Applying Open Quantum Systems Techniques to Density Matrix Minimization

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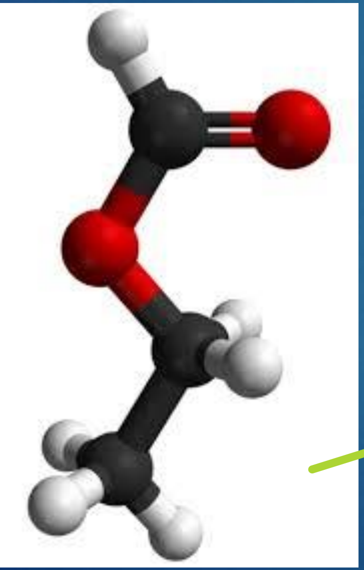
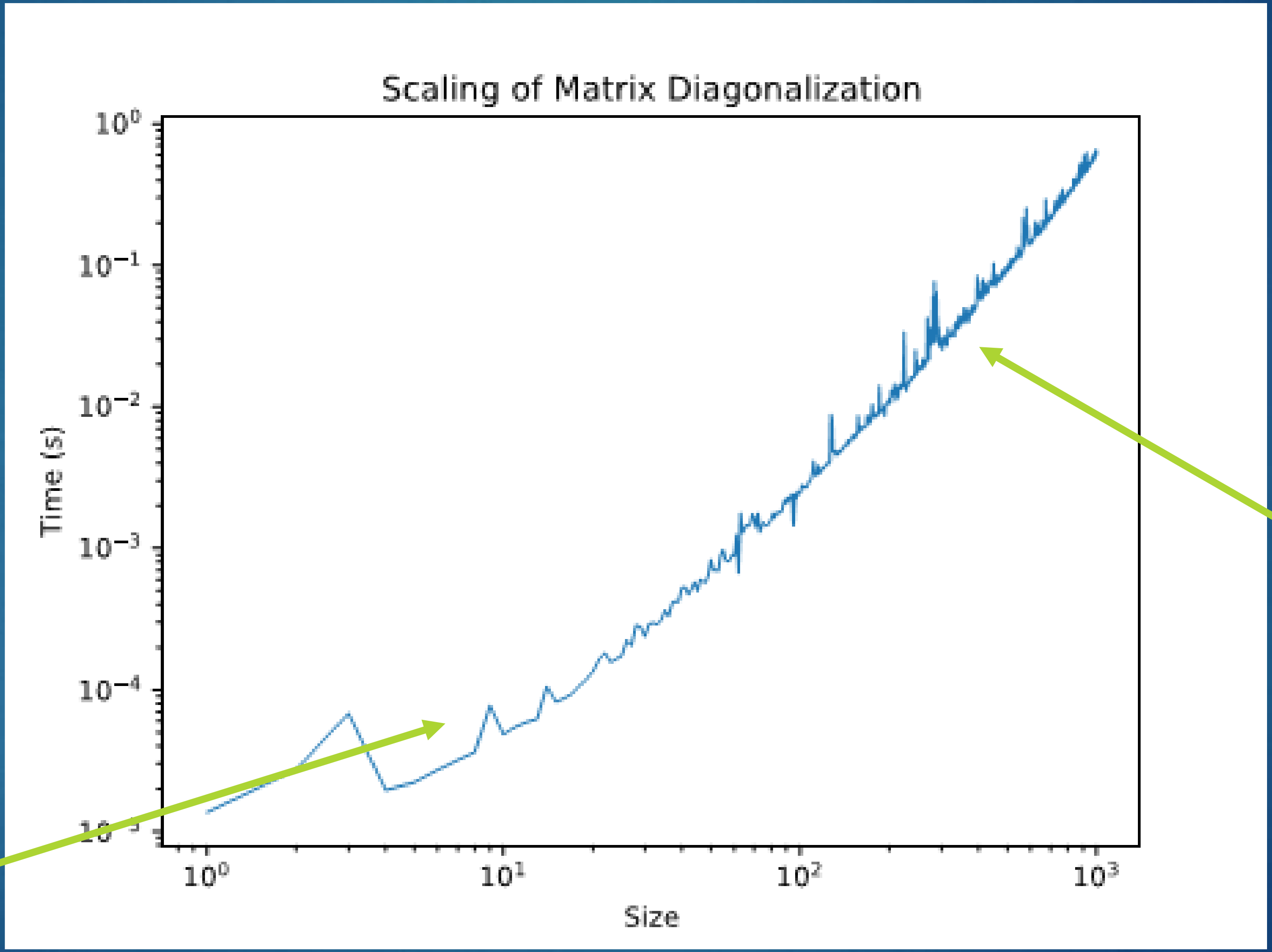
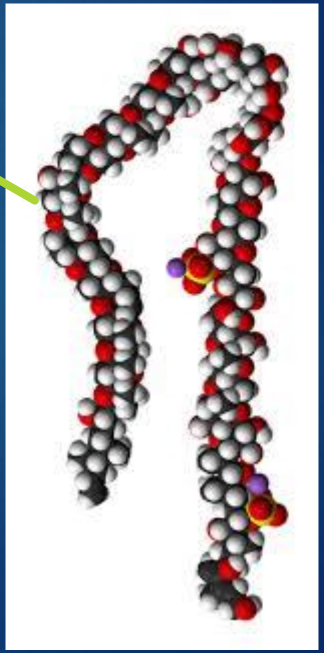
Motivation




Scaling of Matrix Diagonalization
Time (s)
Size
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^1
10^2
10^3



Early DMM

<u>LNV</u>

$$E = Tr[\hat{\rho}\hat{H}]$$

$$\Omega = Tr[\hat{\rho}(\hat{H} - \mu\hat{1})]$$

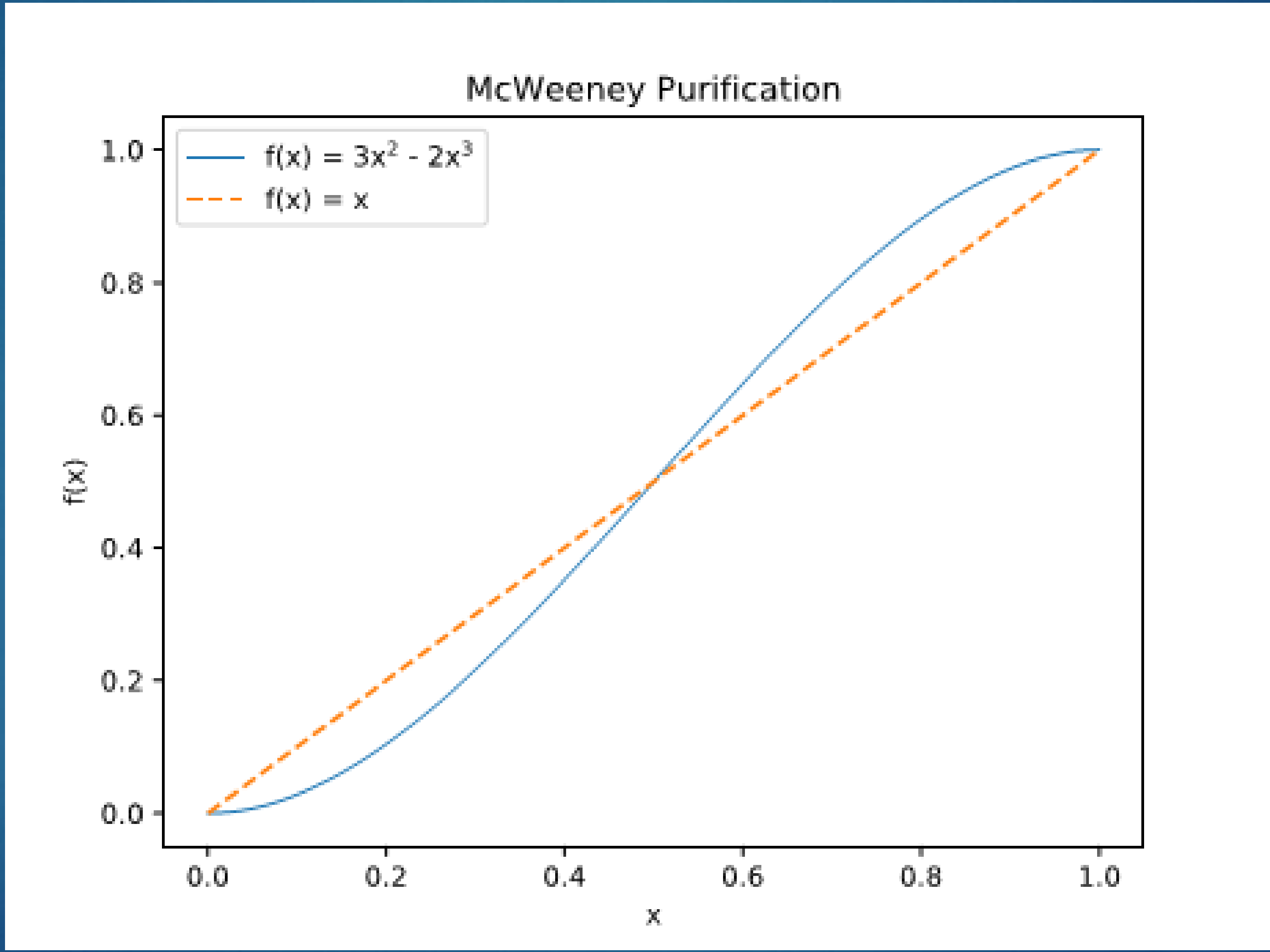
$$\frac{\partial\Omega}{\partial\rho}$$

<u>Daw</u>

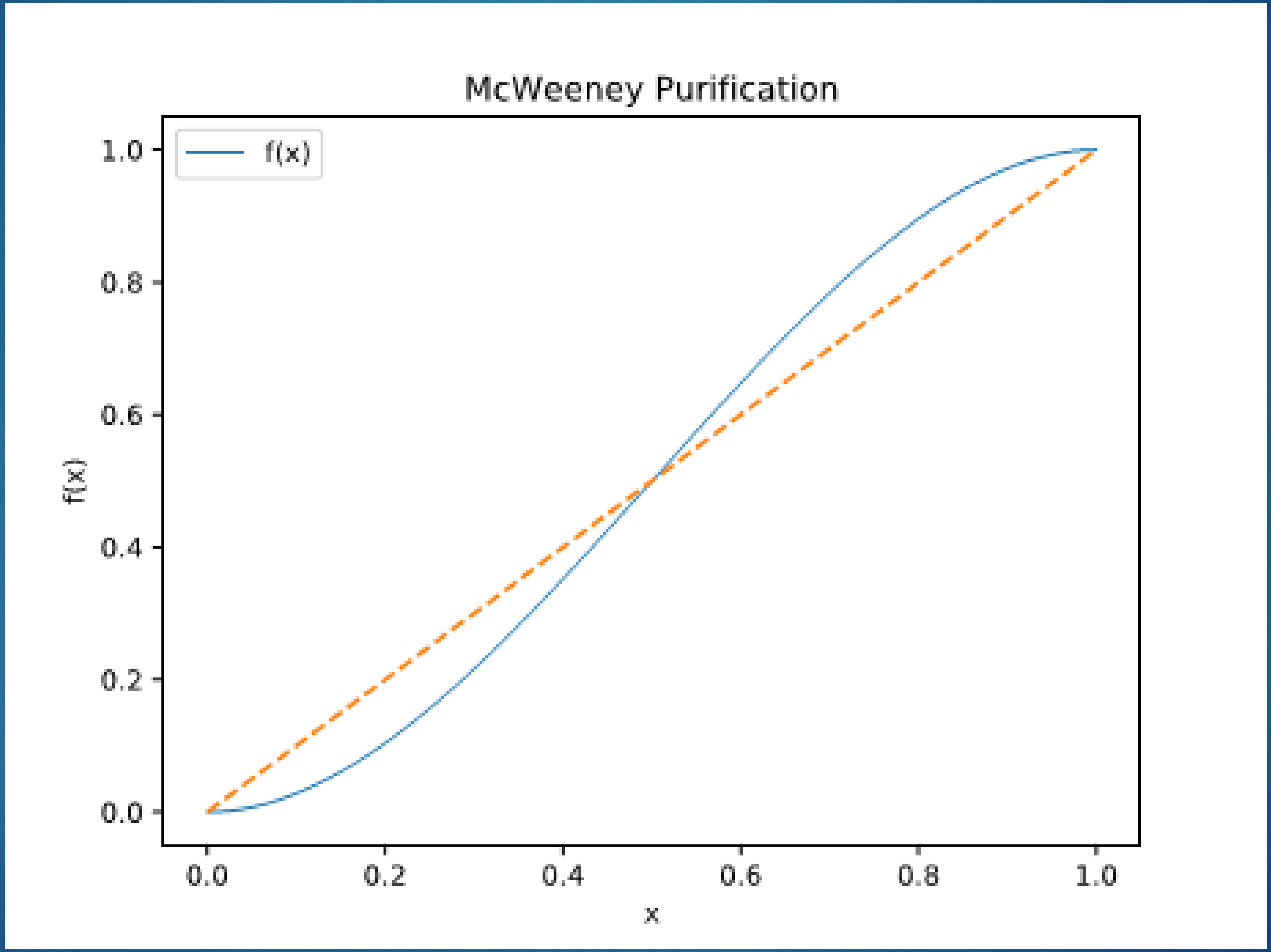
$$E = Tr[\hat{\rho}\hat{H}] \qquad \hat{\rho} = \frac{1}{\hat{1} + \exp\left(\beta(\hat{H} - \mu\hat{1})\right)}$$

$$\frac{\partial\hat{\rho}}{\partial\beta}$$

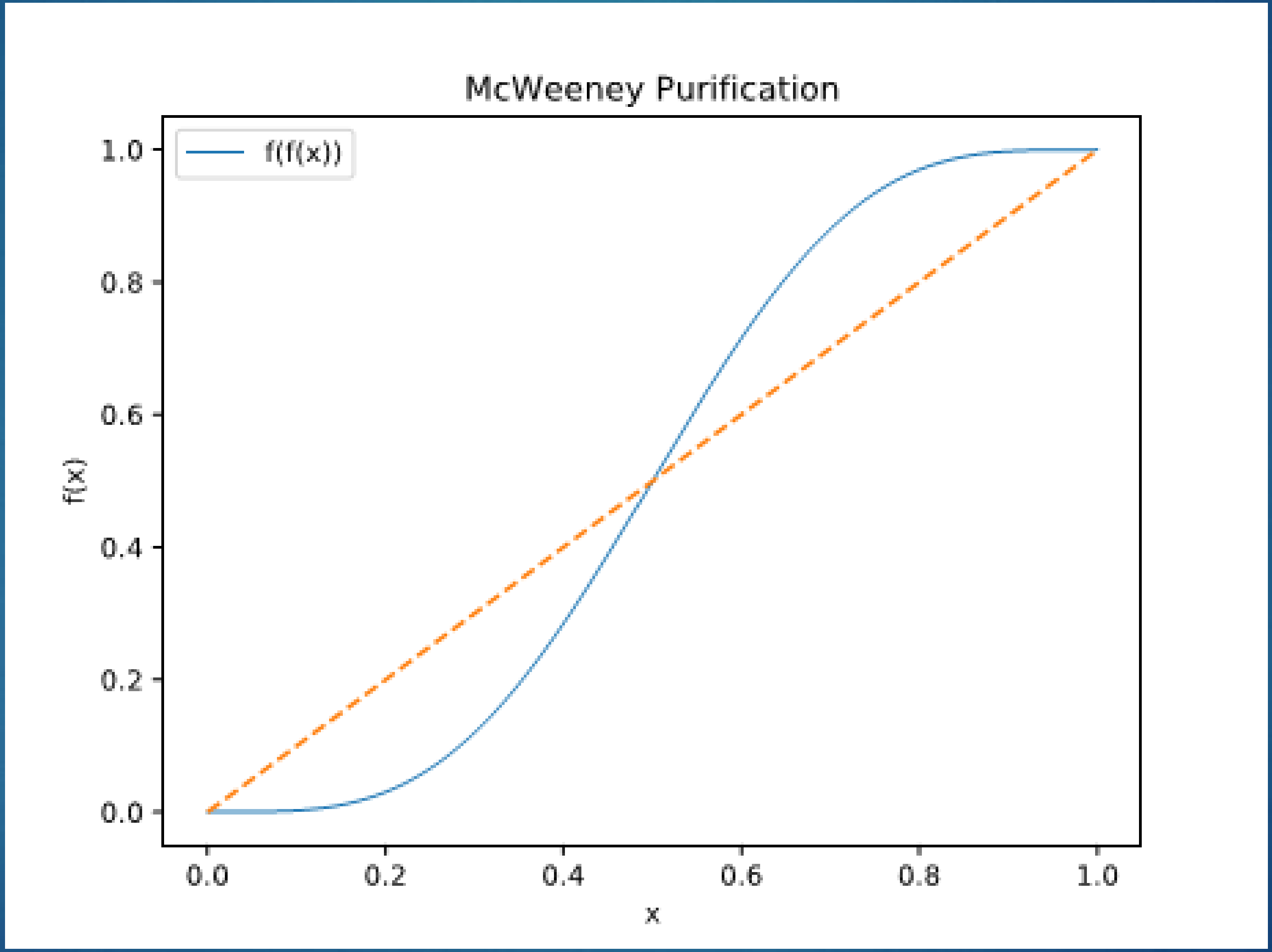
Purification



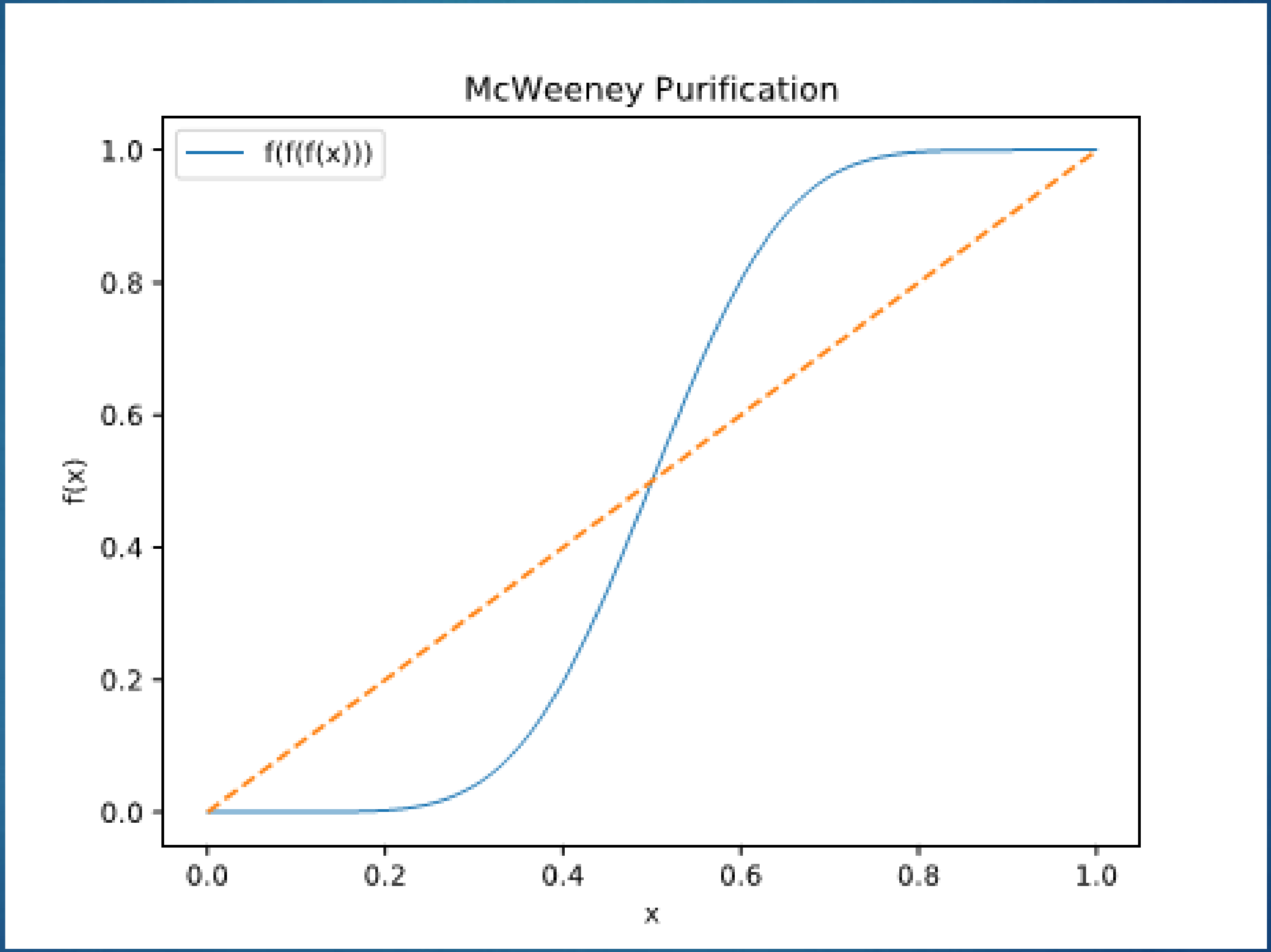
Purification



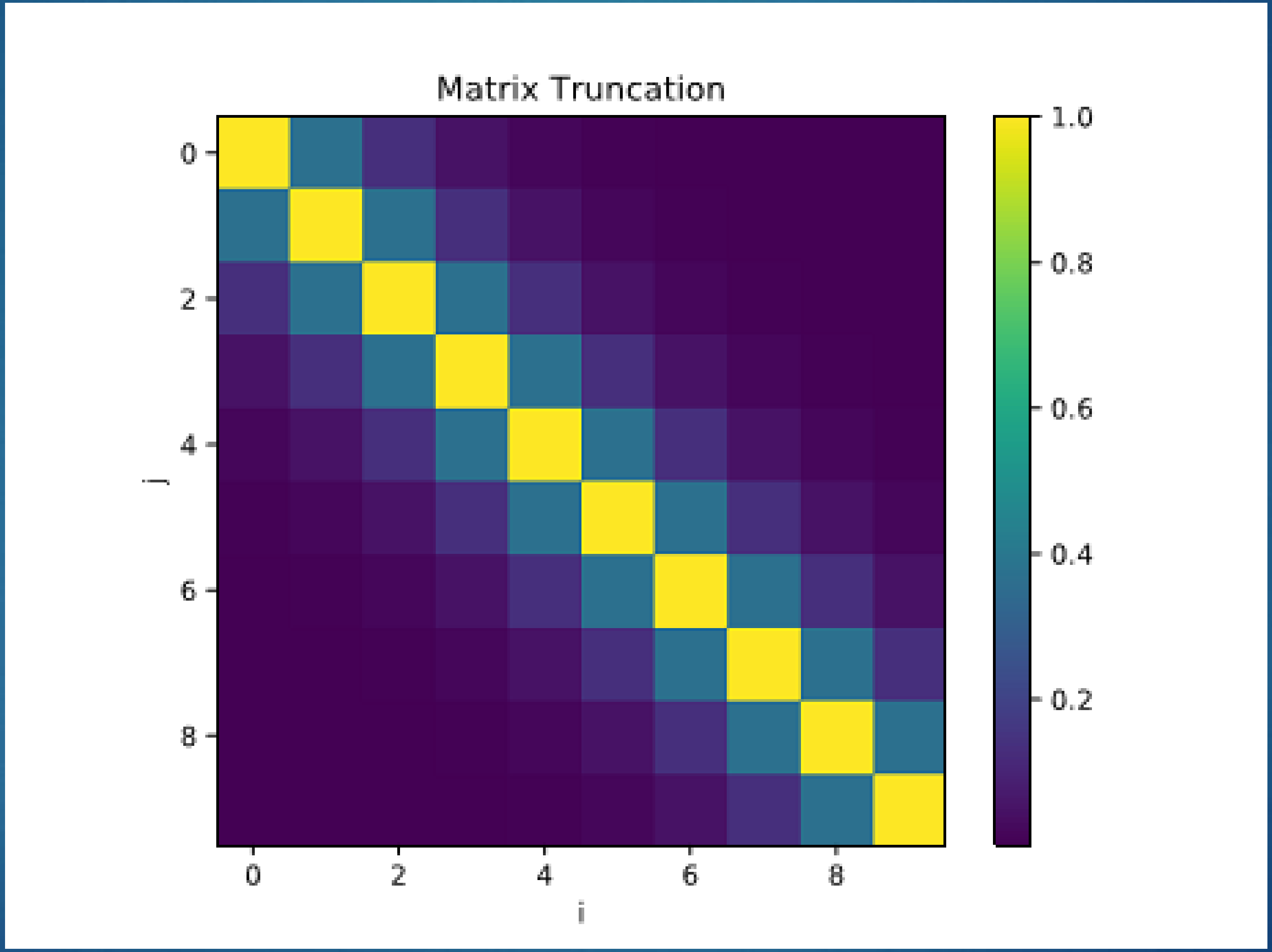
Purification



Purification



Linear-scaling?

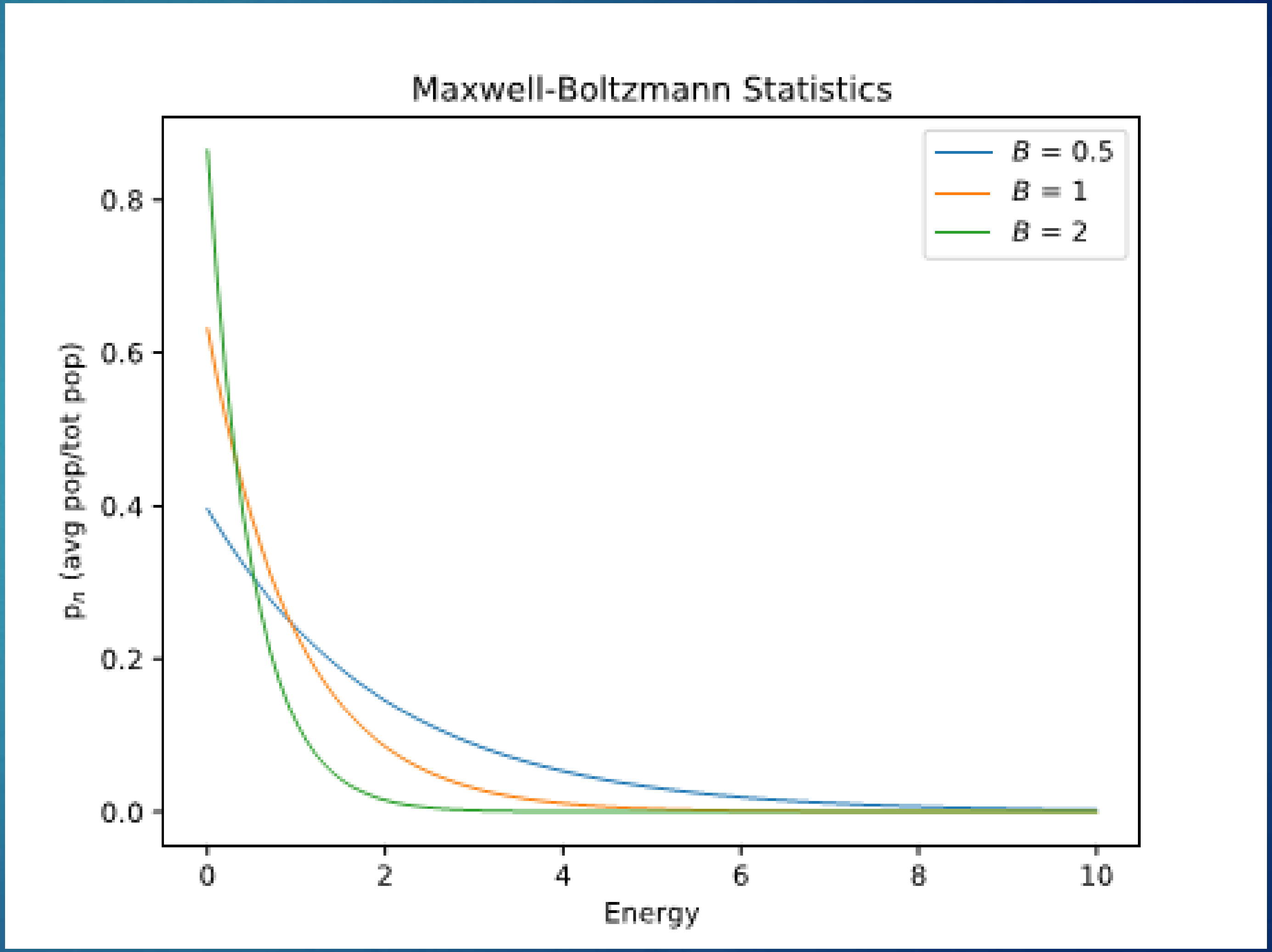


Bloch's Method

$$\hat{\rho} = e^{-\beta \hat{H}}, \qquad \hat{\rho}(0) = 1$$

$$\frac{\partial \hat{\rho}}{\partial \beta} = -\hat{H}\rho$$

$$\frac{\partial \hat{\rho}}{\partial \beta} = -\frac{1}{2}\hat{H}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{H}$$



Bloch's Method

- Let us consider the derivative more closely:

$$\frac{\hat{\rho}(\beta + d\beta) - \hat{\rho}(\beta)}{d\beta} = -\frac{1}{2}\hat{H}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{H} + O(d\beta)$$

$$\hat{\rho}(\beta + d\beta) = \hat{\rho} - \frac{d\beta}{2}\hat{H}\hat{\rho} - \frac{d\beta}{2}\hat{\rho}\hat{H} + O(d\beta^2)$$

$$\hat{\rho}(\beta + d\beta) = (1 - \frac{d\beta}{2}\hat{H})\hat{\rho}(1 - \frac{d\beta}{2}\hat{H})^\dagger + O(d\beta^2)$$

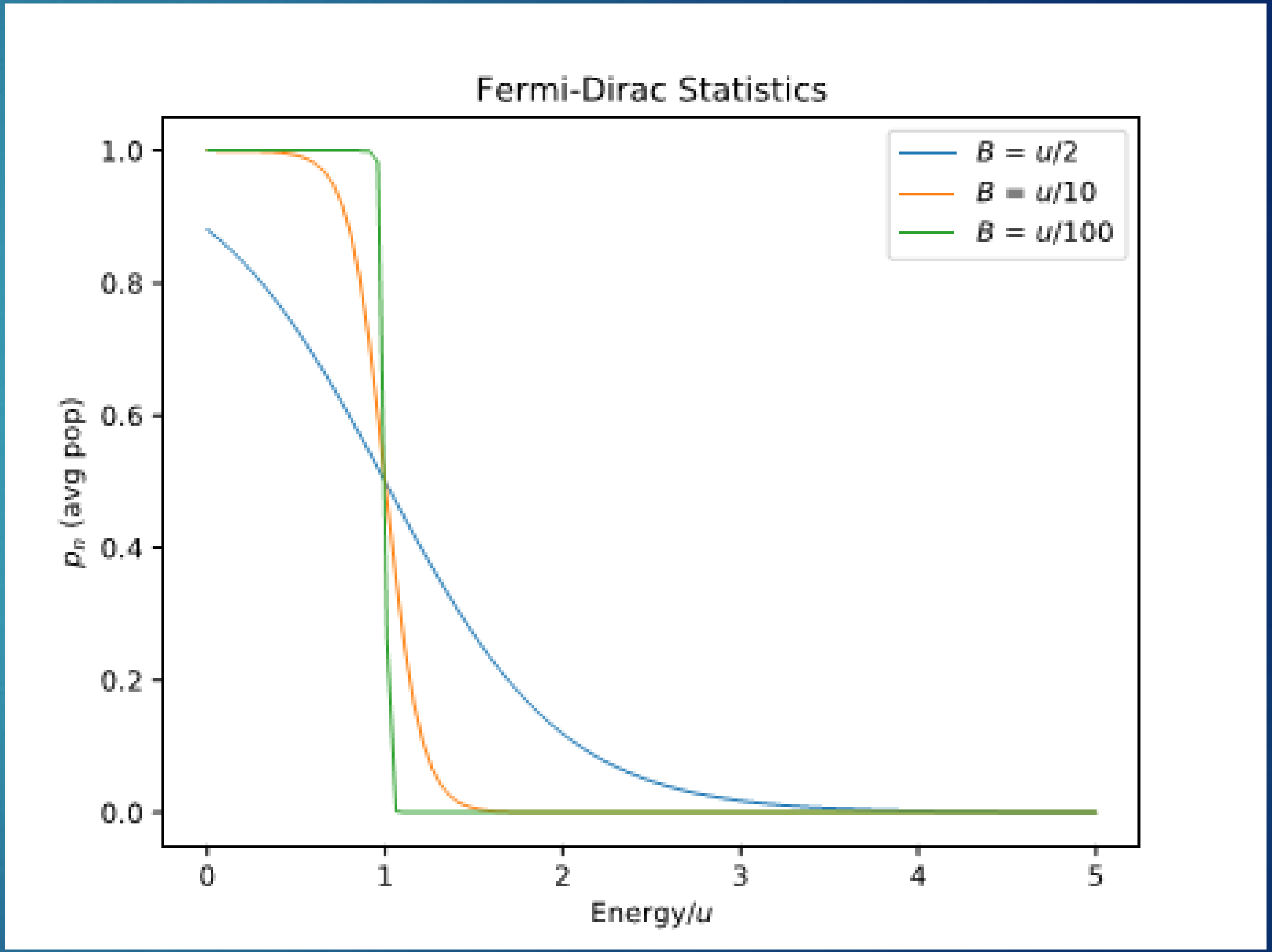
Our DMM

$$\hat{\rho} = \frac{1}{1 + e^{\beta(\hat{H} - \mu)}}, \qquad \hat{\rho}(0) = 1$$

$$\frac{\partial \hat{\rho}}{\partial \beta} = -\left(1 + e^{\beta(\hat{H} - \mu)}\right)^{-2} e^{\beta(\hat{H} - \mu)}\left(\hat{H} - \mu\right)$$

$$\frac{\partial \hat{\rho}}{\partial \beta} = -\hat{\rho}(1 - \hat{\rho})(\hat{H} - \mu)$$

$$\frac{\partial \hat{\rho}}{\partial \beta} = -\frac{1}{2}\left(\hat{H} - \mu\right)(1 - \hat{\rho})\hat{\rho} - \frac{1}{2}\hat{\rho}(1 - \hat{\rho})\left(\hat{H} - \mu\right)$$



Our DMM

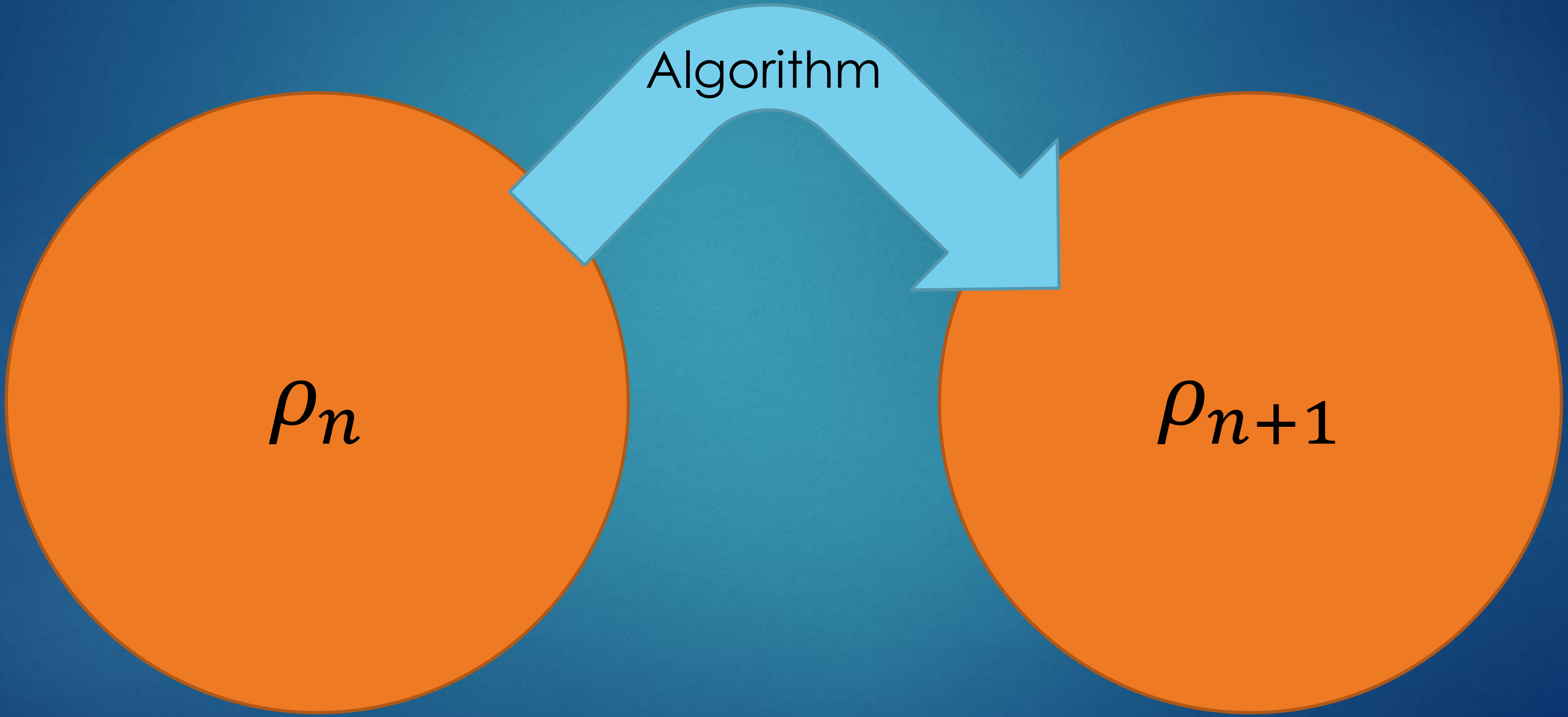
- Let us consider the derivative more closely:

$$\frac{\hat{\rho}(\beta + d\beta) - \hat{\rho}(\beta)}{d\beta} = -\frac{1}{2}(\hat{H} - \mu)(1 - \hat{\rho})\hat{\rho} - \frac{1}{2}\hat{\rho}(1 - \hat{\rho})(\hat{H} - \mu) + O(d\beta)$$

$$\hat{\rho}(\beta + d\beta) = \hat{\rho} - \frac{d\beta}{2}(\hat{H} - \mu)(1 - \hat{\rho})\hat{\rho} - \frac{d\beta}{2}\hat{\rho}(1 - \hat{\rho})(\hat{H} - \mu) + O(d\beta^2)$$

$$\boxed{\hat{\rho}(\beta + d\beta) = \left[1 - \frac{d\beta}{2}(\hat{H} - \mu)(1 - \hat{\rho})\right]\hat{\rho}\left[1 - \frac{d\beta}{2}(\hat{H} - \mu)(1 - \hat{\rho})\right]^{\dagger} + O(d\beta^2)}$$

Quantum Channel



Canonical DMM

- Need to update μ at every step according to:

$$\mu = \frac{Tr\left[\hat{H}\hat{\rho}\left(\hat{1} - \hat{\rho}\right)\right]}{Tr\left[\hat{\rho}\left(\hat{1} - \hat{\rho}\right)\right]}$$

- Additionally,

$$\hat{\rho}(0) = \frac{N_e}{Tr\left[\hat{1}\right]}\hat{1}$$

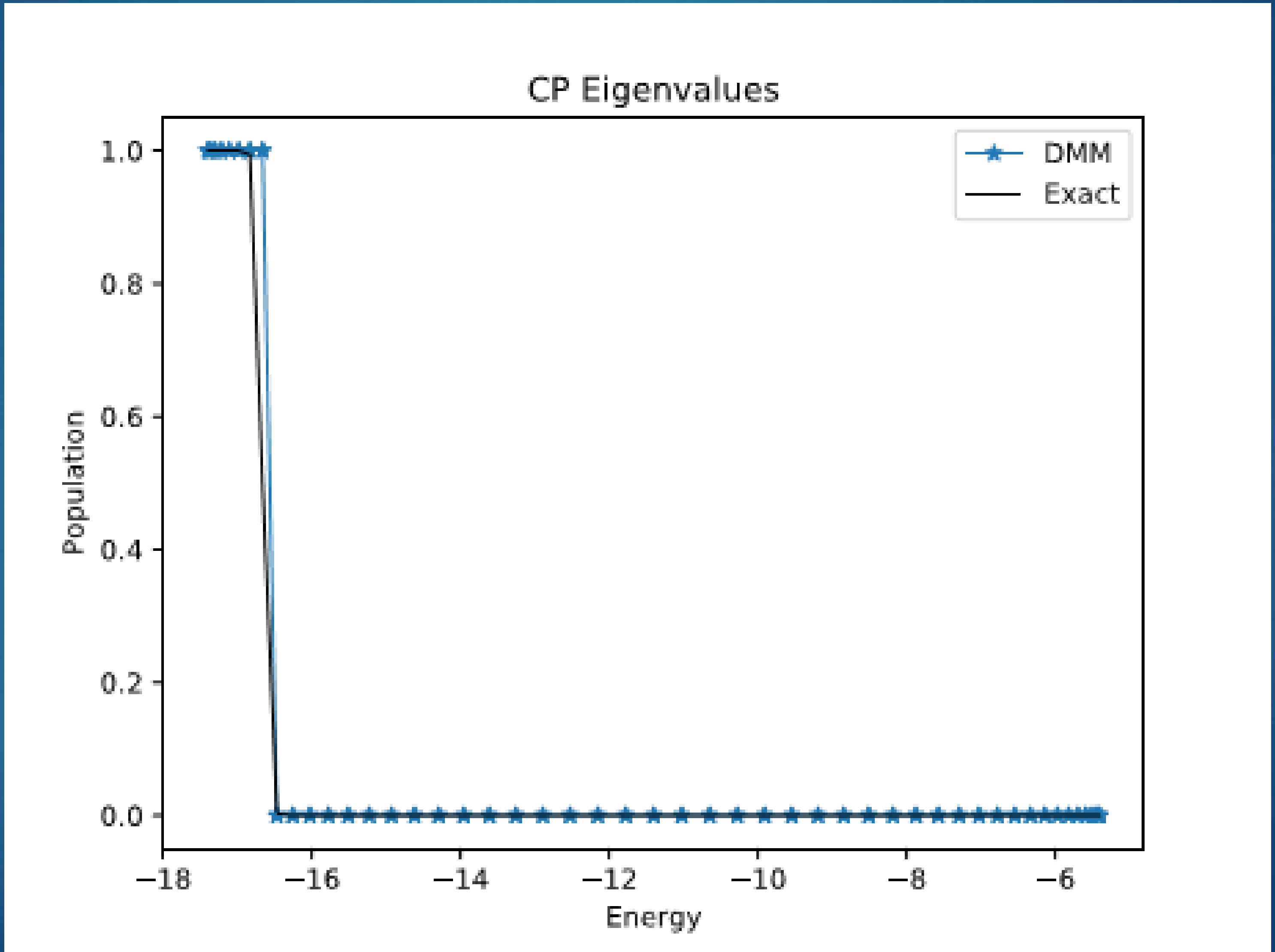
where N_e is the number of electrons in the system

Huckel Theory

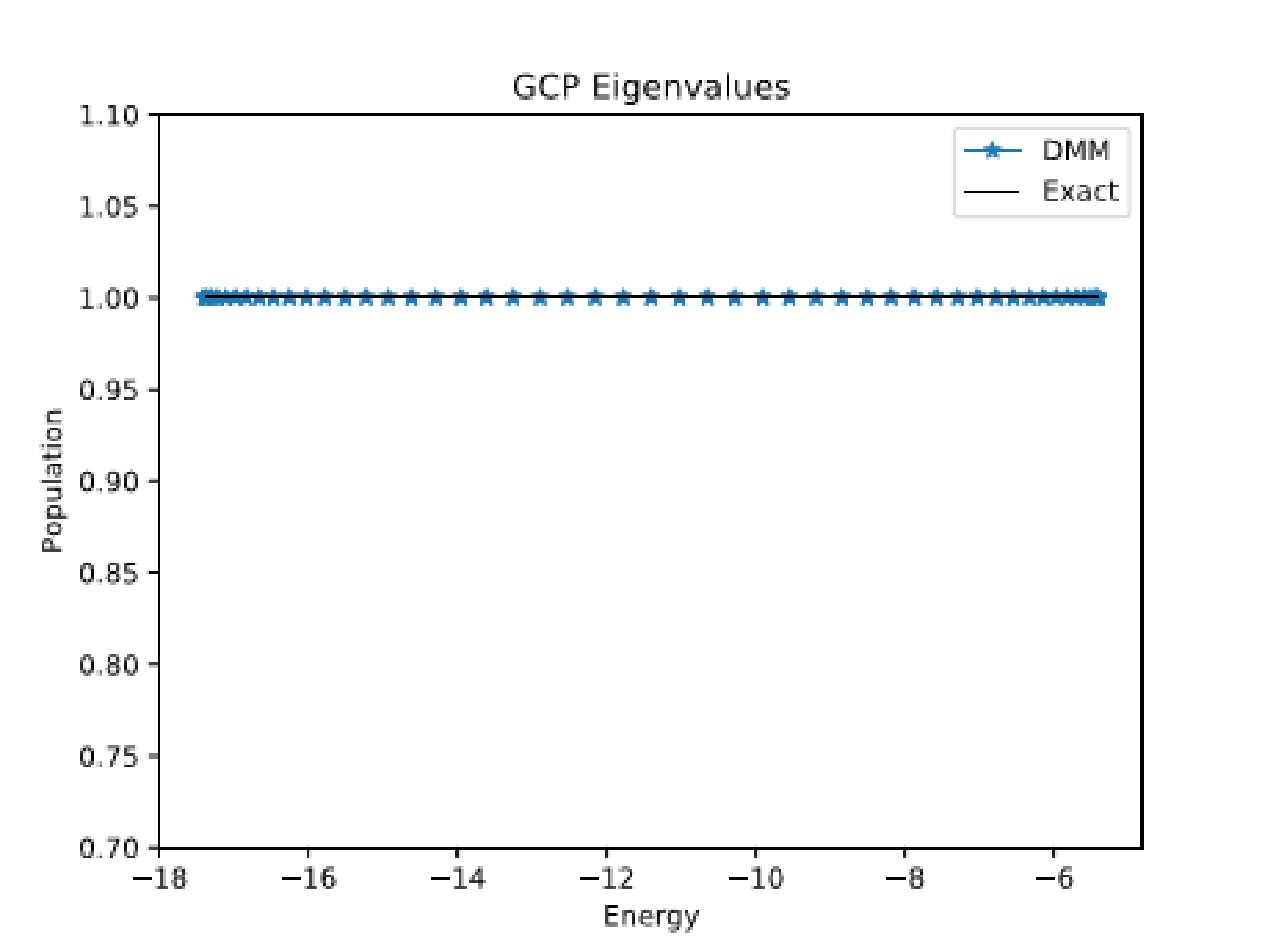
$$\hat{H} = \begin{matrix} \alpha & \gamma & 0 & 0 & 0 & 0 \\ \gamma & \alpha & \gamma & 0 & 0 & 0 \\ 0 & \gamma & \alpha & \gamma & 0 & 0 \\ 0 & 0 & \gamma & \alpha & \gamma & 0 \\ 0 & 0 & 0 & \gamma & \alpha & \gamma \\ 0 & 0 & 0 & 0 & \gamma & \alpha \end{matrix}$$

For ethylene, $\alpha = -11.4\ eV$ and $\gamma = 65\ kcal/mol$

Results - CP


CP Eigenvalues
1.0
0.8
0.6
0.4
0.2
0.0
Population
−18
−16
−14
−12
−10
−8
−6
Energy
DMM
Exact

Results - GCP



GCP Eigenvalues
DMM
Exact
Population
Energy
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
−18
−16
−14
−12
−10
−8
−6

Our DMM – applied to mu

$$\hat{\rho} = \frac{1}{1 + e^{\beta(\hat{H}-\mu)}}, \qquad \hat{\rho}(0) = 1$$

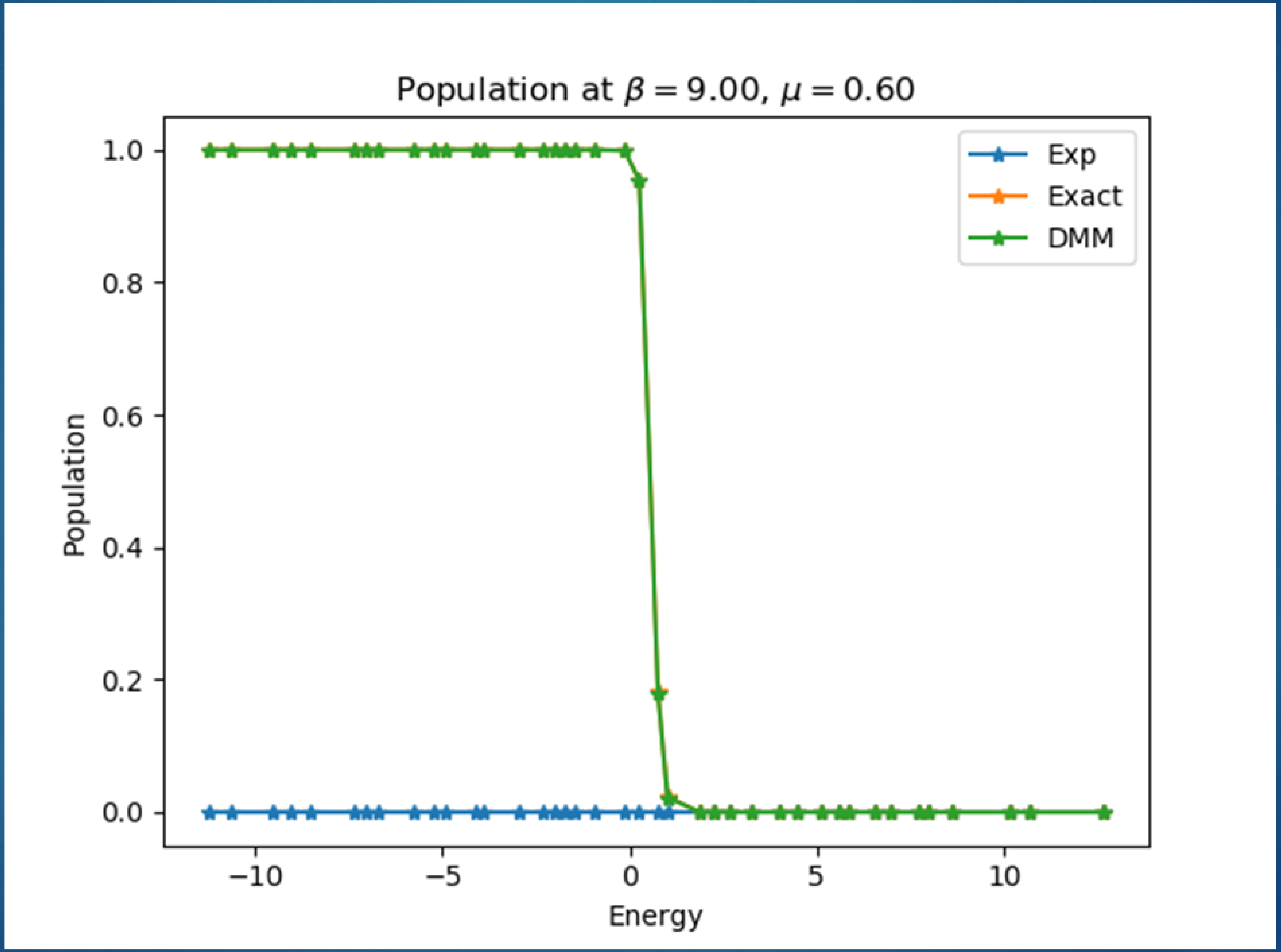
$$\frac{\partial \hat{\rho}}{\partial \mu} = -\left(1 + e^{\beta(\hat{H}-\mu)}\right)^{-2} e^{\beta(\hat{H}-\mu)}(-\beta)$$

$$\frac{\partial \hat{\rho}}{\partial \mu} = \beta \hat{\rho}(1 - \hat{\rho})$$

$$\frac{\partial \hat{\rho}}{\partial \mu} = \frac{\beta}{2}(1 - \hat{\rho})\hat{\rho} + \frac{\beta}{2}\hat{\rho}(1 - \hat{\rho}) + O(d\mu)$$

$$\hat{\rho}(\mu + d\mu) = \left[1 + \frac{\beta d\mu}{2}(1 - \hat{\rho})\right] \hat{\rho} \left[1 + \frac{\beta d\mu}{2}(1 - \hat{\rho})\right]^{\dagger} + O(d\mu^2)$$

Our DMM – applied to mu



Conclusion

- Several goals for the future of this project:
  - Find more realistic models to implement
  - Adopt a non-orthogonal basis version for more general use (very important if we want to compare with DFT methods)
  - Fine tune the code to achieve the maximum speed possible

References

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