Quantum Dot Note

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June 2023

Introduction: difference

Classical

$$H = \sum_{i<j} \frac{1}{|x_i - x_j|} + \sum_i x_i^2.$$

$$\mathcal{L} = \mathbb{E}_{x\sim p(x)}\left[\frac{1}{\beta}\ln p(x) + H(x)\right] \geq -\frac{1}{\beta}\ln Z,$$

$$p(x) = p(z)\left|\frac{\partial z}{\partial x}\right|,$$

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

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

$$f(x) = \tfrac{1}{\beta}\ln p(x) + H(x).$$

Quantum

$$H = -\frac{1}{2}\nabla^2 + V(\boldsymbol{x})$$

$$F = \frac{1}{\beta}\mathrm{Tr}(\rho\ln\rho) + \mathrm{Tr}(\rho H)$$

$$q_n(\boldsymbol{x}) = p_n(f^{-1}(\boldsymbol{x}))\left|\det\left(\frac{\partial f^{-1}(\boldsymbol{x})}{\partial \boldsymbol{x}}\right)\right|$$

$$\nabla_{\boldsymbol{\phi}} F = \mathop{\mathbb{E}}_{n\sim\mu_n}\left[\left(\frac{1}{\beta}\ln\mu_n + \mathop{\mathbb{E}}_{\boldsymbol{x}\sim q_n(\boldsymbol{x})}\left[E_n^{\mathrm{loc}}(\boldsymbol{x})\right]\right)\nabla_{\boldsymbol{\phi}}\ln\mu_n\right],$$

$$\nabla_{\boldsymbol{\theta}} F = \mathop{\mathbb{E}}_{n\sim\mu_n}\mathop{\mathbb{E}}_{\boldsymbol{x}\sim q_n(\boldsymbol{x})}\left[E_n^{\mathrm{loc}}(\boldsymbol{x})\nabla_{\boldsymbol{\theta}}\ln q_n(\boldsymbol{x})\right].$$

Theory

- ✓ Hamiltonian:
  - ➢ Continuous space
  - ➢ d-dimensional
  - ➢ N fermions

$$H = -\frac{1}{2}\sum_{i}^{N}\nabla^2 + \sum_{i}^{N}\frac{1}{2}x_i^2 + \sum_{i<j}^{N}\frac{\kappa}{|x_i - x_j|}$$

$$E(x) = -\frac{1}{2}\sum_{i}^{N}\nabla^2$$

$$V(x) = \sum_{i}^{N}\frac{1}{2}x_i^2 + \sum_{i<j}^{N}\frac{\kappa}{|x_i - x_j|}$$

Theory

✓ Ground state of non-interacting system:

2D harmonic oscillator Hamiltonian:

$$H = -\frac{1}{2}\sum_i^N \nabla^2 + \sum_i^N \frac{1}{2}(x_i^2 + y_i^2)$$

Ground state

(1) 1D case, wave function:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\frac{1}{\pi^{1/4}}H_n(x)\exp(-\frac{x^2}{2})$$

Hermite polynomial $H_n(x)$ ("HermiteH" in Mathematica):

$$\begin{aligned}
H_0(x) &= 1\\
H_1(x) &= 2x\\
H_2(x) &= 4x^2 - 2\\
H_3(x) &= 8x^3 - 12x\\
H_4(x) &= 16x^4 - 28x^2 + 12\\
H_5(x) &= 32x^5 - 160x^3 + 120x\\
H_6(x) &= 64x^6 - 480x^4 + 720x^2 - 120\\
H_7(x) &= 128x^7 - 1344x^5 + 3360x^3 - 1680x
\end{aligned}$$

(2) 2D case

$$\begin{aligned}
\Psi_{n_x,n_y}(x,y) &= \psi_{n_x}(x)\psi_{n_y}(y)\\
&= \frac{1}{2^n n!\sqrt{\pi}}H_{n_x}(x)H_{n_y}(y)\exp\left(-\frac{x^2+y^2}{2}\right)
\end{aligned}$$

Theory

✓ Ground state of non-interacting system:

N points

The ground state can be described by Slater determinants $|\phi_j(x_i)|$.

Example:

$$\Psi(x) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \phi_0(x_0) & \phi_1(x_0) & \phi_2(x_0) & \phi_3(x_0) & \phi_4(x_0) & \phi_5(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \phi_2(x_1) & \phi_3(x_1) & \phi_4(x_1) & \phi_5(x_1) \\ \phi_0(x_2) & \phi_1(x_2) & \phi_2(x_2) & \phi_3(x_2) & \phi_4(x_2) & \phi_5(x_2) \\ \phi_0(x_3) & \phi_1(x_3) & \phi_2(x_3) & \phi_3(x_3) & \phi_4(x_3) & \phi_5(x_3) \\ \phi_0(x_4) & \phi_1(x_4) & \phi_2(x_4) & \phi_3(x_4) & \phi_4(x_4) & \phi_5(x_4) \\ \phi_0(x_5) & \phi_1(x_5) & \phi_2(x_5) & \phi_3(x_5) & \phi_4(x_5) & \phi_5(x_5) \end{vmatrix}$$

Probability:

$$\log(p(z)) = \log(|\Psi(z)|^2) = 2\log(|\Psi(z)|)$$

$$f = -\log|\Phi(x)|^2$$

Theory

✓ Model：

$$x_i^{l+1} = x_i^l + \sum_{i \neq j} \eta(|x_i^l - x_j^l|)(x_i^l - x_j^l)$$

$$p(x) = p(z) \left| \frac{\partial z}{\partial x} \right|,$$

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

$$\ln p(x) = \ln p(z) + \ln \left| \frac{\partial z}{\partial x} \right|$$

Results: Xiehao’s Work

Journal of Machine Learning

ISSN: 2790-2048(e), 2790-203X(p)

Ab-initio Study of Interacting Fermions at Finite Temperature with Neural Canonical Transformation

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Abstract. We present a variational density matrix approach to the thermal properties of interacting fermions in the continuum. The variational density matrix is parametrized by a permutation equivariant many-body unitary transformation together with a discrete probabilistic model. The unitary transformation is implemented as a quantum counterpart of neural canonical transformation, which incorporates correlation effects via a flow of fermion coordinates. As the first application, we study electrons in a two-dimensional quantum dot with an interaction-induced crossover from Fermi liquid to Wigner molecule. The present approach provides accurate results in the low-temperature regime, where conventional quantum Monte Carlo methods face severe difficulties due to the fermion sign problem. The approach is general and flexible for further extensions, thus holds the promise to deliver new physical results on strongly correlated fermions in the context of ultracold quantum gases, condensed matter, and warm dense matter physics.

Keywords:
Interacting fermions,
Thermodynamics,
Variational free energy,
Normalizing flows.

Article Info.:
Volume: 1
Number: 1
Pages: 38- 59
Date: March/2022
doi.org/10.4208/jml.220113

Article History:
Received: 22/11/2021
Accepted: 19/3/2022

Communicated by:
Weinan E

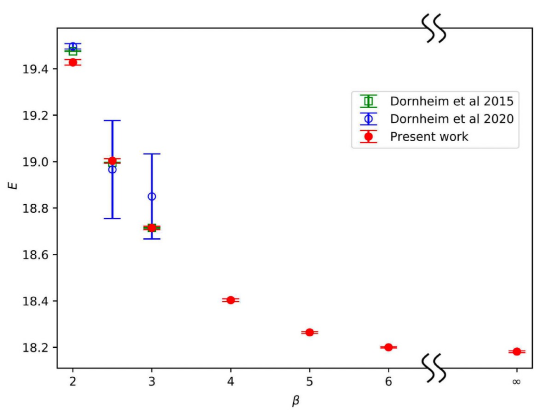

Figure 4.1: Energy E versus inverse temperature β for 6 spin-polarized electrons in a two-dimensional quantum dot with $\kappa = 0.5$. The green and blue points are benchmark data from two different variants of PIMC [68, 69], while the red points are results of the present approach, including the zero-temperature limit.

B Some more benchmark data for 2D quantum dot

The following table summarizes our results for the energy of a two-dimensional quantum dot at $\beta = 10$, for various electron number N and interaction strength κ. PIMC results from [74] are also listed when available. All data correspond to the fully spin-polarized case. Our finite-temperature calculations indicate that the entropy is negligible for a temperature as low as $\beta = 10$, so our energy results can be treated as variational. We anticipate these results (as well as those presented in the main text) can be further improved by adopting better model architecture and optimization schemes. We also note the results reported in Figure 4.8 of [83] for $\beta = 10$, $N = 3$, $\kappa = 2$ show that the data in [74] may be subject to slight systematic errors.

N	κ	This work	[74]
3	2	8.331(3)	8.37(1)
3	4	11.070(4)	11.05(1)
3	6	13.495(6)	13.43(1)
3	8	15.653(7)	15.59(1)
4	2	14.336(4)	14.30(5)
4	4	19.517(7)	19.42(1)
4	6	24.060(9)	23.790(12)
4	8	28.178(12)	27.823(11)
6	0.5	18.179(4)	–
6	1	22.003(6)	–
6	1.5	25.600(8)	–
6	2	28.994(9)	–
6	3	35.241(10)	–
6	4	41.012(11)	–
6	5	46.385(13)	–
6	6	51.448(13)	–
6	7	56.270(16)	–
6	8	60.837(15)	60.42(2)

Some results: T=0

Shape: [8192, 6, 2]
Hidden: [2, 32]
Params: 194

$\beta = 10$

N	κ	This work	[74]
3	2	8.331(3)	8.37(1)
3	4	11.070(4)	11.05(1)
3	6	13.495(6)	13.43(1)
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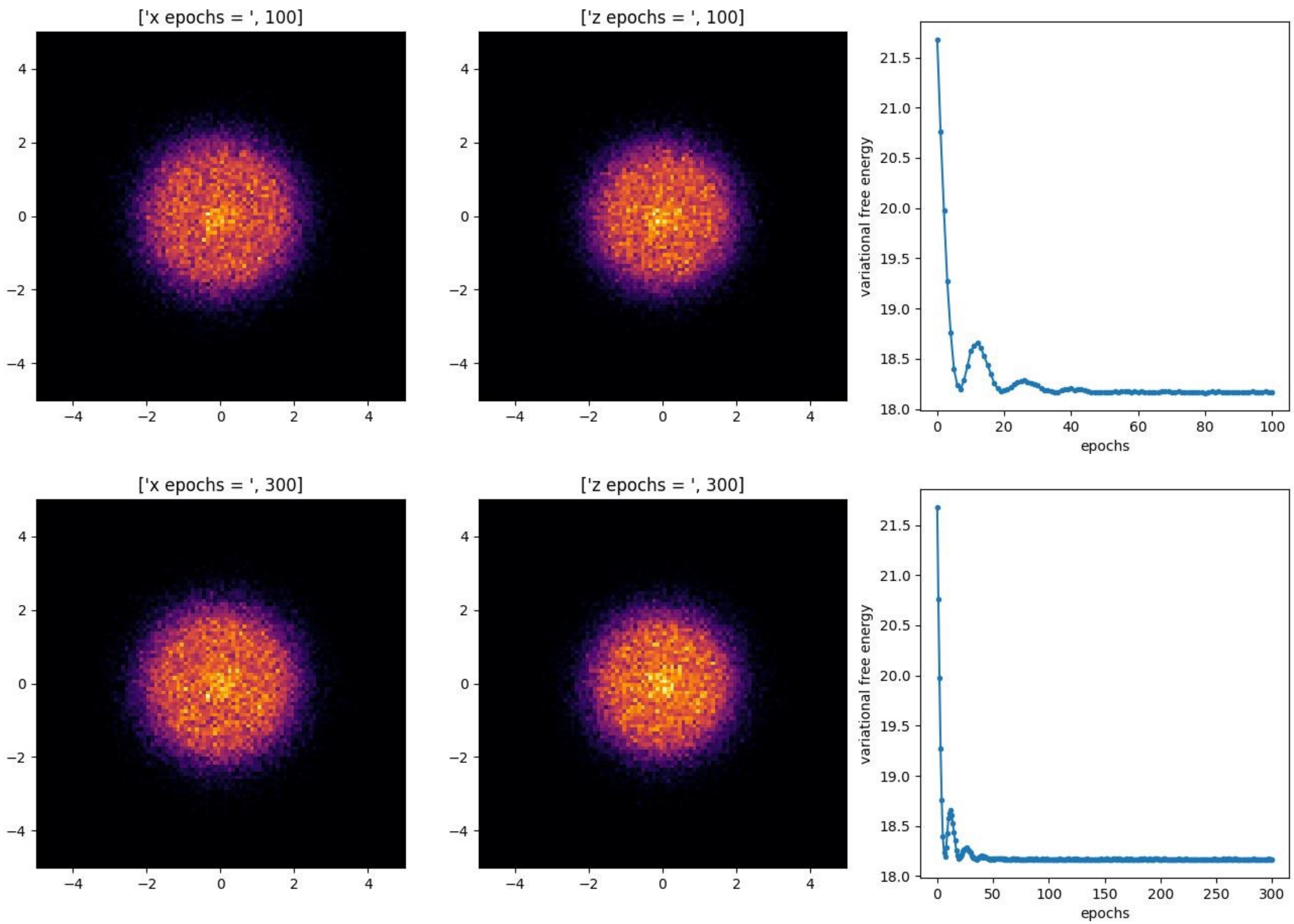
6	6	51.448(13)	–
6	7	56.270(16)	–
6	8	60.837(15)	60.42(2)

N	k	Epoch = 100	Epoch = 300
3	2.0		8.354 ± 0.005
3	4.0		
3	6.0		
3	8.0		
6	0	14.000 ± 0.000	14.000 ± 0.000
6	0.5	18.167 ± 0.004	18.162 ± 0.004
6	1.0	22.030 ± 0.007	22.022 ± 0.006
6	1.5	25.655 ± 0.010	25.628 ± 0.009
6	2.0	29.069 ± 0.012	29.040 ± 0.011
6	3.0		
6	4.0		
6	5.0		
6	6.0		
6	7.0		
6	8.0	63.267 ± 0.057	61.382 ± 0.030

Some results: T=0

Shape: [8192, 6, 2]
Kappa: 0.5
Hidden: [2, 32]
Params: 194

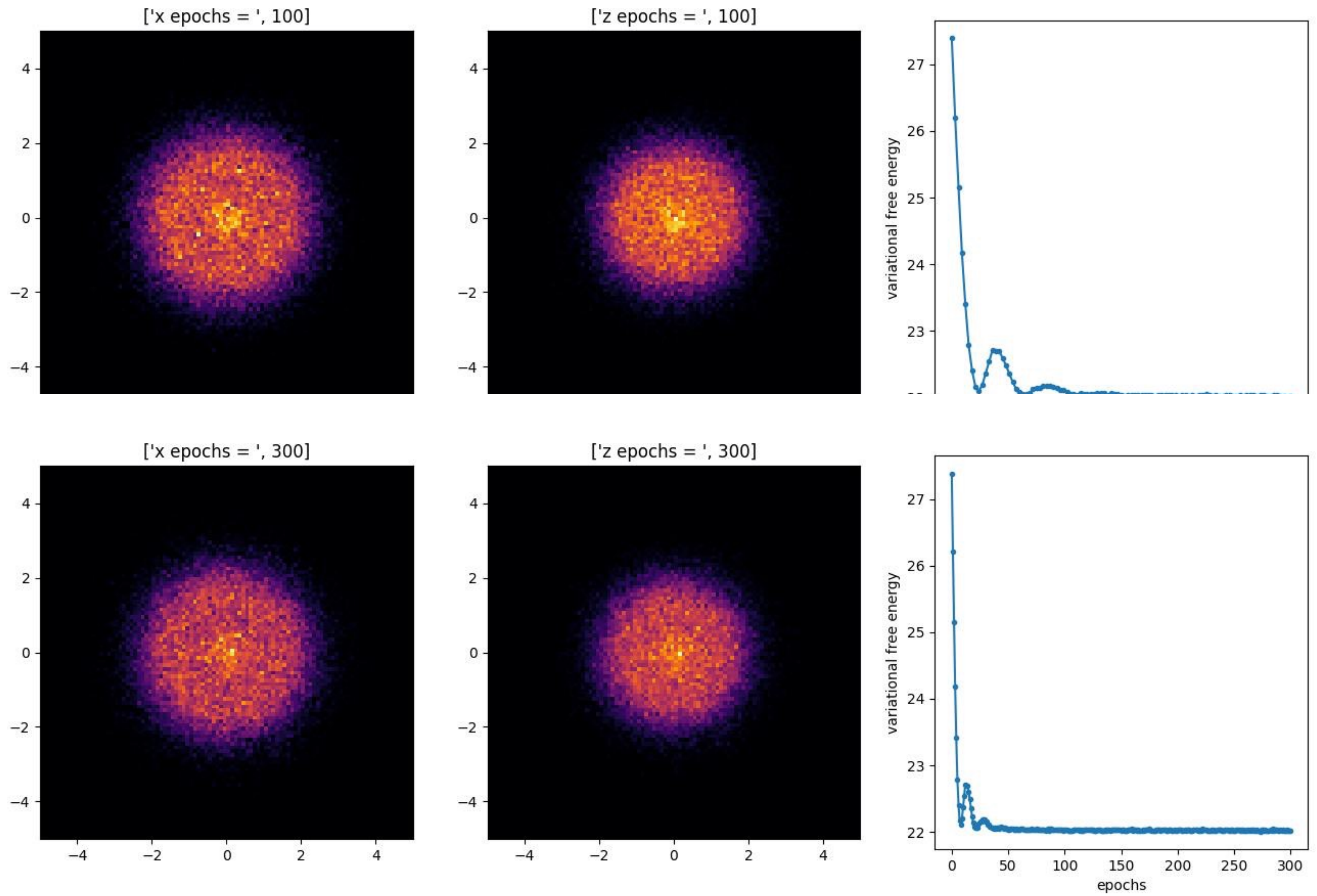
100 . E = 18.167 , err = 0.004 , Ek = 6.075 , Ep = 12.092
300 . E = 18.162 , err = 0.004 , Ek = 6.049 , Ep = 12.113



Some results: T=0

Shape: [8192, 6, 2]
Kappa: 1.0
Hidden: [2, 32]
Params: 194

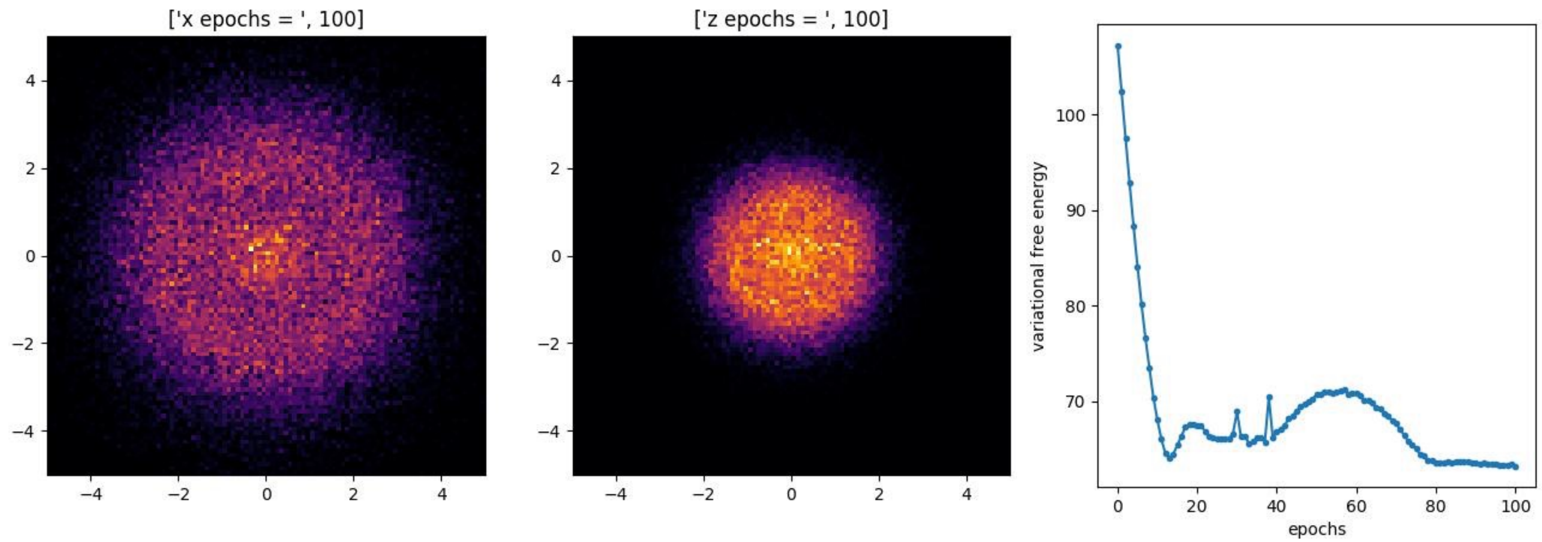
100 . E = 22.030 , err = 0.007 , Ek = 5.380 , Ep = 16.650
300 . E = 22.022 , err = 0.006 , Ek = 5.423 , Ep = 16.599

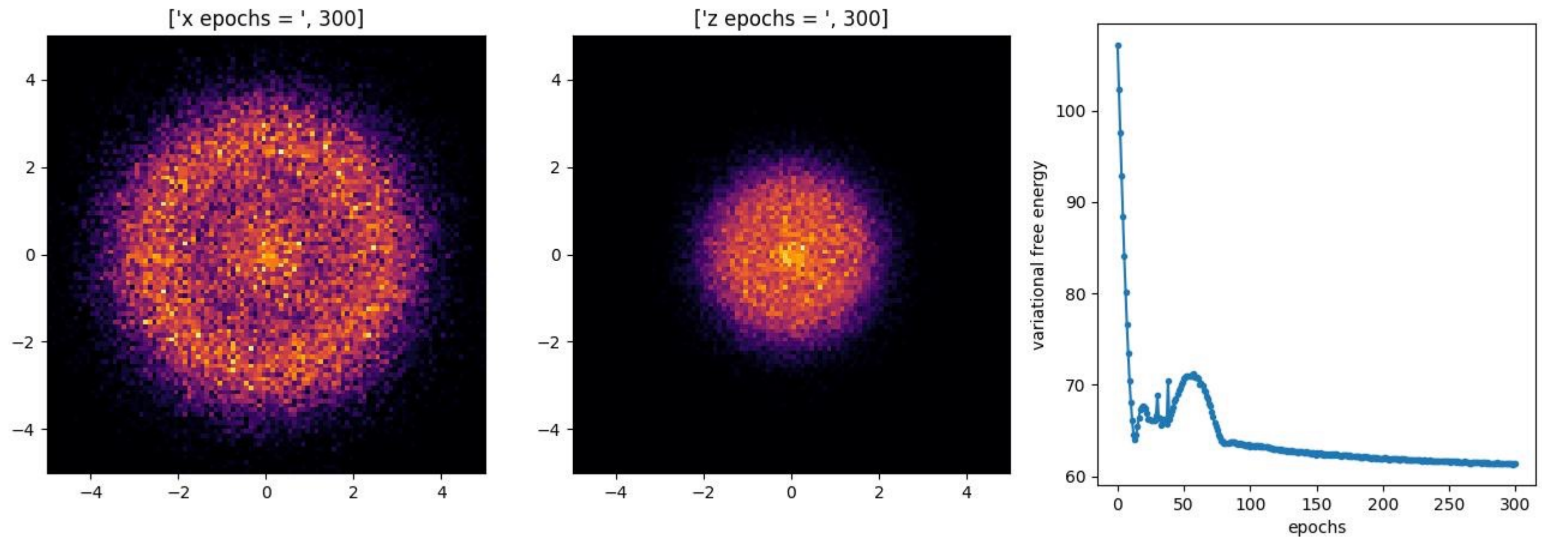


Some results: T=0

Shape: [8192, 6, 2]
Kappa: 8.0
Hidden: [2, 32]
Params: 194

100. E = 63.267 , err = 0.057 , Ek = 2.562 , Ep = 60.705
300. E = 61.382 , err = 0.030 , Ek = 2.720 , Ep = 58.662





Some results: T=0

Shape: [8192, 6, 2]
Hidden: [4, 64]
Params: 772

$\beta = 10$

N	κ	This work	[74]
3	2	8.331(3)	8.37(1)
3	4	11.070(4)	11.05(1)
3	6	13.495(6)	13.43(1)
3	8	15.653(7)	15.59(1)
4	2	14.336(4)	14.30(5)
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6	5	46.385(13)	–
6	6	51.448(13)	–
6	7	56.270(16)	–
6	8	60.837(15)	60.42(2)

N	k	Epoch = 100	Epoch = 300	Epoch = 1000
3	2.0	8.354+-0.006	8.356+-0.006	
3	4.0			
3	6.0			
3	8.0			
6	0			
6	0.5	18.165+-0.004	18.167+-0.004	
6	1.0	22.032+-0.007	22.026+-0.007	
6	1.5			
6	2.0			
6	3.0			
6	4.0	41.254+-0.020	41.227+-0.018	
6	5.0			
6	6.0			
6	7.0			
6	8.0			