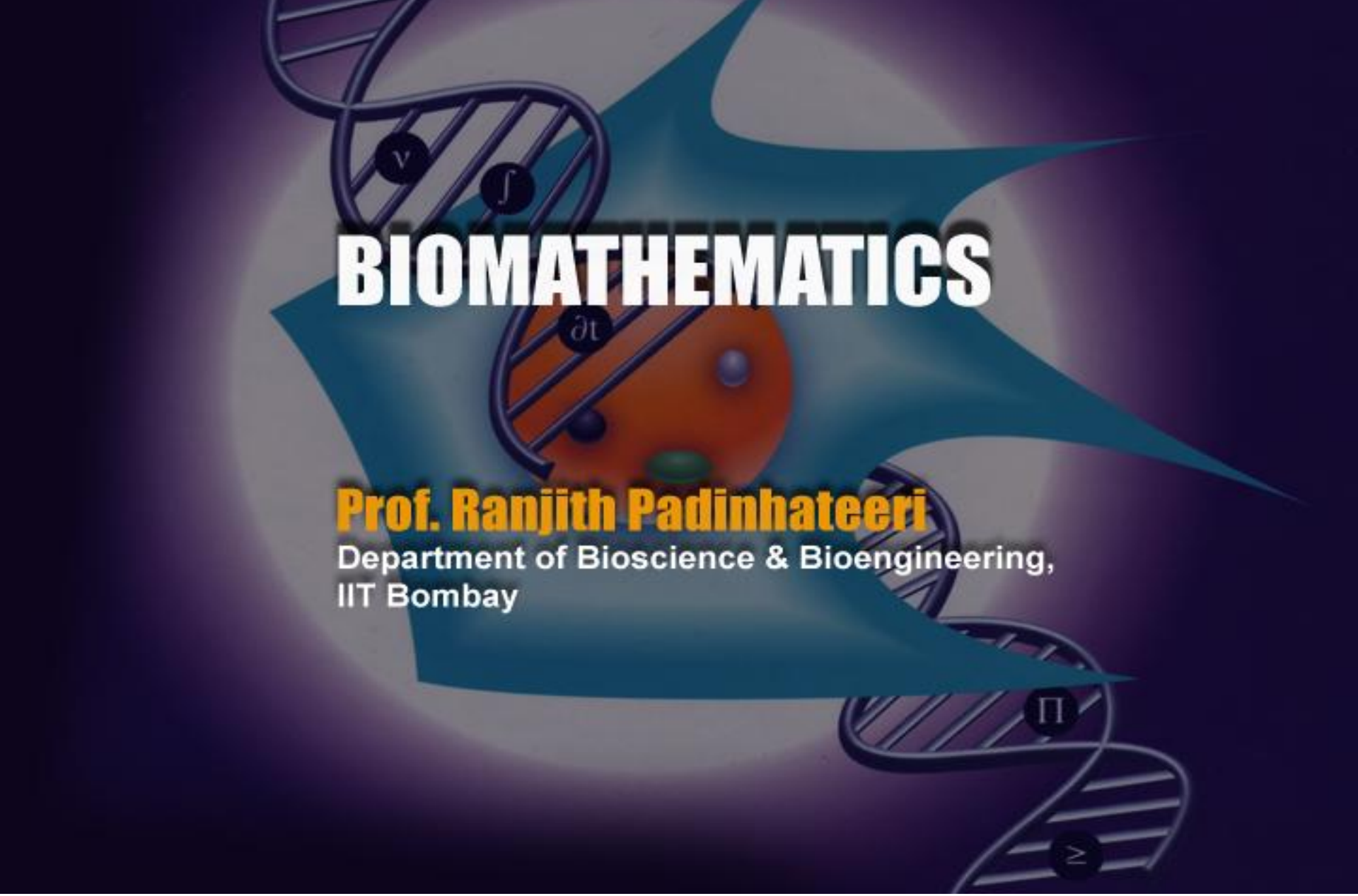
BIOMATHEMATICS
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IIT Bombay

Lecture 38

Statistical thermodynamics of biological systems

Thermodynamics of protein organization along DNA

Total number of arrangements possible, When there are N binding sites and m proteins

$$\Omega = \frac{N!}{m!(N-m)!}$$

Entropy

$$S = k_B \ln \Omega = k_B \ln \left(\frac{N!}{m!(N-m)!} \right)$$

$$S = -k_B N \left[\rho \ln \rho + (1-\rho) \ln (1-\rho)\right]$$

When there are m proteins bound, the energy is given by

$$E = -m\ \epsilon\ k_B T = -N \rho \epsilon\ k_B T$$

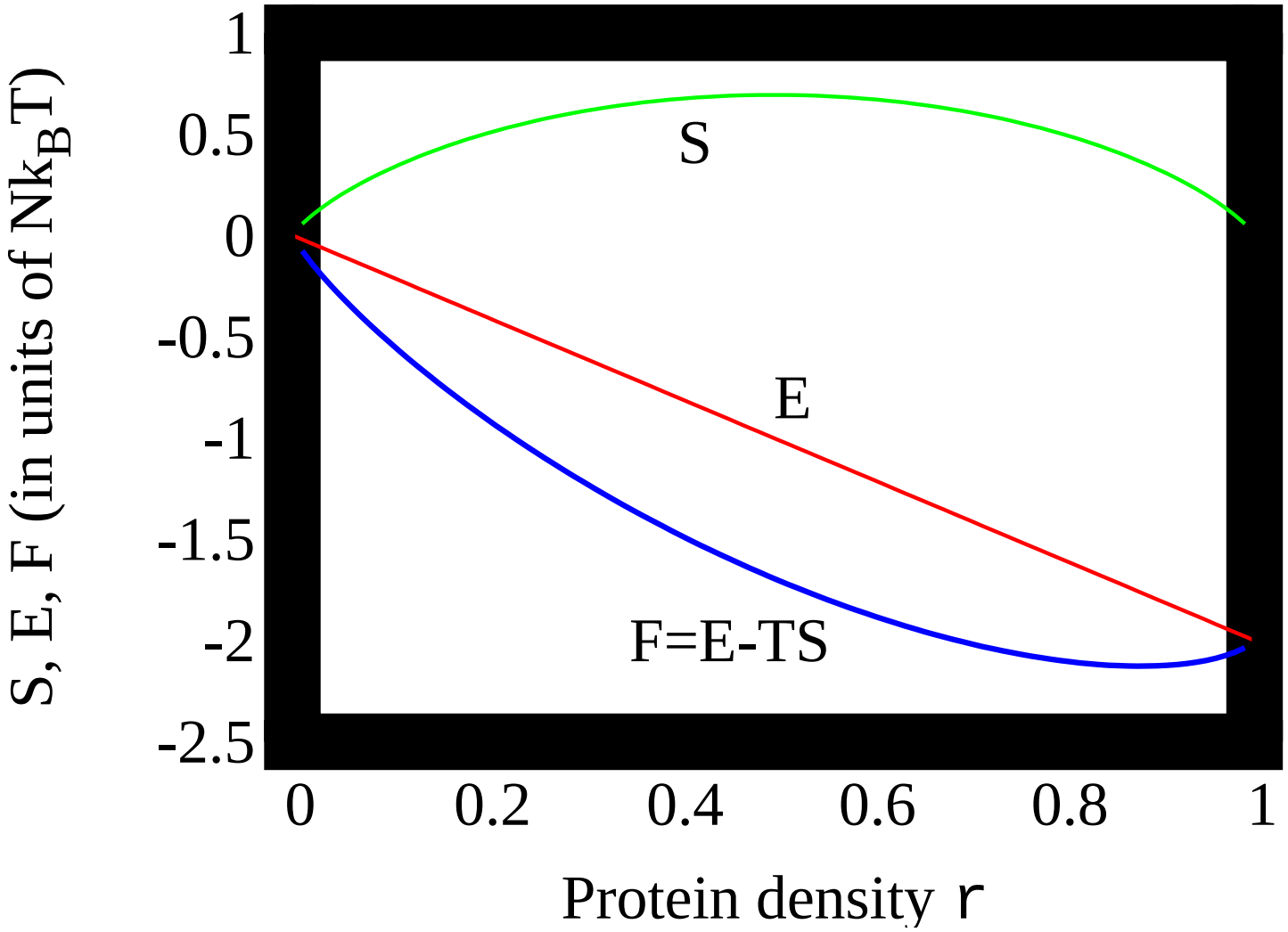
Free energy (F)

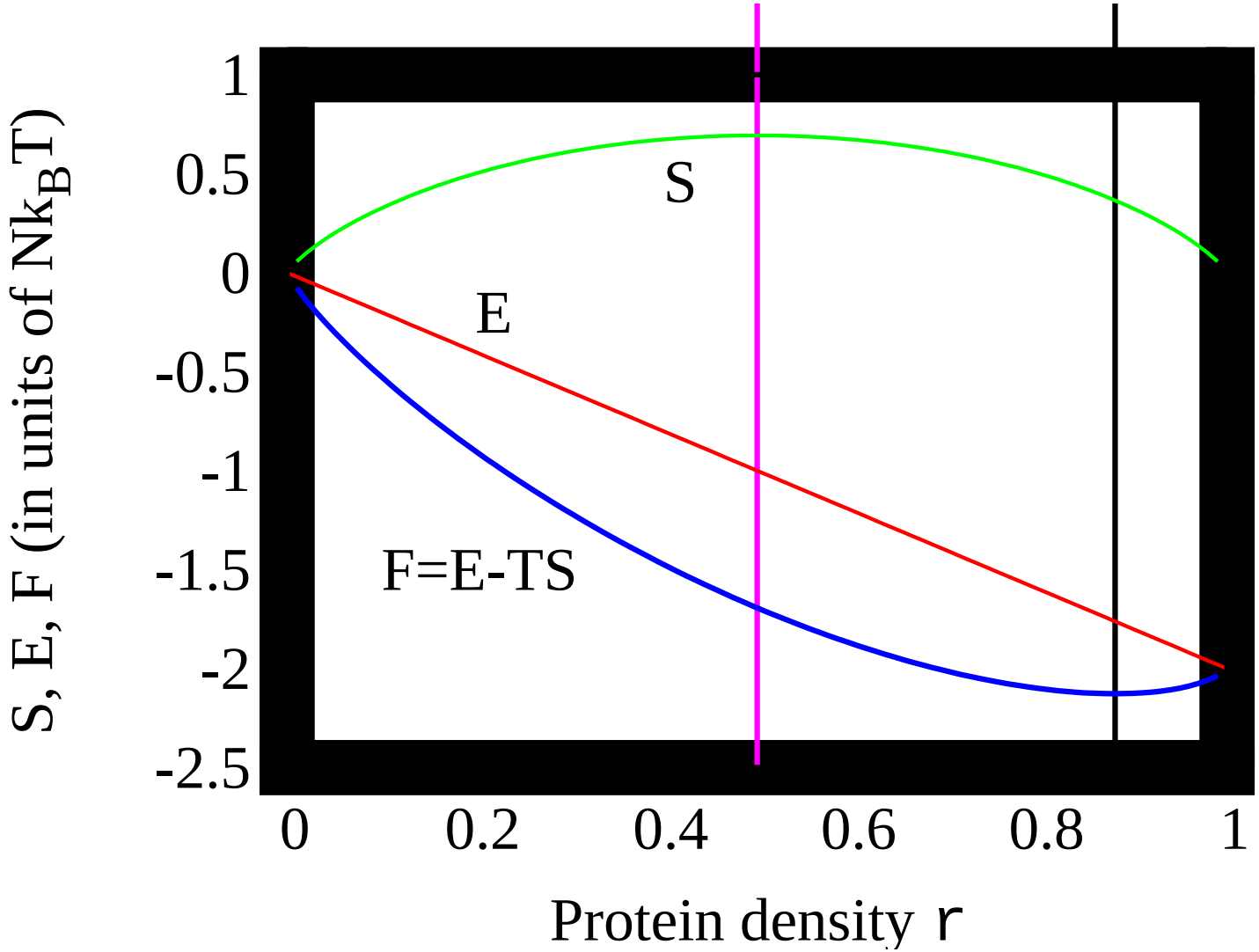
$$F = E - TS$$

$$F = -N\rho\epsilon\ k_B T + k_B T N\left[\rho \ln \rho + (1-\rho)\ln(1-\rho)\right]$$

Free energy per binding site, in units of k_BT, is given by

$$\frac{F}{Nk_BT} = -\rho\epsilon + \rho \ln \rho + (1-\rho) \ln (1-\rho)$$


S, E, F (in units of Nk_BT)
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
0
0.2
0.4
0.6
0.8
1
Protein density r
S
E
F=E-TS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Protein density r
S
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F=E-TS

The free energy is minimum when

$$\frac{\partial F}{\partial \rho} = 0$$

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$$\Rightarrow \rho = \frac{e^{\epsilon}}{1 + e^{\epsilon}}$$

For $\epsilon = 2$