Electrons in a Quantum Dot

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Main task: Learn the probability distribution from a Hamiltonian

Goal: $p(x) = e^{-\beta H(x)}/Z$ Normalization factor Z is unknown

K-L divergence

$$\boldsymbol{KL}(p_\theta||p) \equiv \int dx p_\theta(x)[\ln p_\theta(x) - \ln p(x)] \geq 0$$ equal to zero iff $p_\theta(x) = p(x)$

$$\min_\theta \left\{ \int dx\, p_\theta(x) \left[\frac{1}{\beta} \ln p_\theta(x) + H(x) \right] \right\} \geq -\frac{1}{\beta} \ln Z = F$$

$$\Longleftrightarrow \min_\theta \left\{ \mathop{\mathbb{E}}_{\boldsymbol{x} \sim p_\theta(\boldsymbol{x})} \left[H(\boldsymbol{x}) + k_B T \ln p_\theta(\boldsymbol{x}) \right] \right\}$$

How to parametrize the distribution p_θ ?

One possible way is to generate the $p_\theta(x)$ from a simple distribution $N(z)$.

$$z \xrightarrow{\mathrm{g}} x$$

$$p_\theta(x) = N(z)\left|\frac{\partial z}{\partial x}\right|$$

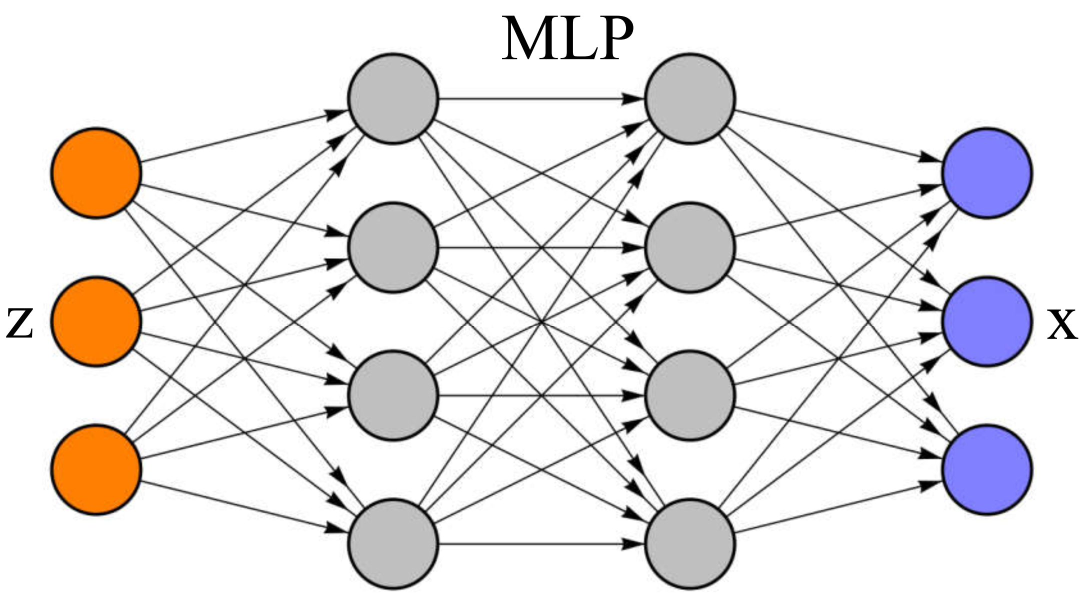
$$\ln p_\theta(x) = \ln N(z) - \ln\left|\frac{\partial x}{\partial z}\right|$$

$$\nabla \mathcal{L} = \mathbb{E}_{\boldsymbol{z} \sim \boldsymbol{\mathcal{N}}(\boldsymbol{z})}\left[\nabla f\left(g(\boldsymbol{z})\right)\right]$$

$$\text{where } f(x) = \frac{1}{\beta}\ln p_\theta(x) + H(x)$$

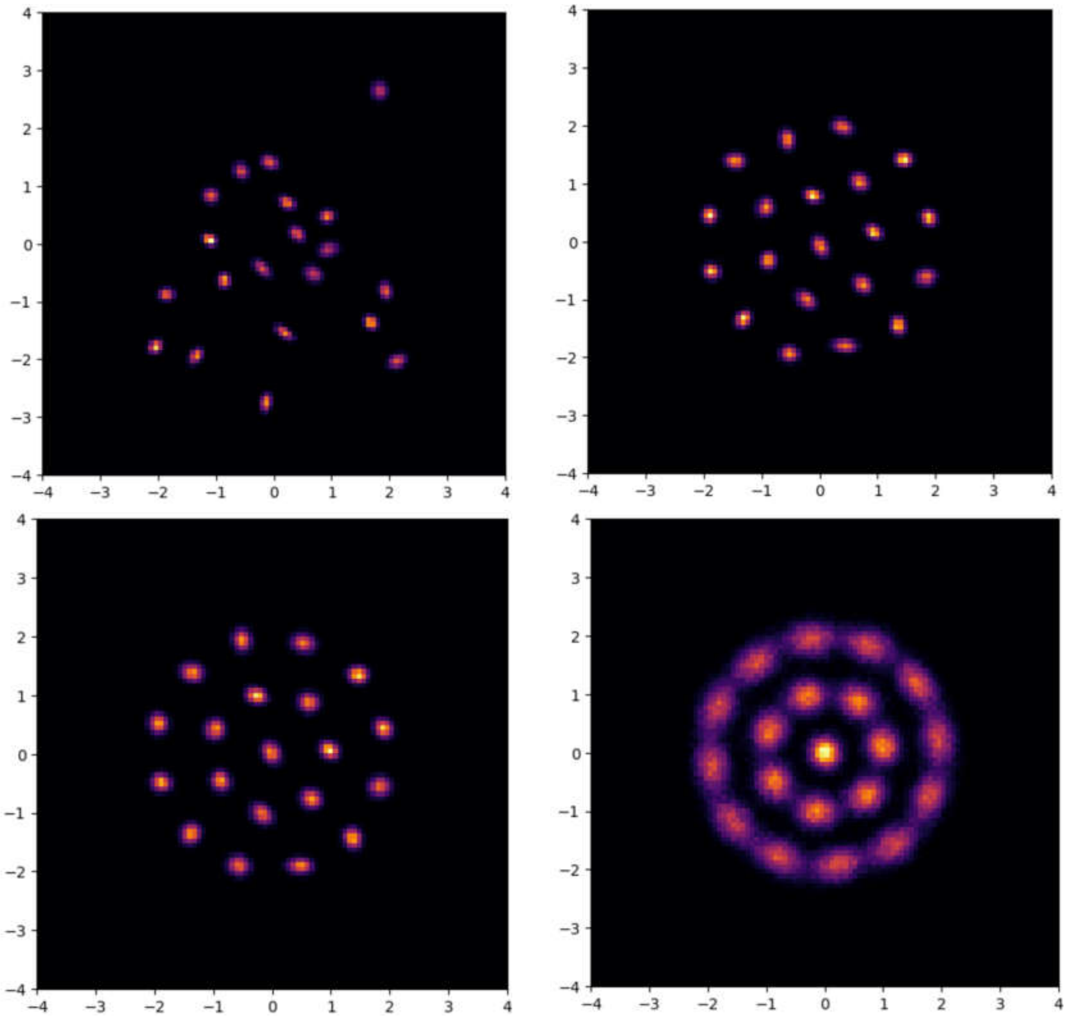
Network

$$z \to z_1 = \sigma(W_1 z + b_1) \to \cdots \to x = W_n z_{n-1} + b_{n-1}$$



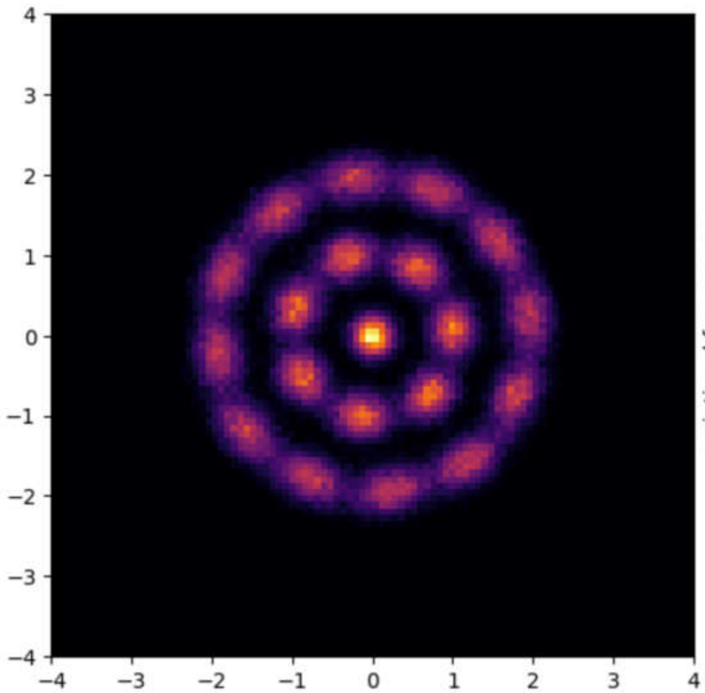
n*dim + hidden layers + n*dim

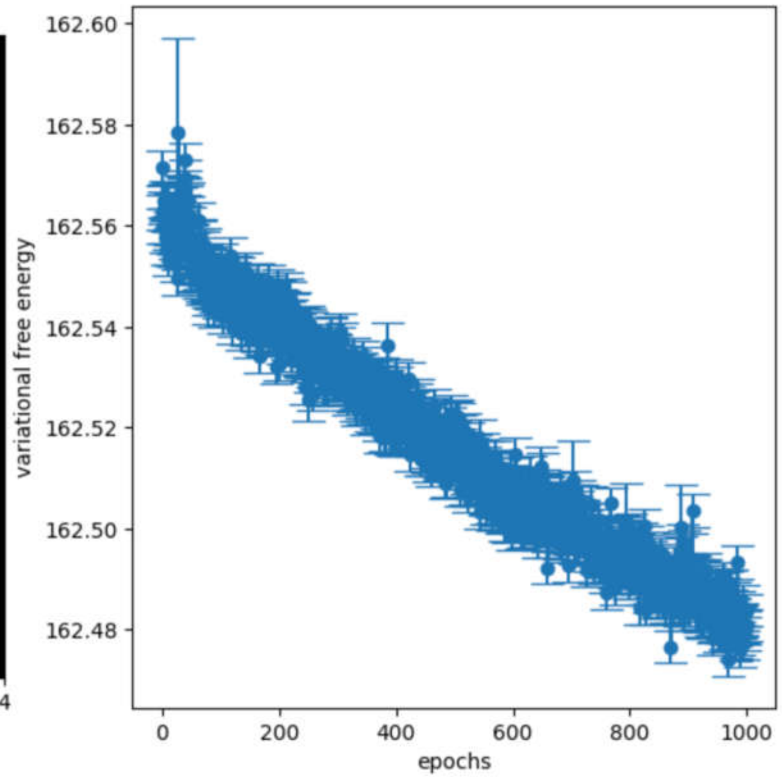
$n = 20, \beta = 10$



Final result

$n = 20, \beta = 10$



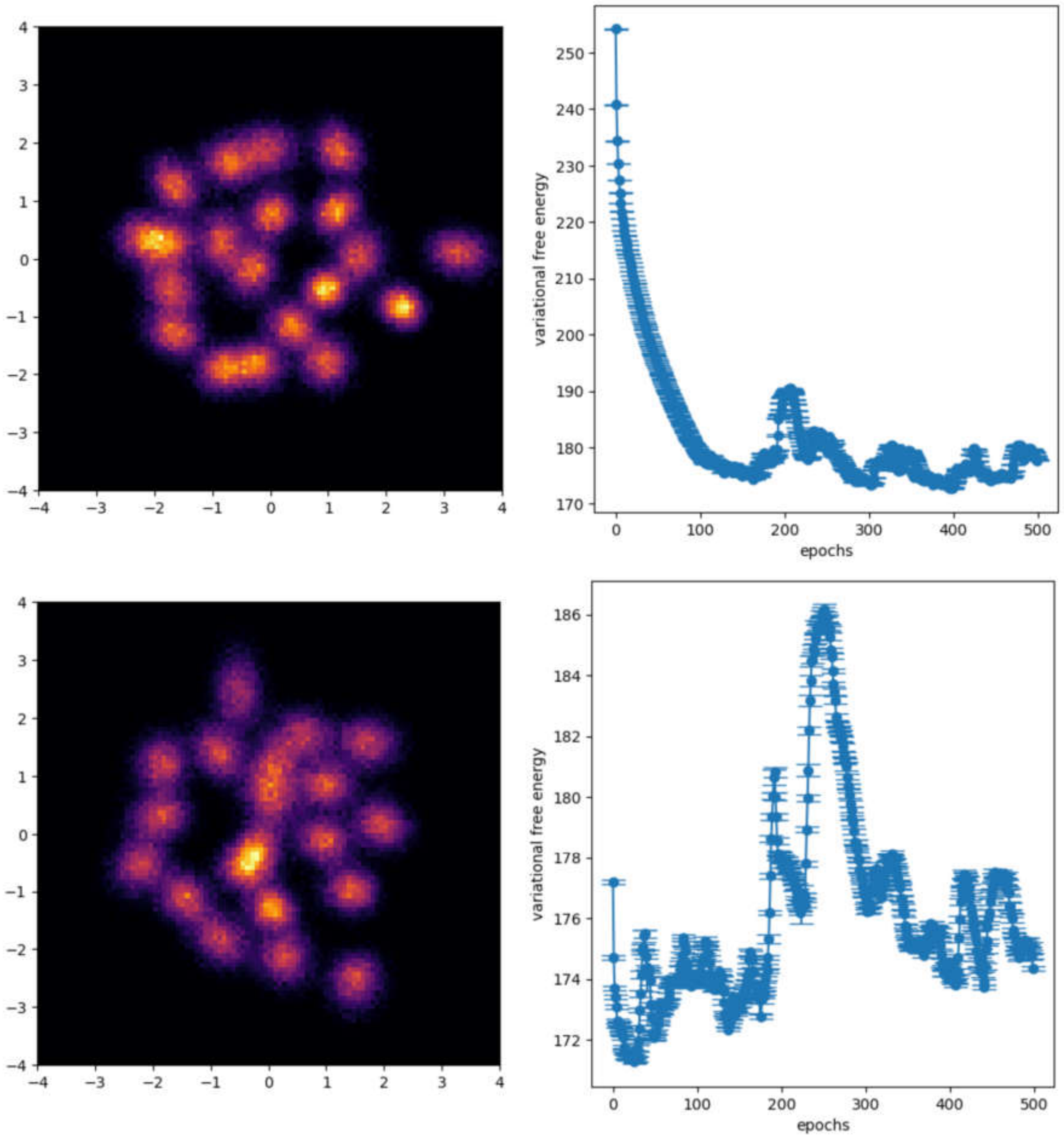


$F = 162.4838 \pm 0.0032$

$\langle E \rangle = 160.8027$

$n = 20, \beta = 1.5$

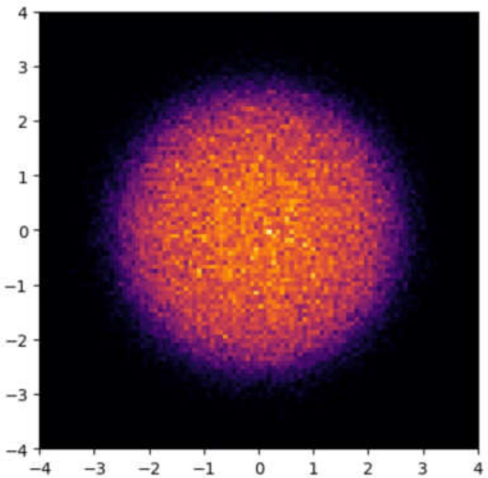
$[40, 64, 64, 40]$

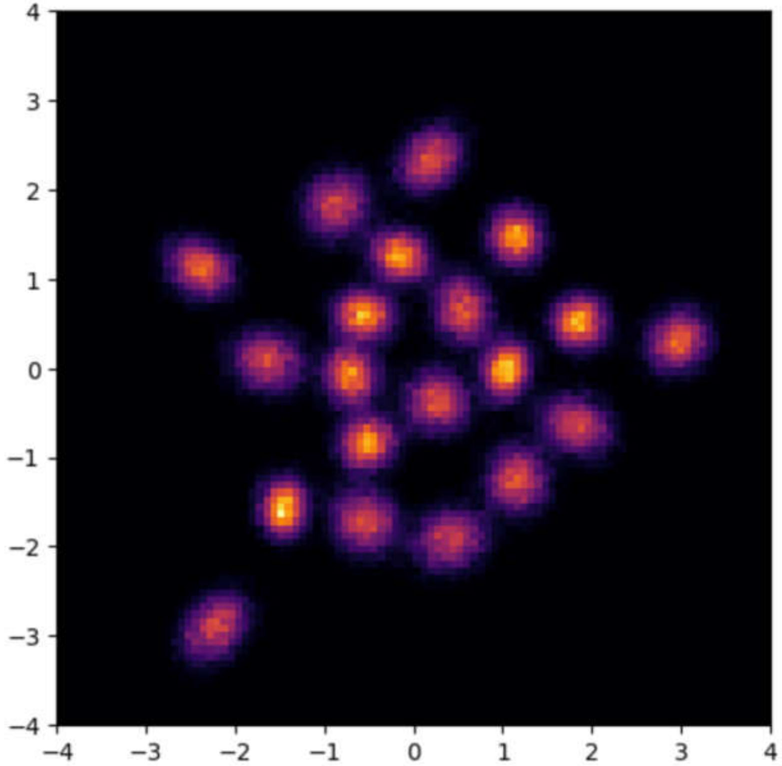


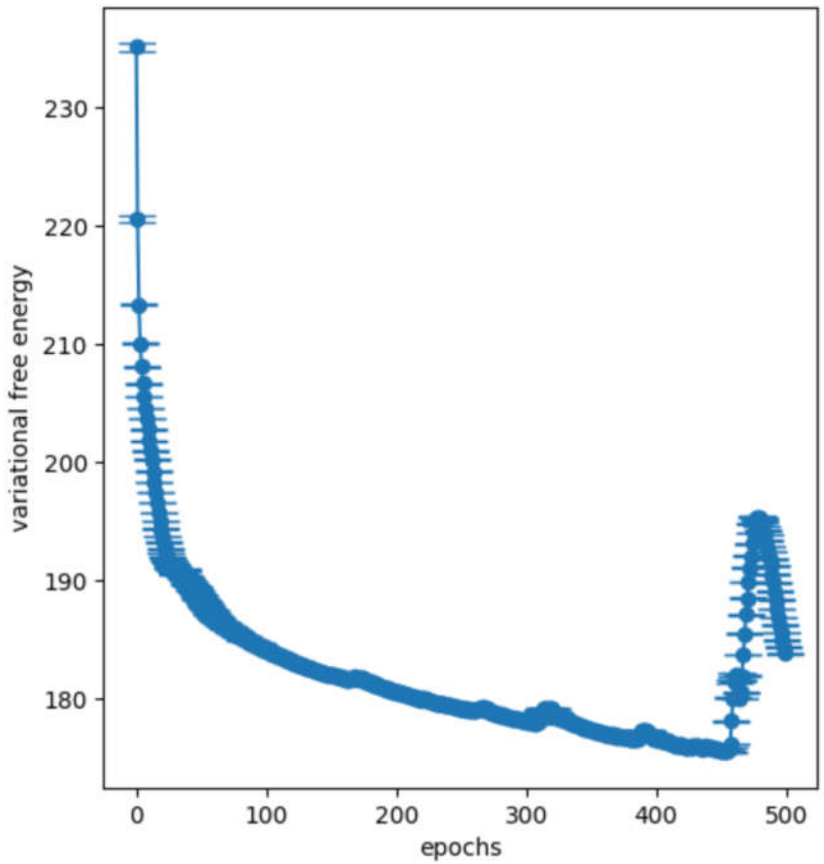
$n = 20, \beta = 1.5$

$[40, 128, 128, 40]$

MC

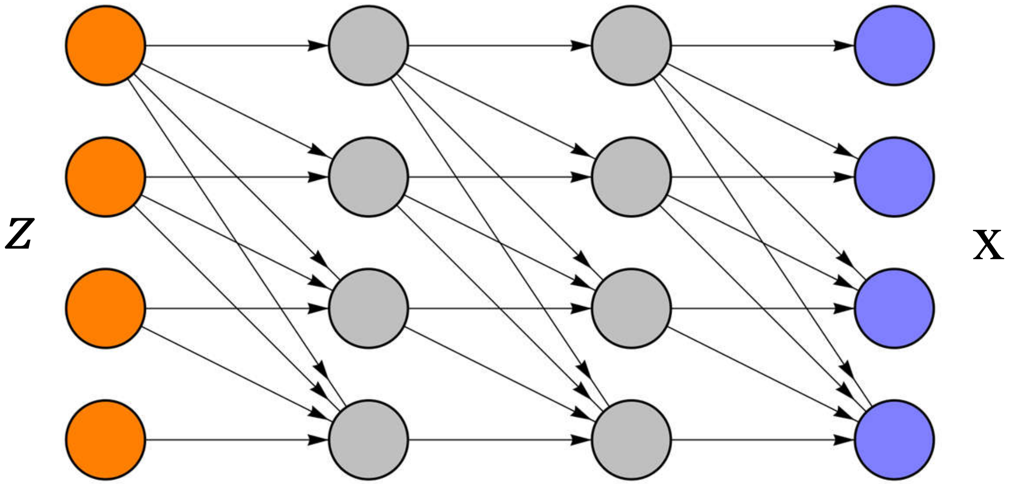




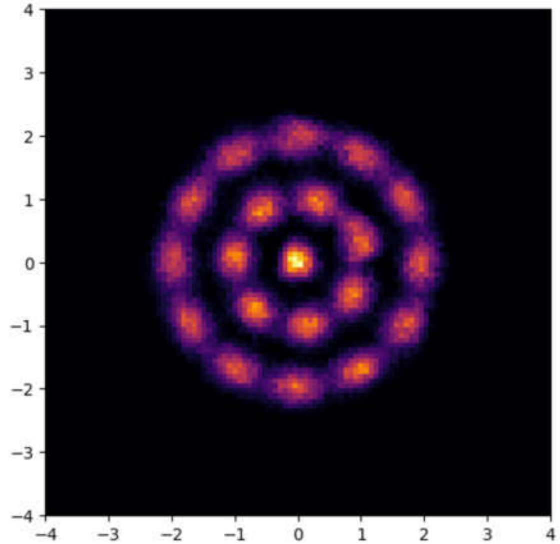


Network

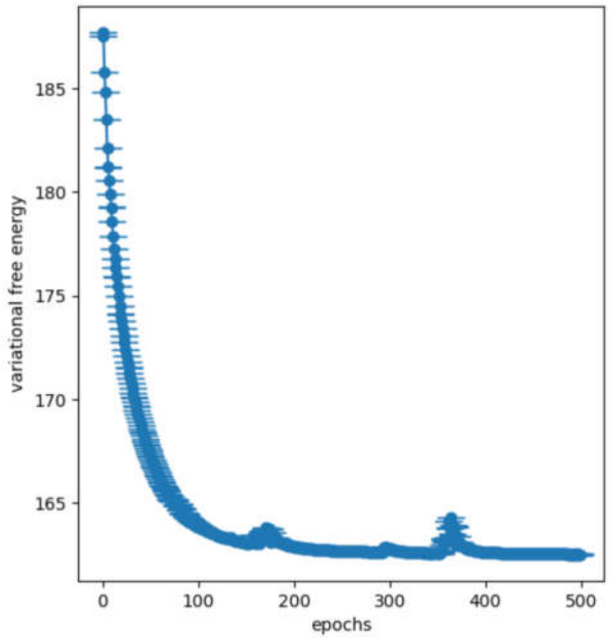
Autoregressive MLP



$[40, 40, 40, 40, 40]$



$n = 20, \beta = 10$

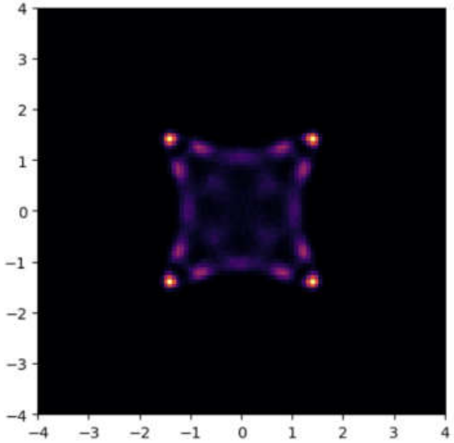


Steps: 200+500

Symmetry

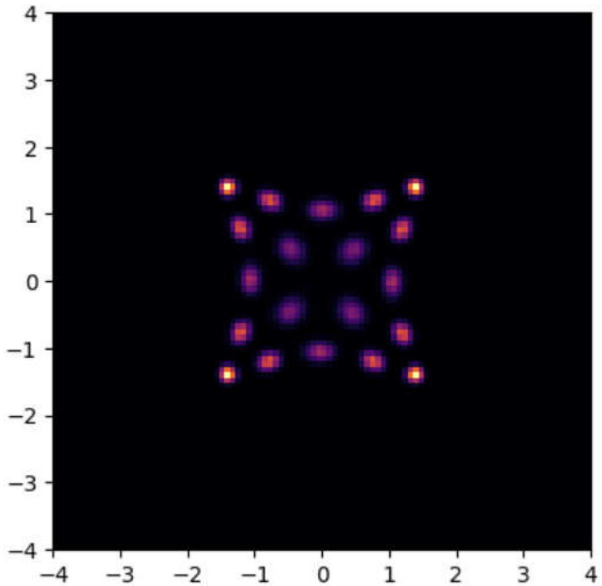
Potential: $V = x^4 + y^4 - x^2y^2$ C_4

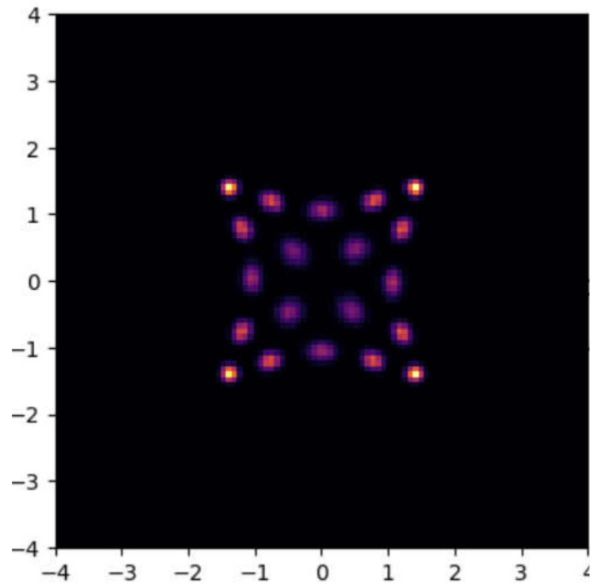
MC

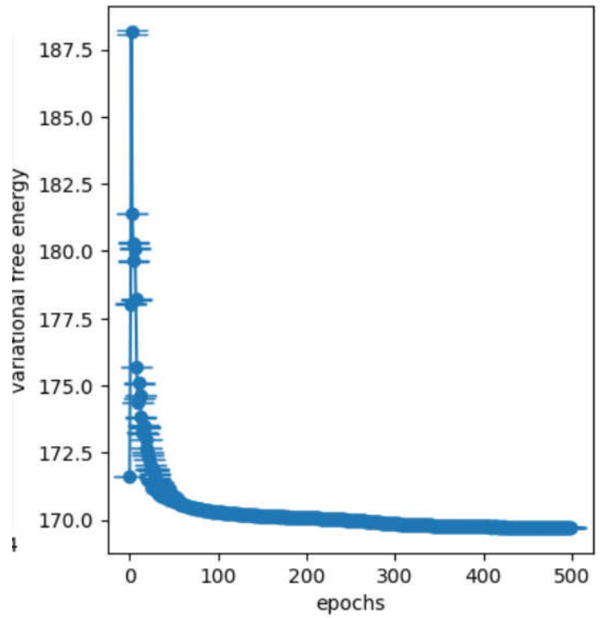


$$p_{\text{sym}}(\boldsymbol{x}) = \frac{1}{N_g}\sum_g p(g\boldsymbol{x})$$

$$\mathscr{L} - \mathscr{L}_{\text{sym}} = \int d\boldsymbol{x}\, p(\boldsymbol{x})\left[\ln p(\boldsymbol{x}) - \ln p_{\text{sym}}(\boldsymbol{x})\right] \geq 0$$







Symmetry

$$x = \sigma(Wz + b), p(x) = N(z)\left|\frac{\partial z}{\partial x}\right|$$

With $Gx = \sigma(WGz + b)$

$$[G, W] = 0, Gb = b$$

$G = P$

$G = R$

$$\boxed{\begin{gathered} W = I \otimes \lambda_{d\times d} + \left(11^T\right) \otimes \gamma_{d\times d} \\ b = I \otimes C_{d\times 1} \end{gathered}}$$

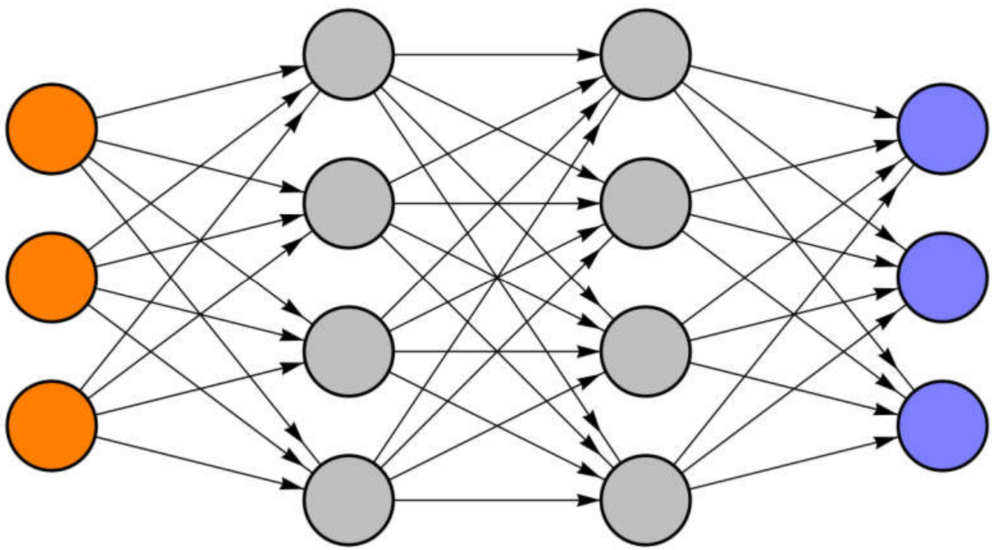
We will have $p(Sx) = p(x),\ while\ N(Sz) = N(z)$

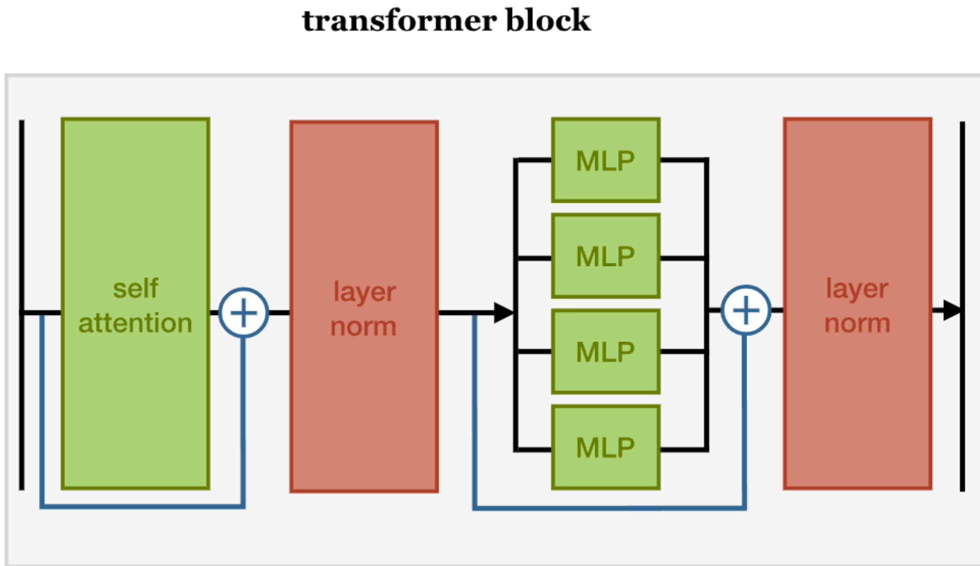
N particles, one layer has $d + 2d^2$ parameters

$$\boxed{\begin{gathered} W = \begin{pmatrix} w_{11} & \cdots & w_{1n} \\ \vdots & \ddots & \vdots \\ w_{n1} & \cdots & \cdots w_{nn} \end{pmatrix} \\ w_{ij} = \begin{pmatrix} a_{ij} & b_{ij} \\ -b_{ij} & a_{ij} \end{pmatrix} \\ b = 0 \end{gathered}}$$

Network

MLP + Transformer





Better behavior at high temperatures!

$$n = 20, \beta = 1.5$$