Machine learning quantum mechanics of materials.

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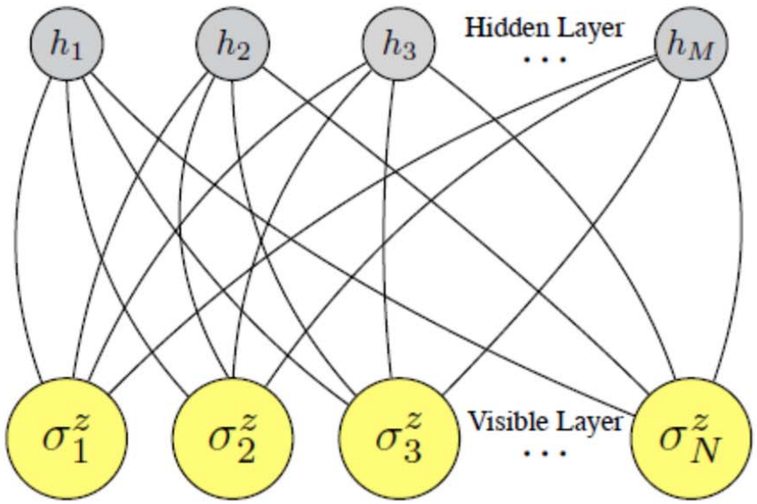
Classification

Expressive power

Wave function by Restricted Boltzmann Machine



G. Carleo and M. Troyer, Science **355,** 602 (2017)

No intra-layer Ising coupling:
bipartite Ising model with local field

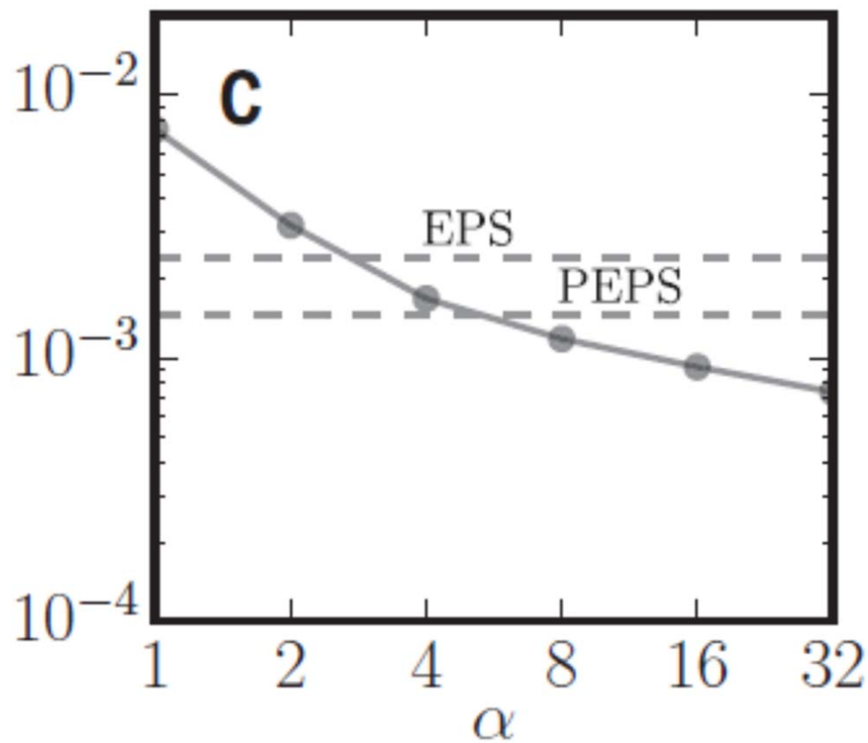
$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z},$$

$$E(\mathcal{W}) = \langle \Psi_M | \mathcal{H} | \Psi_M \rangle / \langle \Psi_M | \Psi_M \rangle$$

$$R(\dot{\mathcal{W}}(t)) = \mathrm{dist}(\partial_t \Psi, -i\mathcal{H}\Psi)$$

Wave function by Restricted Boltzmann Machine

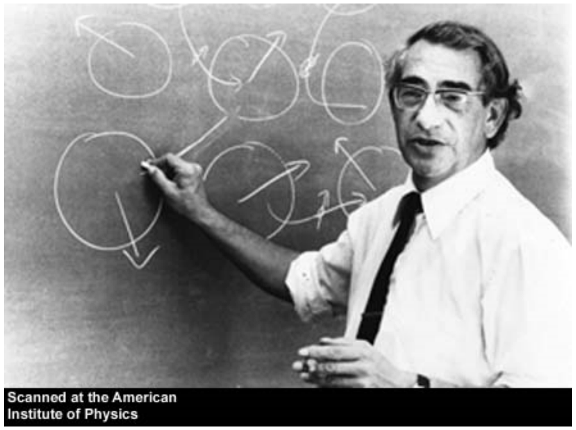
- More compact representation of many-body states
- 1000 fewer variational parameters than MPS for example.



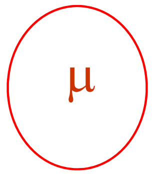
Tensor networks vs RBM: Chen et al. PRB **97**, 085104 (2018)

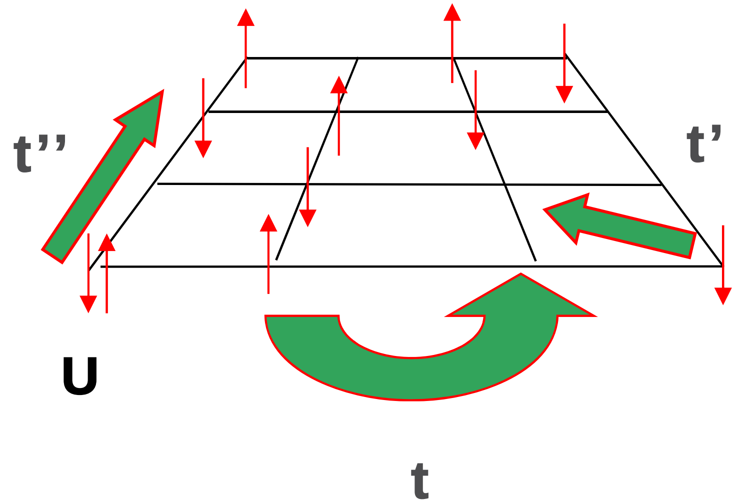
Policy (recommander)

Hubbard model



1931-1980

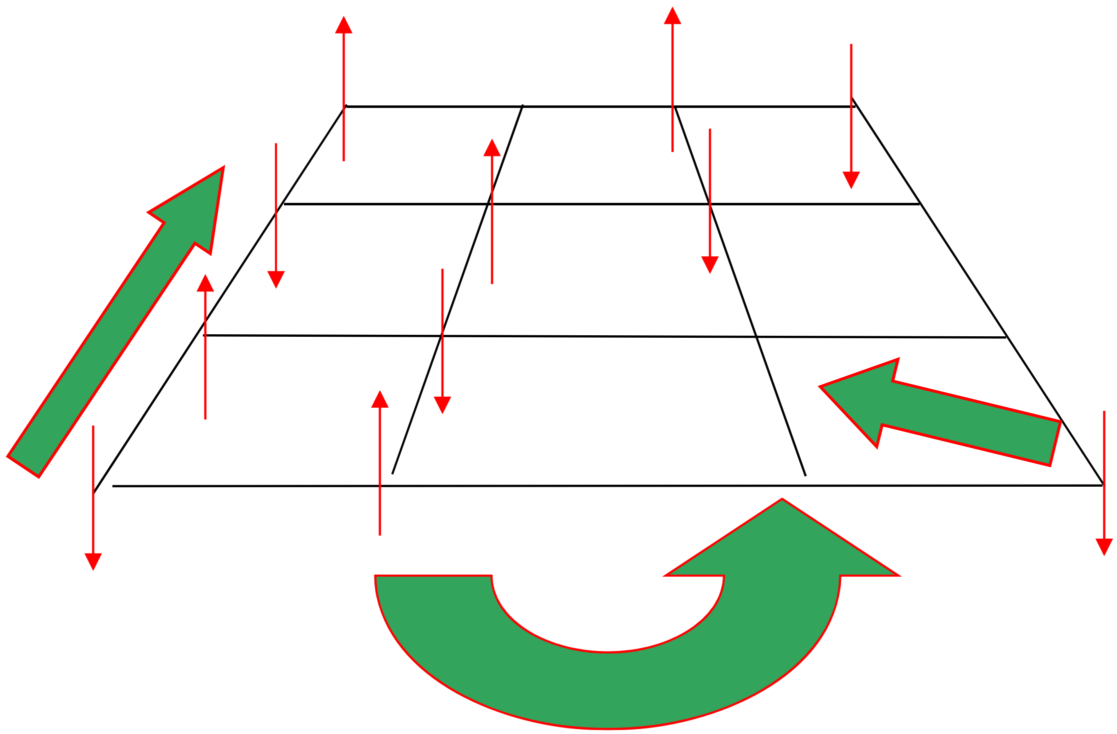




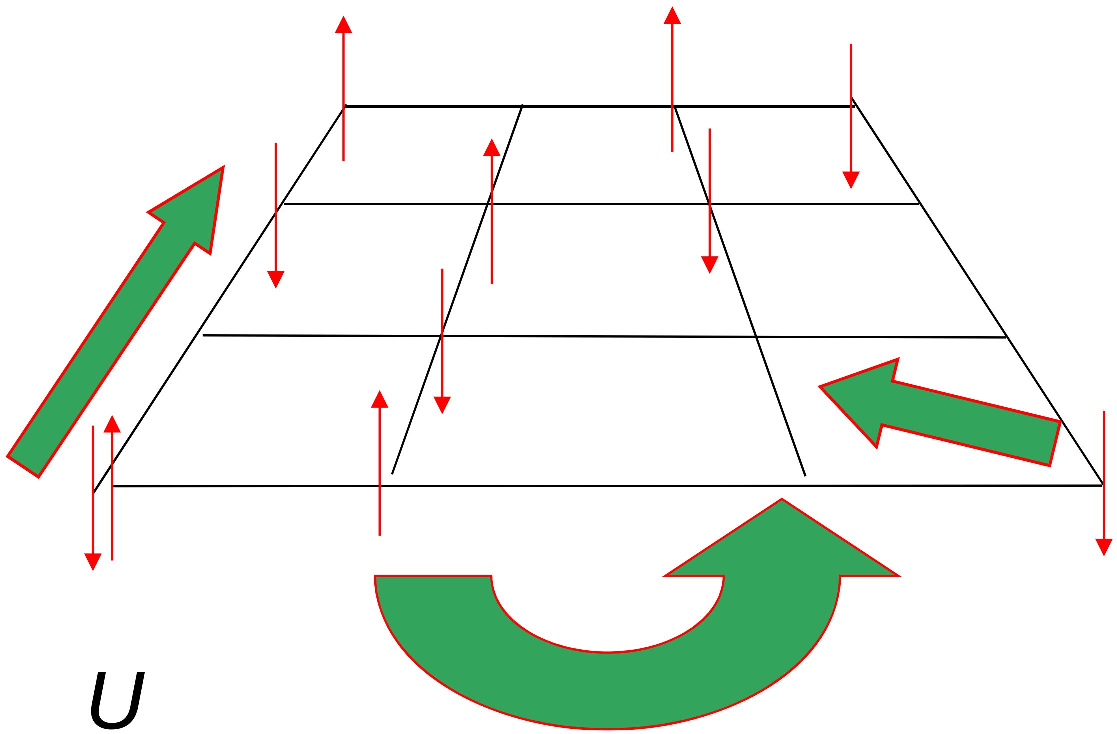
$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}\right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

4^N states

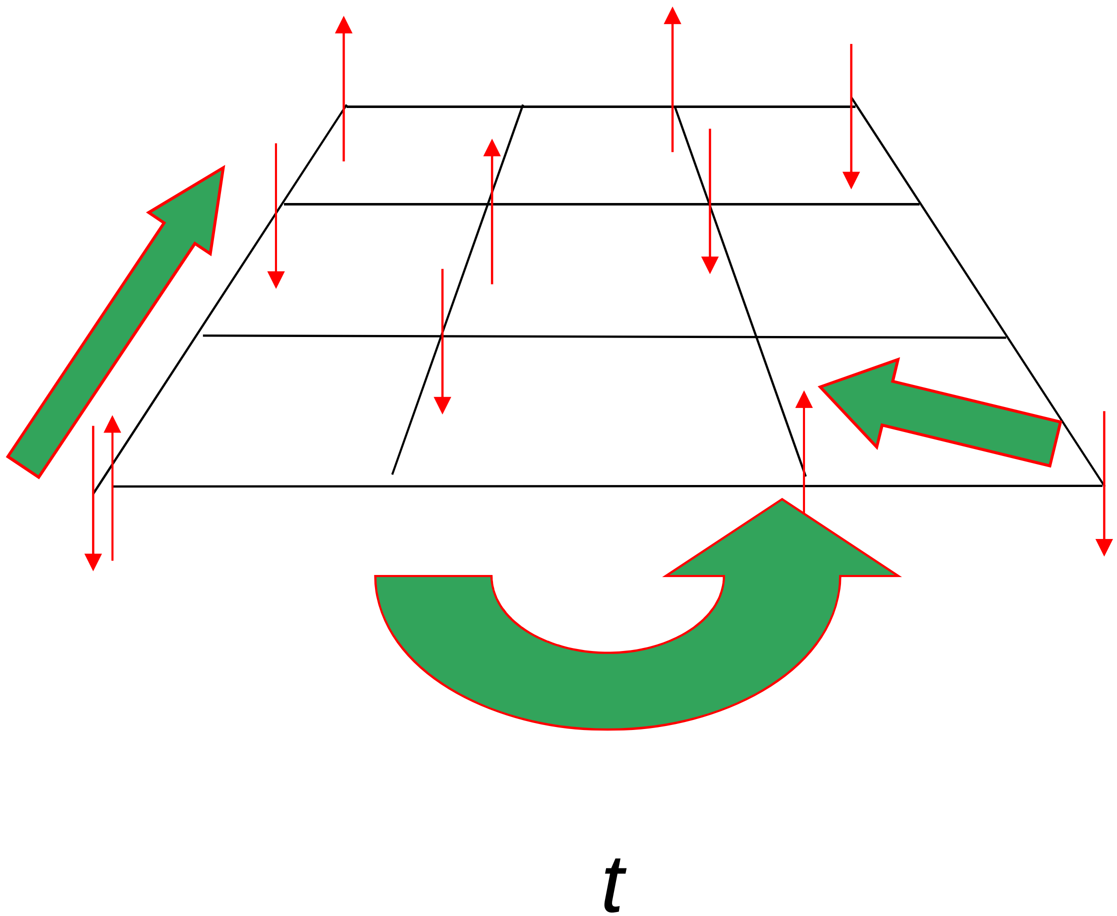
What is inside?



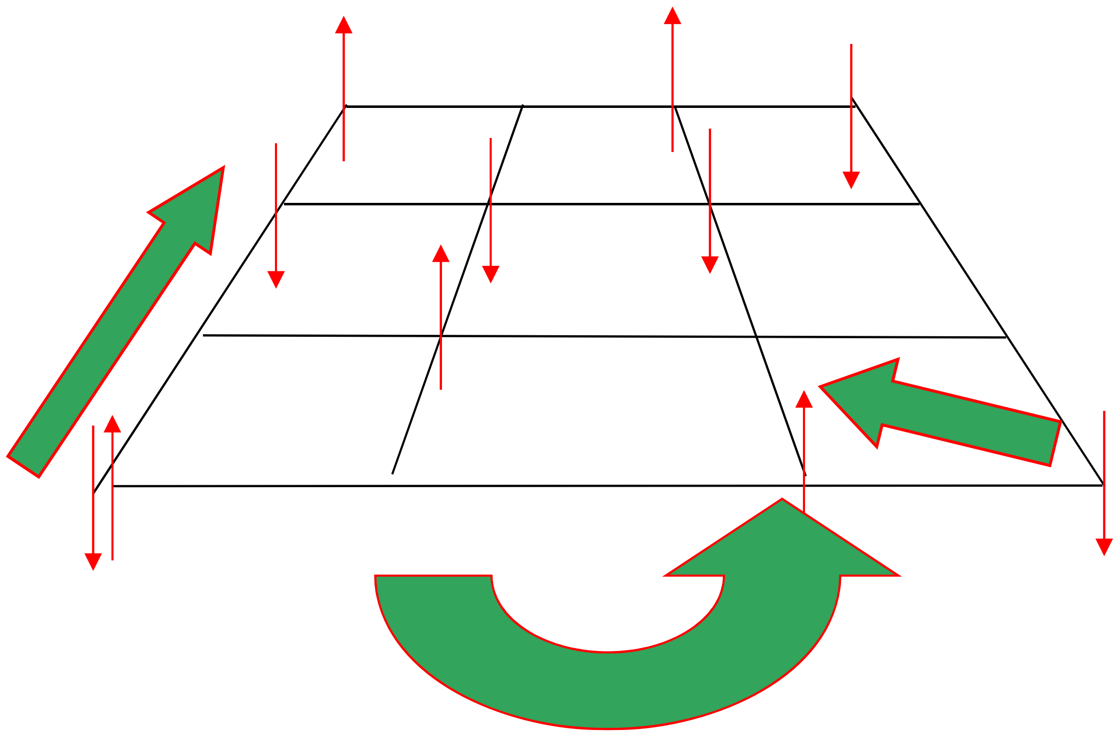
What is inside?



What is inside?



What is inside?



Minus sign

Importance of this « class » of models

- Ferromagnetism
- High-temperature superconductivity
- Improvements to density functional theory for realistic materials simulations:
  - Magnetocaloric materials
  - Quantum chemistry
  - Drug design
  - Oxygen absorption by hemoglobin …

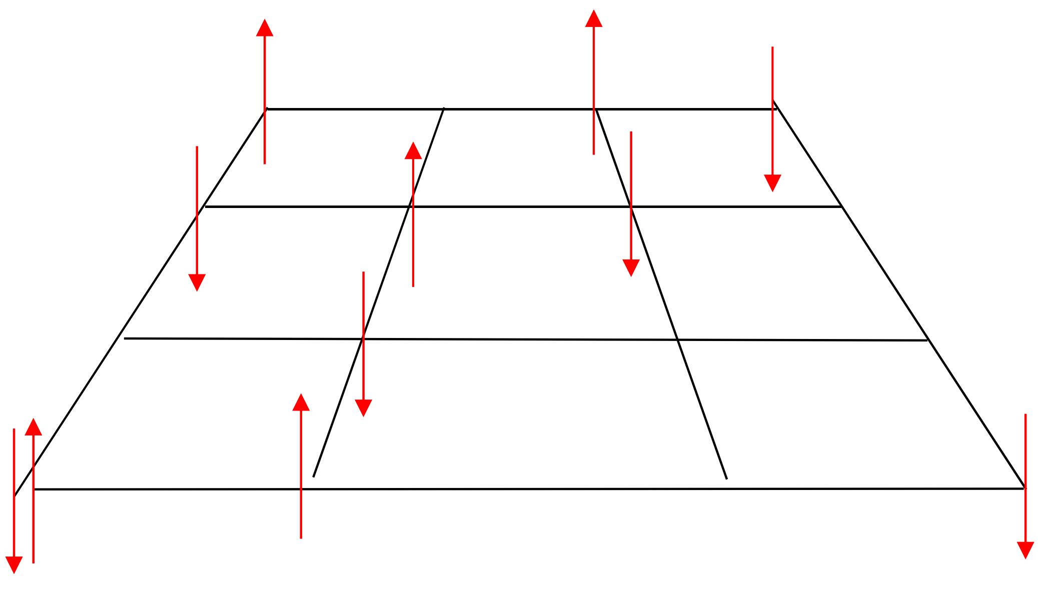
Quantum Monte Carlo

- Metropolis-Hastings Algorithm for Markov Chains

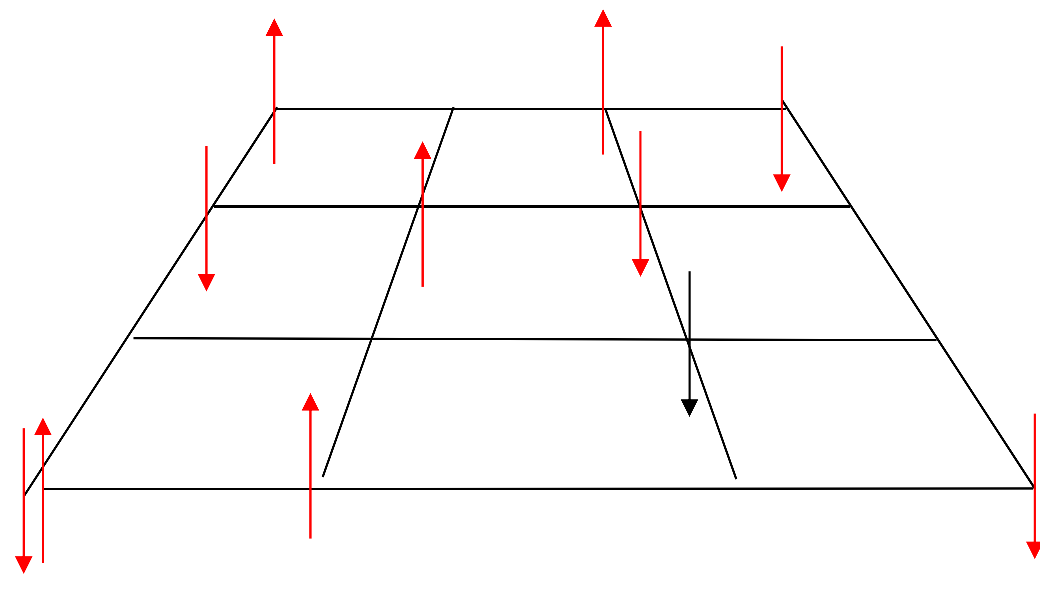
$$P(C)\,W(C\to D) = P(D)\,W(D\to C)$$

$$W(C\to D) = \min\left[1, \frac{P(D)}{P(C)}\right]$$

Problems
- *P(C)/P(D)*
- correlations
- ergodicity



C



D

Quantum Monte Carlo

$$P(C)\,W(C \to D) = P(D)\,W(D \to C)$$

$$W(C \to D) = W_{proposal}(C \to D)\,W_{accept}(C \to D)$$

$$W(C \to D) = \min\left[1, \frac{P(D)}{P(C)}\right]$$

$$W(C \to D) = \min\left[1, \frac{P(D)\,W_{proposal}(D \to C)}{P(C)\,W_{proposal}(C \to D)}\right]$$

Self-learning Quantum Monte Carlo

$$W\left(C \to D\right) = \min\left[1, \frac{P\left(D\right) W_{proposal}\left(D \to C\right)}{P\left(C\right) W_{proposal}\left(C \to D\right)}\right]$$

$$W_{proposal}\left(D \to C\right) = P_{learned}\left(C\right)$$

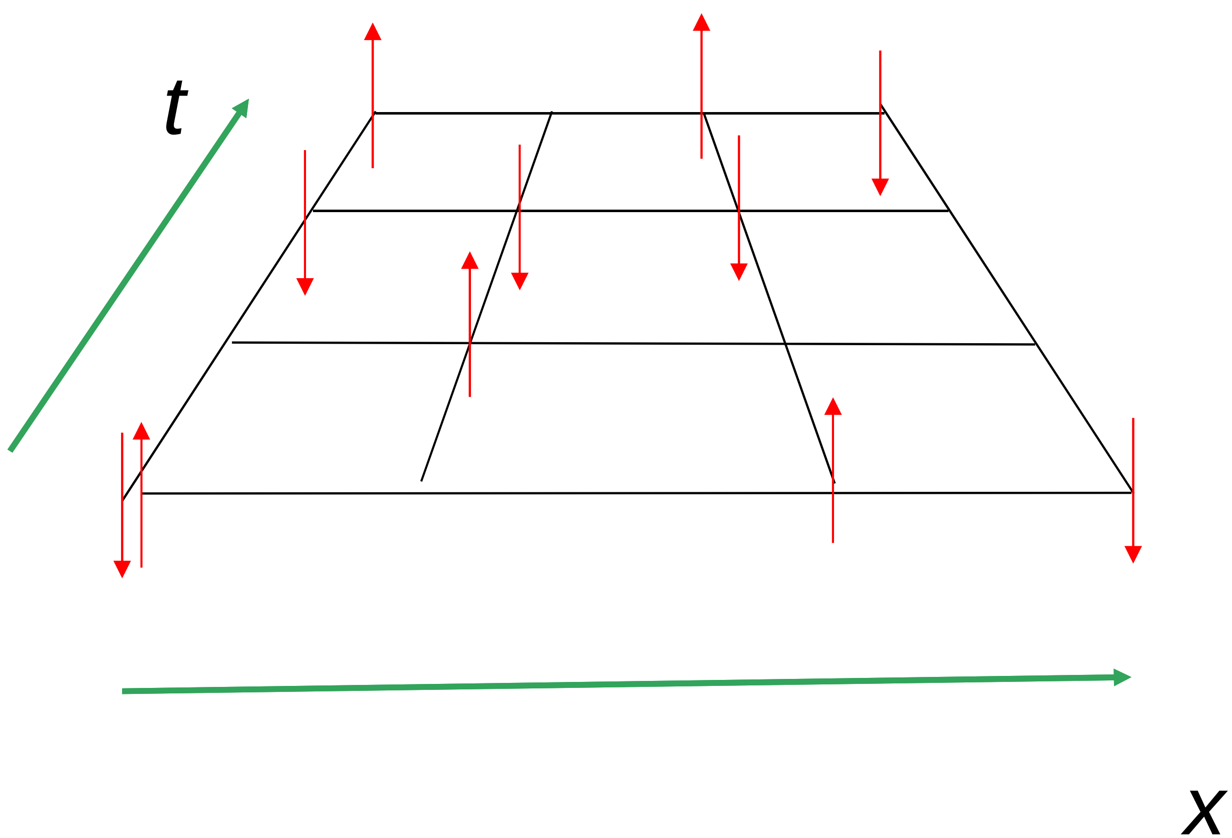
$$W\left(C \to D\right) = \min\left[1, \frac{P\left(D\right) P_{learned}\left(C\right)}{P\left(C\right) P_{learned}\left(D\right)}\right]$$

Solves some problems

- *High acceptance rate*
- *$P_{learned}(C)/P_{learned}(D)$ easy*
- *« Global moves » -- decorrelation, ergodicity*

Self-Learning Quantum Monte-Carlo

- Determinant quantum Monte Carlo
  - Learn configurations of fields (1,-1) on a discrete space-time lattice.



Self-learning Quantum Monte-Carlo

$$P_{learned}(C) = \exp[-\beta\ H^{eff}(C)]$$

$$H^{\text{eff}} = E_0 + \sum_{(i\tau);(j,\tau')} J_{i,\tau;j\tau'} s_{i,\tau} s_{j,\tau'} + \cdots\ ,$$

X.Y. Xu et al. PHYSICAL REVIEW B **96**, 041119(R) (2017)

Self-learning continuous time quantum Monte Carlo (CTQMC)

- Auxiliary field CTQMC
  - Learn likelihood of configurations of fields (1,-1) on *discrete spacial lattice* and *continuous-time* label for arbitrary order in perturbation theory

$$\frac{Z}{Z_0} = \mathrm{Tr}\left[e^{-\beta H_0} T_\tau e^{-\int_0^\beta d\tau H_1(\tau)}\right]$$

$$Z_n(\{s_i,\tau_i\})/Z_0 \simeq e^{-\beta H_n^{\mathrm{eff}}(\{s_i,\tau_i\})}, \tag{7}$$

$$-\beta H_n^{\mathrm{eff}}(\{s_i,\tau_i\}) \equiv \frac{1}{n}\sum_{i,j} J(\tau_i-\tau_j)s_i s_j + \frac{1}{n}\sum_{i,j} L(\tau_i-\tau_j) + f(n). \tag{8}$$

Y. Nagai et al. PHYSICAL REVIEW B **96**, 161102(R) (2017)

Also

- Regression with constraint: inversion of Fredholm integrals of the first kind

$$G(\tau) = -\int \mathrm{d}\omega \frac{e^{-\omega\tau}}{1 + e^{-\hbar\omega/k_B T}} A(\omega)$$

L.-F. Arsenault https://arxiv.org/abs/1506.08858v1

Questions

- Would deep-learning or other method improve the accuracy of the learned probability?
- Is there a way to improve the choice of basis states? (« minus sign problem »)
- Can RBM be generalized to « dynamical mean field » (Green's functions)?

A useful reference for AI-Physics http://wangleiphy.github.io/lectures/DL.pdf

Merci

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