right)$

Equation 1: $\Delta F_{to} = N\left(F_p(L_p) - F_s(L_p)\right) + (N-1)F_{spring}(L_s, l)$

Where:

L_p is contour length per pit, L_s is contour length per linker (stretched segment between neighbouring pits), l is pit spacing (centre-to-centre distance between neighbouring pits)

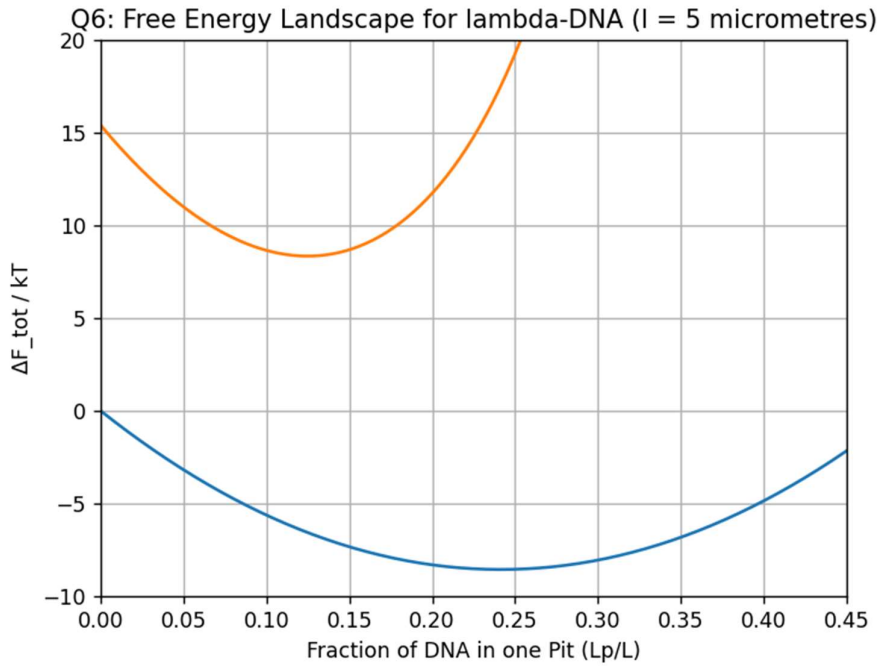
Furthermore, we are given that: $L = NL_p + (N-1)L_s$, such that: $L_s = \frac{L-NL_p}{N-1}$

Equation 3 states that for $h \gg P$: $A_s \sim \frac{P}{h^2}$

Equation 5 states: $A_p \sim P\left(\frac{1}{(h+d)^2} + \frac{2}{a^2}\right)$

$$A = A_s - A_p$$

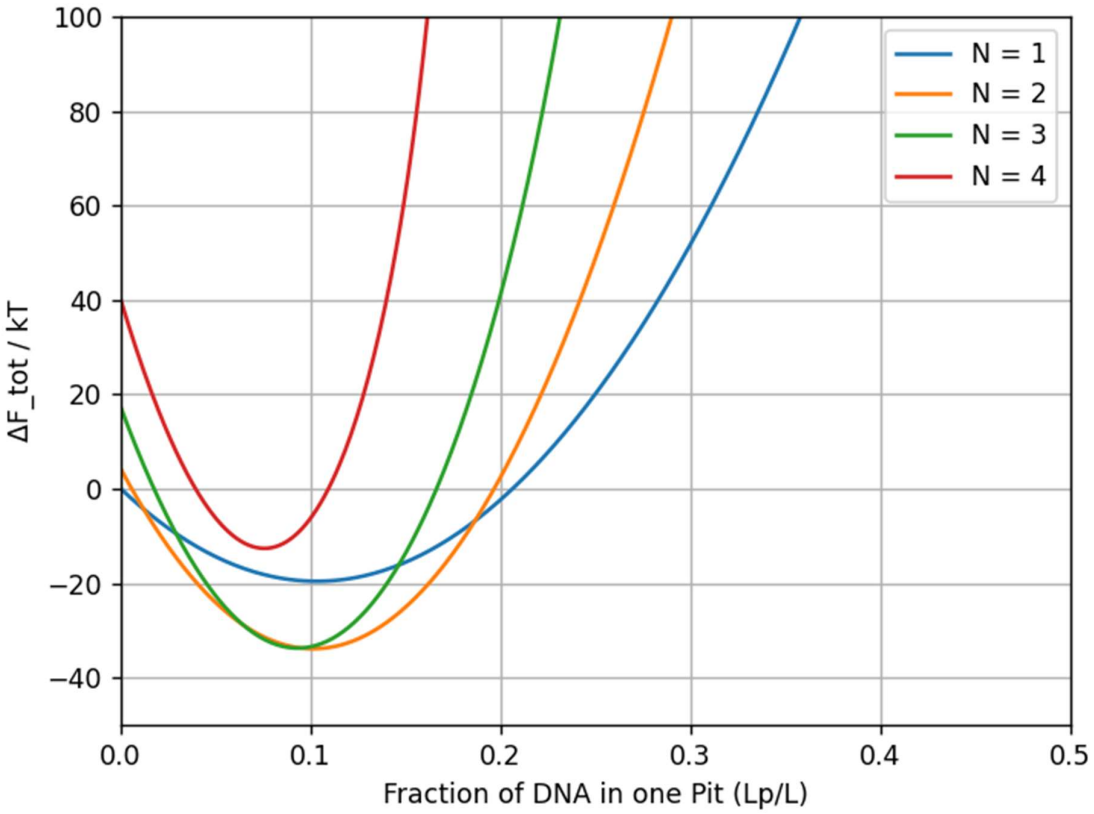
Combining everything, and plotting $\frac{L_p}{L}$ at $N = 1$ and $N = 2$:



7.)

Now we must adjust parameters ($h, d, a\ or\ l$) so that $N = 2$ and $N = 3$ are both the most stable configurations. To this logically, one must understand how changing one of the parameters would affect the DNA's preferred contour per pit. My strategy here is simple. By reducing h, we know that the preferred contour per pit would increase, as DNA "would dislike" being in the slit, and therefore it there is "more incentive" for it to go into the pits. This is shown as: $A_s \sim \frac{P}{h^2}$.

Parameters used: $h = 86.355\ nm,\ \ d = 100\ nm,\ \ a = 300\ nm,\ \ l = 5\ \mu m$



8.)

Printing out $\frac{L_p}{L}$ at the stable configuration in python:

For $N = 2,\ \ \frac{L_p}{L} = 0.102$

For $N = 3,\ \ \frac{L_p}{L} = 0.093$

Appendix:

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

kT = 1.0  # Working in units of kT makes things simpler
L_A = 21.0e-6   # lambda
L_T4 = 71.8e-6  # T4
P = 64e-9
w_eff = 6e-9   # Adjusted
h = 100e-9
d = 100e-9
a = 300e-9
l = 5.0e-6
A_s = P / h**2
A_p = P * (1.0 / (h + d)**2 + 2.0 / a**2)
A = A_s - A_p
B = w_eff / ((h + d) * a**2)
L = 21e-6

def F_spring(L_spring, l, P):
    return ((l**2) / (2 * P * L_spring)) * (1 + 1 / (2 * (1 - (l /
L_spring))))

def F_pit(L_p):
    F_p = A_p * L_p + B * L_p**2   # Pit energy
    F_s = A_s * L_p  # Slit energy
    return F_p - F_s   # The relevant energy is the DIFFERENCE (Gain from
moving Slit -> Pit)

def Ftot(L_p, N):

    if N == 1:
        return F_pit(L_p)

    L_spring = (L - N * L_p) / (N - 1)

    if L_spring <= l:
        # Not enough contour to span the distance -> unphysical
        return np.nan

    return N * F_pit(L_p) + (N-1) * F_spring(L_spring, l, P)

Lp_frac = np.linspace(0.0, 1.0, 1000)  # Lp/L

F1 = []
F2 = []
```

```
for x in Lp_frac:
    Lp = x * L          # convert fraction to actual contour per pit
    F1.append(Ftot(Lp, 1))  # N = 1
    F2.append(Ftot(Lp, 2))  # N = 2

plt.ylim(-10, 20)
plt.xlim(0, 0.45)

plt.plot(Lp_frac, F1, label="N = 1")
plt.plot(Lp_frac, F2, label="N = 2")
plt.xlabel("Fraction of DNA in one Pit (Lp/L)")
plt.ylabel("ΔF_tot / kT")
plt.title("Q6: Free Energy Landscape for lambda-DNA (l = 5 micrometres)")
plt.grid(True)
plt.show()

##################################################

h = 86.355e-9
d = 100e-9
a = 300e-9
l = 5.0e-6
A_s = P / h**2
A_p = P * (1.0 / (h + d)**2 + 2.0 / a**2)
A = A_s - A_p
B = w_eff / ((h + d) * a**2)
L = 71.8e-6 # T4 length

Ns = [1, 2, 3, 4]

plt.figure()

for N in Ns:
    F_vals = []
    for x in Lp_frac:
        Lp = x * L
        F_vals.append(Ftot(Lp, N))

    F_vals = np.array(F_vals)

    valid = np.isfinite(F_vals) # mask out NaNs (where L_spring <= l)
    F_valid = F_vals[valid]
    x_valid = Lp_frac[valid]

    idx_min = np.argmin(F_valid)
    Lp_over_L_min = x_valid[idx_min]
    F_min = F_valid[idx_min]
```

```
    print(f"N = {N}: L_p/L at minimum = {Lp_over_L_min:.3f},  F_min =
{F_min:.2f} kT")

    plt.plot(Lp_frac, F_vals, label=f"N = {N}")

plt.xlabel("Fraction of DNA in one Pit (Lp/L)")
plt.ylabel("ΔF_tot / kT")
plt.ylim(-50, 100)
plt.xlim(0, 0.5)
plt.legend()
plt.grid(True)
plt.show()
```