Title: Bridging physical intuition and neural networks for variational wave-functions

Speakers: Agnes Valenti

Series: Machine Learning Initiative

Date: October 14, 2022 - 3:00 PM

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Abstract: Variational methods have proven to be excellent tools to approximate the ground states of complex many-body Hamiltonians. Generic tools such as neural networks are extremely powerful, but their parameters are not necessarily physically motivated. Thus, an efficient parametrization of the wave function can become challenging. In this talk I will introduce a neural-network-based variational ansatz that retains the flexibility of these generic methods while allowing for a tunability with respect to the relevant correlations governing the physics of the system. I will illustrate the ansatz on a model exhibiting topological phase transitions: The toric code in the presence of magnetic fields. Additionally, I will talk about the use of variational wave functions to gain physical insights beyond lattice models, in particular for the real use-case of two-dimensional materials.

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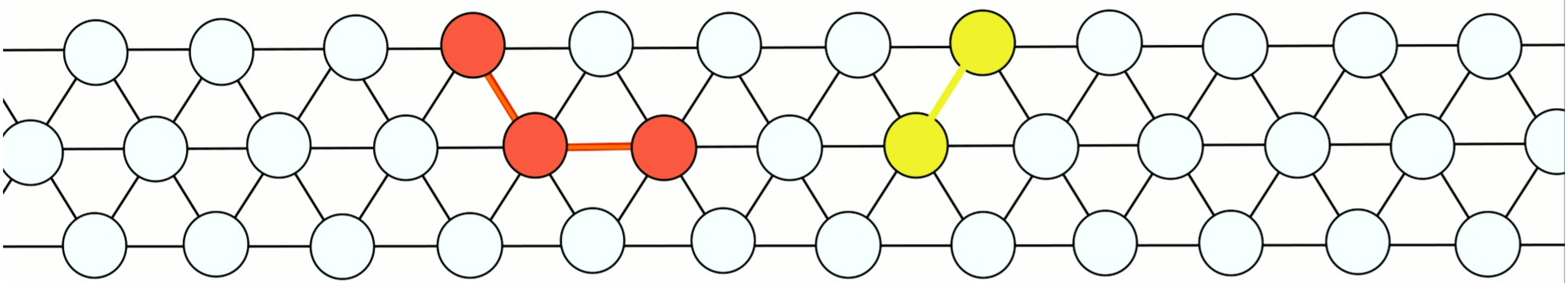
Bridging physical intuition and neural networks for variational wave-functions

Agnes Valenti



AV, E Greplova, NH Lindner, SD Huber, PRR 4 (2022)

Collaborators

Eliška Greplová
TU Delft

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Technion, Haifa

Erez Berg
Weizmann Institute

Sebastian Huber
ETH Zurich

Part I: Variational wave-functions: Neural Networks and physical intuition

Part II: Variational wave-functions: Physical insights beyond lattice models

AV, E Greplova, NH Lindner, SD Huber, PRR 4 (2022)

The quantum many-body problem

Schroedinger's equation

$$\frac{d}{dt}|\Psi(t)\rangle = -iH|\Psi(t)\rangle$$

$$H|\Psi\rangle = E|\Psi\rangle$$

$$H \longrightarrow \Psi$$

The quantum many-body problem

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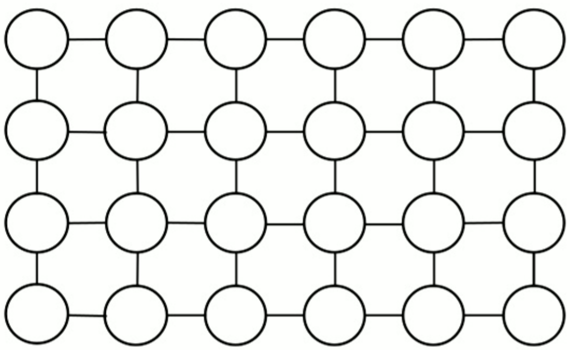
$$H \longrightarrow \Psi$$

N spins

Hilbert space dimension: 2^N



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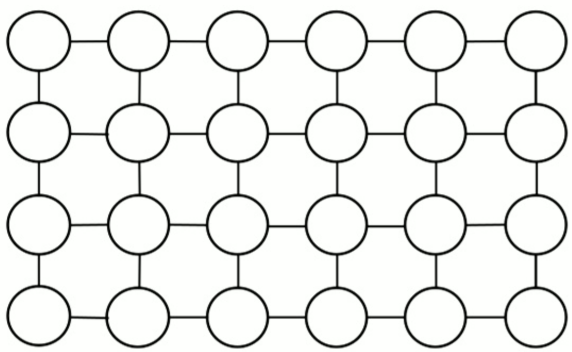
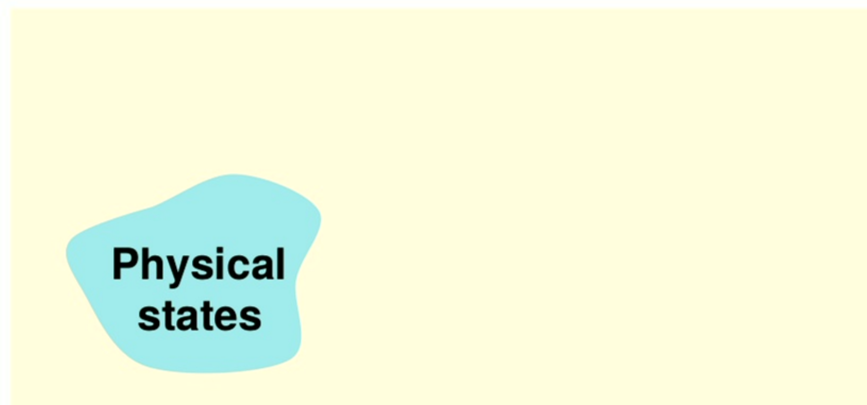




↳ Poly(N) parameters?

Variational formulation

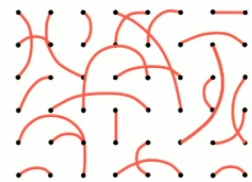
$$|\Psi\rangle = \sum_S \Psi(S)|S\rangle$$

parametrize: $\Psi(S) \approx \Psi_W(S)$

Variational principle

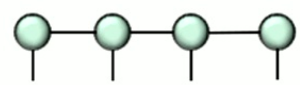
$$E_{var}(W) = \frac{\langle\Psi_W|H|\Psi_W\rangle}{\langle\Psi_W|\Psi_W\rangle} \geq E_G$$

Variational wave functions



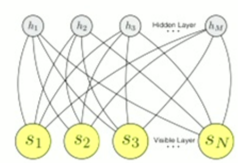
Motivated by physics of model:
RVB, Slater-Jastrow...

[P Anderson, Science (1987)]
[R Jastrow, PR (1955)]



Area law entanglement:
MPS, PEPS...

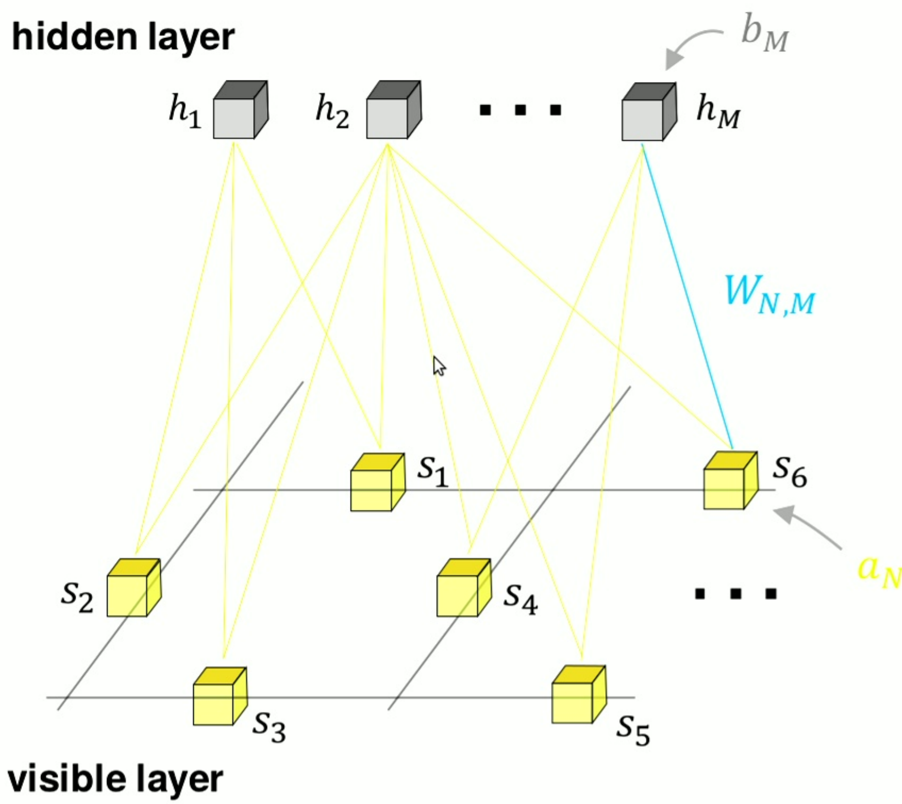
[A Klümper et al., J. Phys. A (1991)]
[S R White, PRL (1992)], [R Orus, AoP (2014)]



Generic:
Neural Networks

[G Carleo and M Troyer, Science (2017)]

Restricted Boltzmann Machine (RBM)

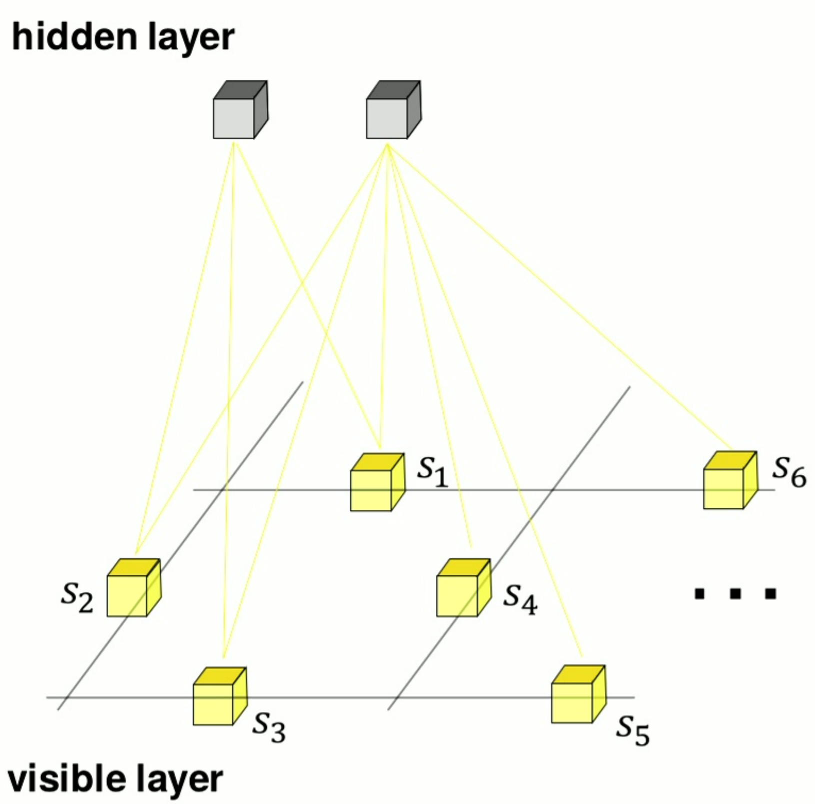


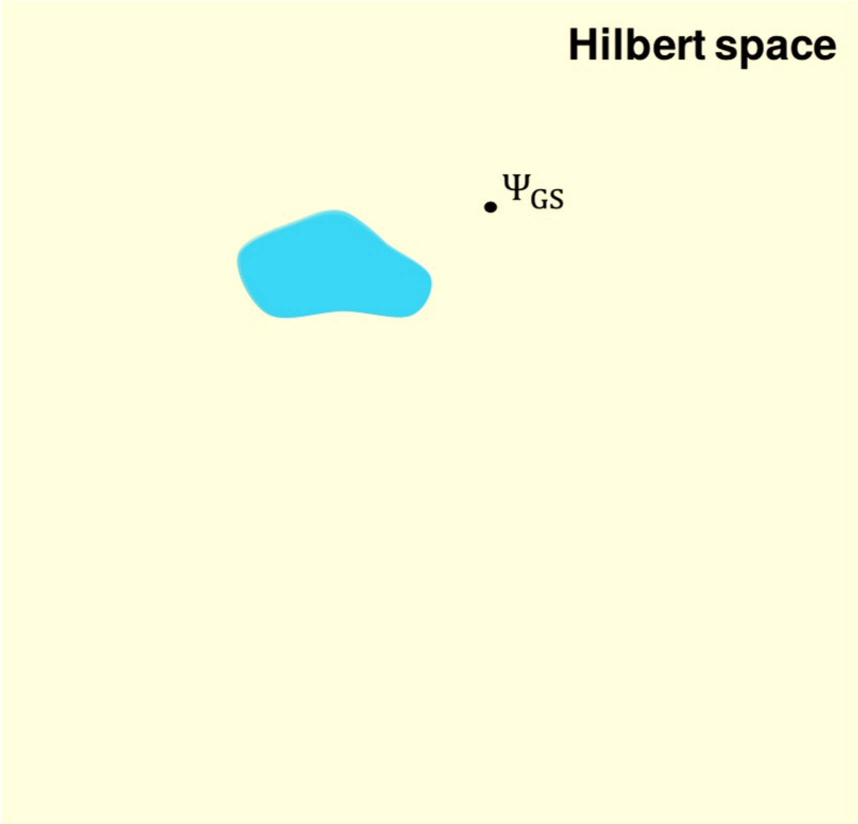
- Variational state: $\Psi_W(S) = \sum_h \exp(E_{RBM})$,

  $E_{\mathrm{RBM}} = \sum_k a_k s_k + \sum_j b_j h_j + \sum_{k,j} W_{k,j} s_k h_j$

[G Carleo and M Troyer, Science (2017)]

Restricted Boltzmann Machine (RBM)





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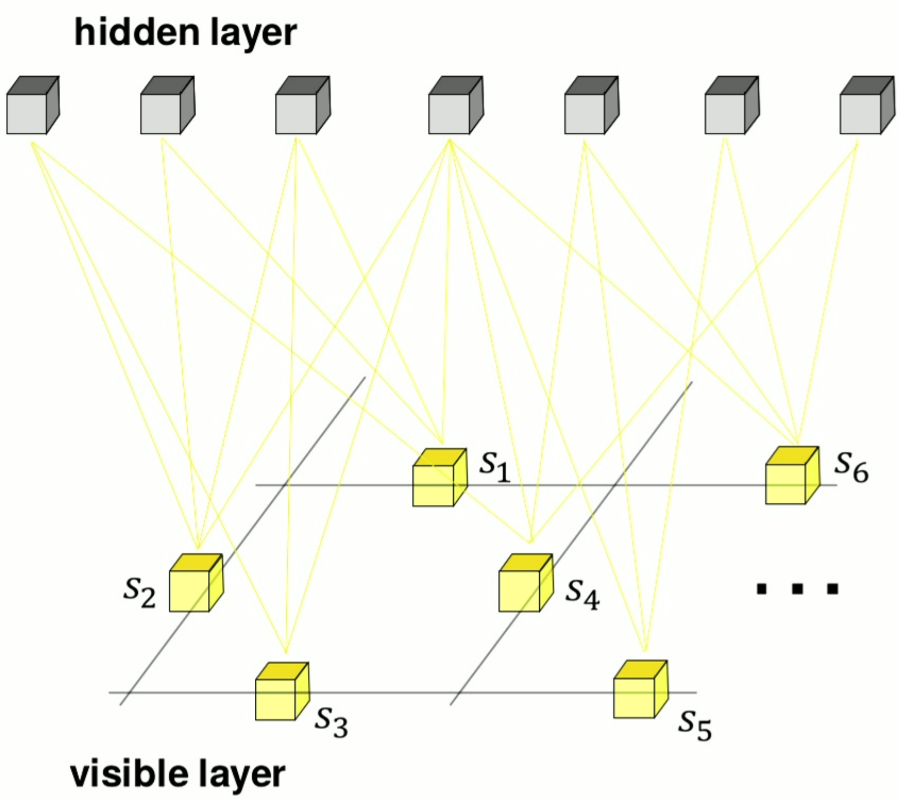
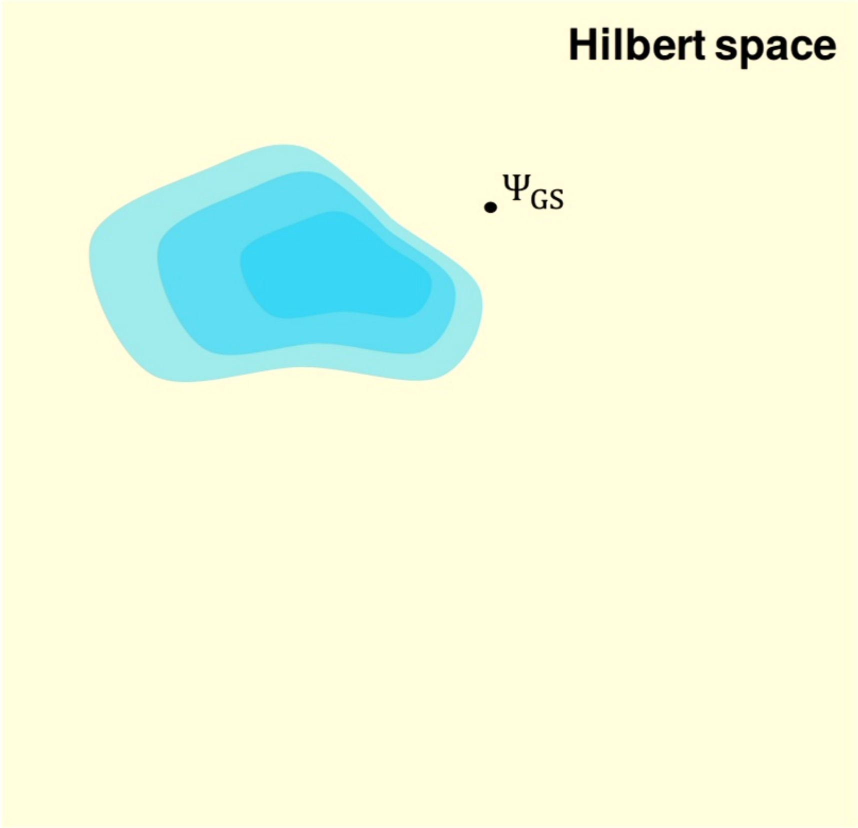
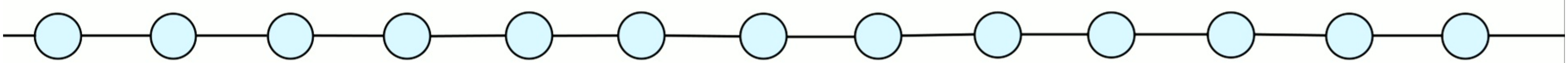
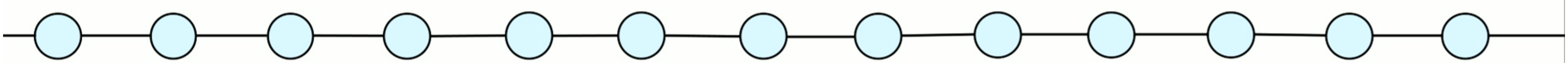




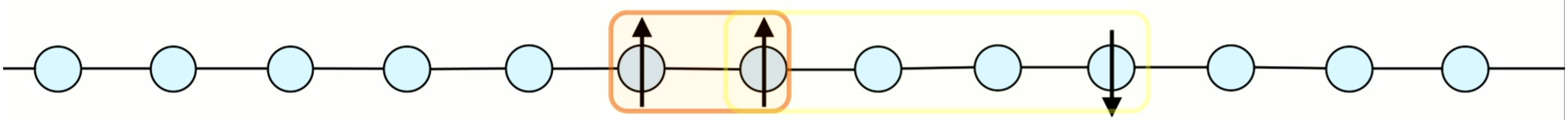
Bringing physical intuition to Neural Networks: Correlated RBMs



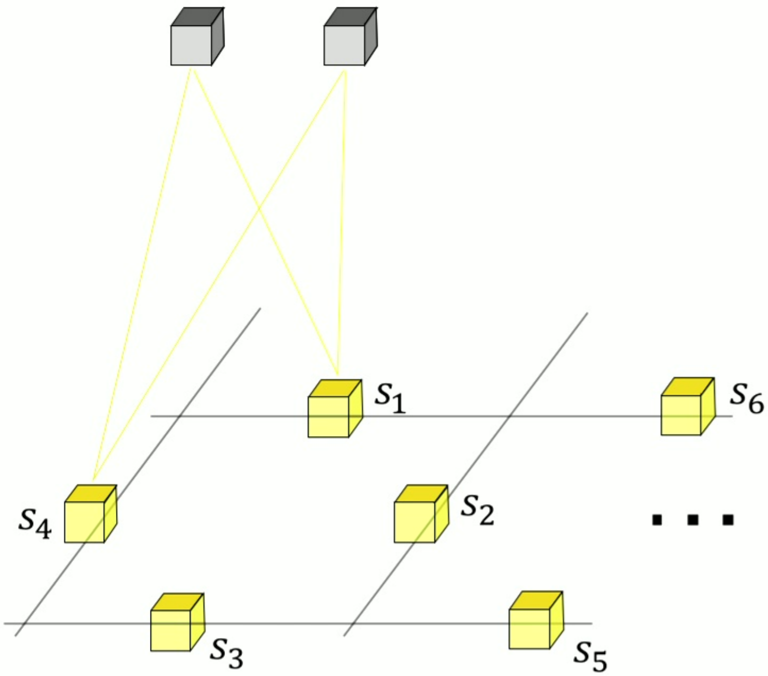
Bringing physical intuition to Neural Networks: Correlated RBMs

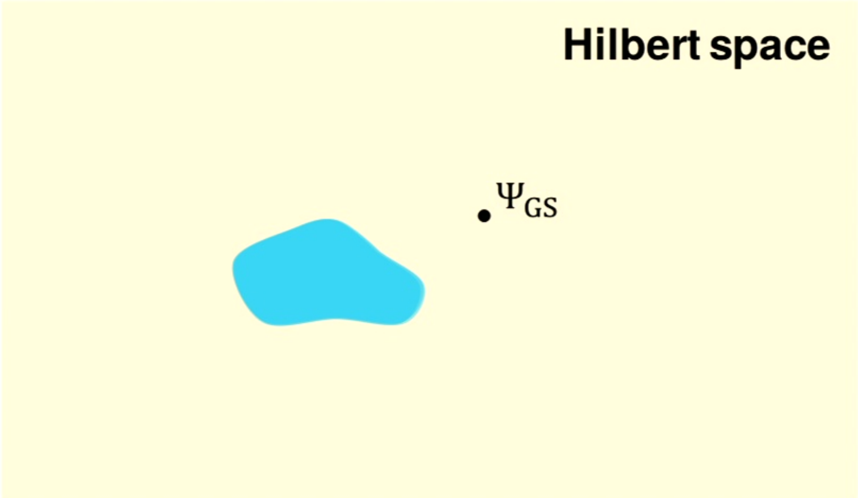


Bringing physical intuition to Neural Networks: Correlated RBMs



Restricted Boltzmann Machine (RBM)

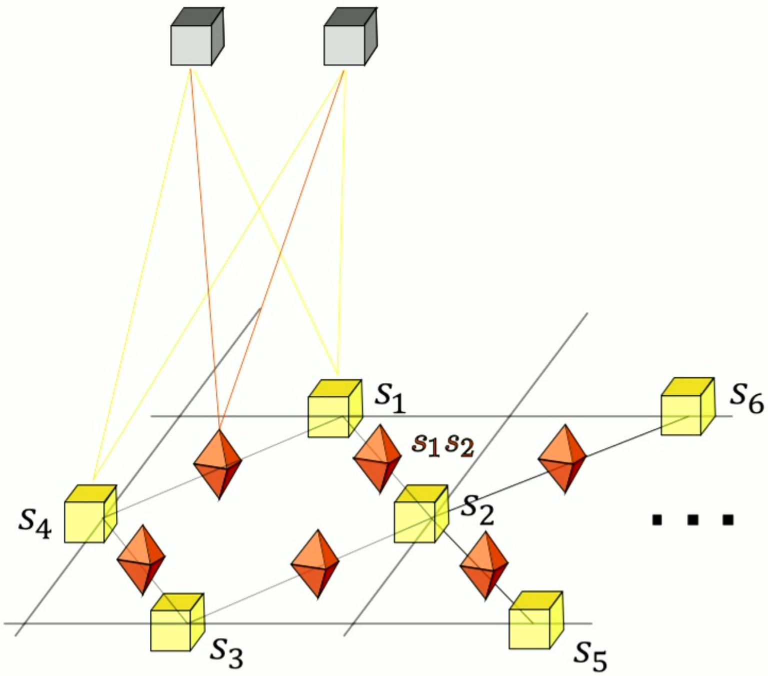


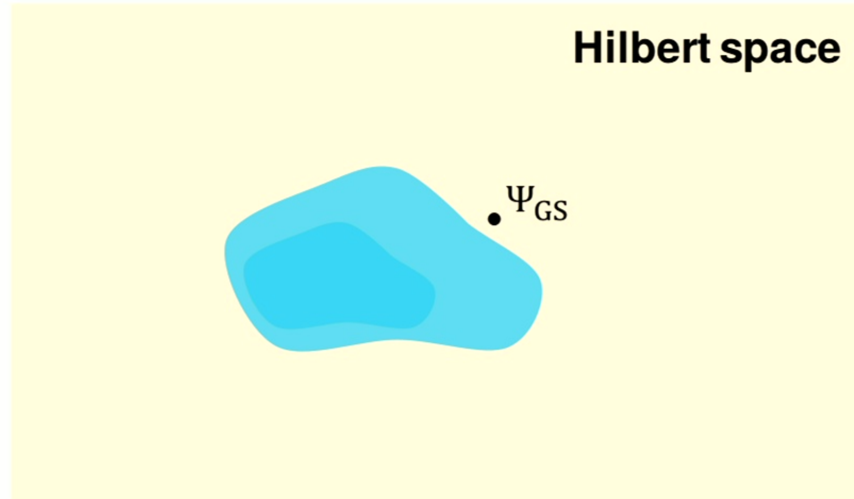


$$\Psi_W(S) = \sum_h \exp(E_{cRBM}),$$

$$E_{cRBM} = E_{RBM}$$

Restricted Boltzmann Machine (RBM)



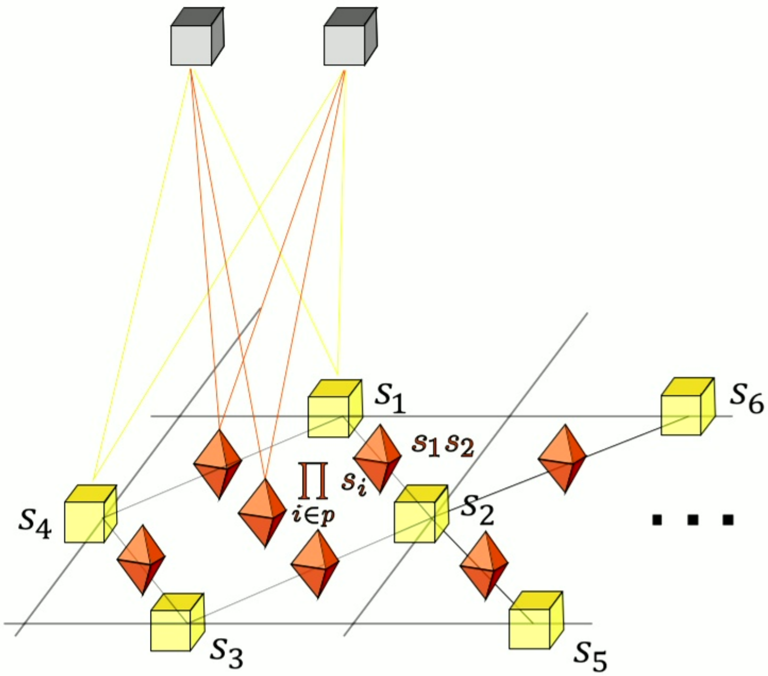


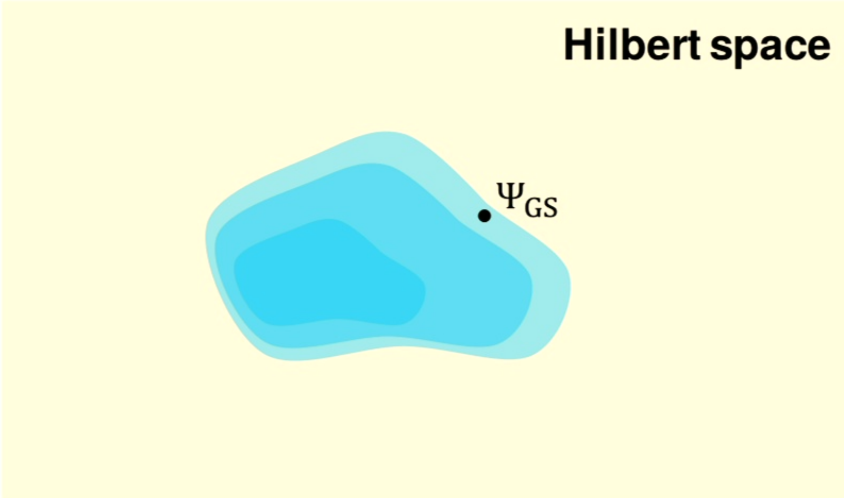
- Introduce Correlators $C_i = s_{i_1} \cdot \ldots \cdot s_{i_n}$ to the visible layer

$$\Psi_W(S) = \sum_h \exp(E_{cRBM}),$$

$$E_{cRBM} = E_{RBM} + \sum_i a_i^{corr} C_i + \sum_{i,j} W_{i,j}^{corr} C_i h_j$$

Restricted Boltzmann Machine (RBM)





- Introduce Correlators $C_i = s_{i_1} \cdot \ldots \cdot s_{i_n}$ to the visible layer

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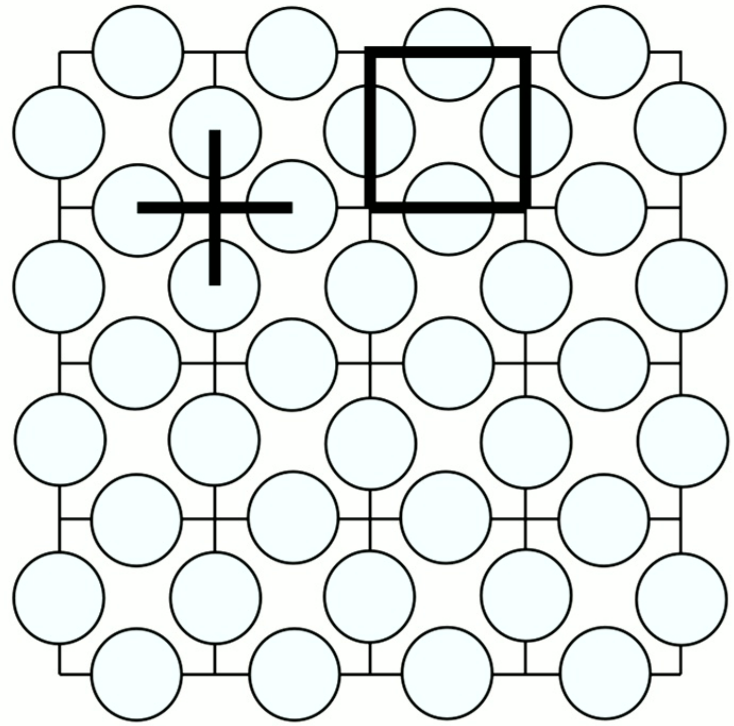
Testing correlated RBMs on

- *Topological phases*: Toric code with magnetic fields
- *Frustrated magnetism*: Heisenberg model (triangular lattice)

Toric code model

$$A_s = \prod_{i \in s} \sigma_i^x \qquad B_p = \prod_{i \in p} \sigma_i^z$$

$$H_{TC} = -\sum_s A_s - \sum_p B_p$$



- Ground state: $|TC\rangle = \prod_s (1 + A_s)|0\rangle$

  Stabilizer constraints: $A_s|TC\rangle = |TC\rangle$, $B_p|TC\rangle = |TC\rangle$

[AY Kitaev, Ann. Phys. (2003)]

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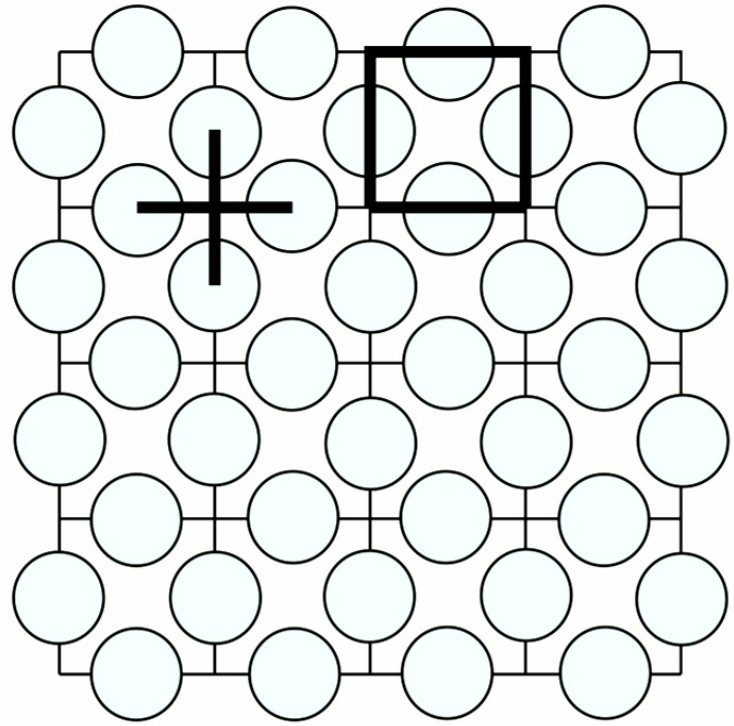
Toric code model

$$A_s = \prod_{i \in s} \sigma_i^x \qquad B_p = \prod_{i \in p} \sigma_i^z$$



$$H_{TC} = -\sum_s A_s - \sum_p B_p \quad + \vec{h} \cdot \sum_i \vec{\sigma}_i$$

- Ground state: $|TC\rangle = \prod_s (1 + A_s)|0\rangle$

  Stabilizer constraints: $A_s|TC\rangle = |TC\rangle$, $B_p|TC\rangle = |TC\rangle$

⟹ How stable is the topological phase against perturbations?

[AY Kitaev, Ann. Phys. (2003)]

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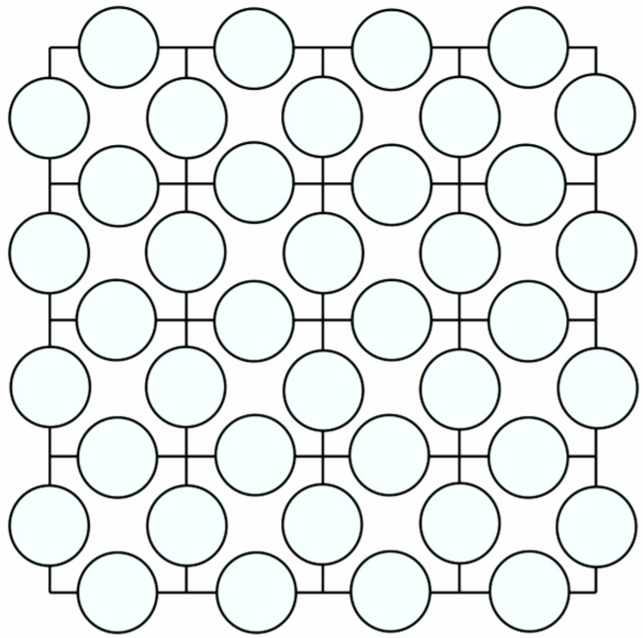
Toric code, magnetic fields and correlated RBMs (I)



- cRBM ansatz: $\Psi_W(S) = \sum_h \exp(E_{cRBM})$, $E_{cRBM} = E_{RBM} + \sum_i a_i^{corr} C_i + \sum_{i,j} W_{i,j}^{corr} C_i h_j$

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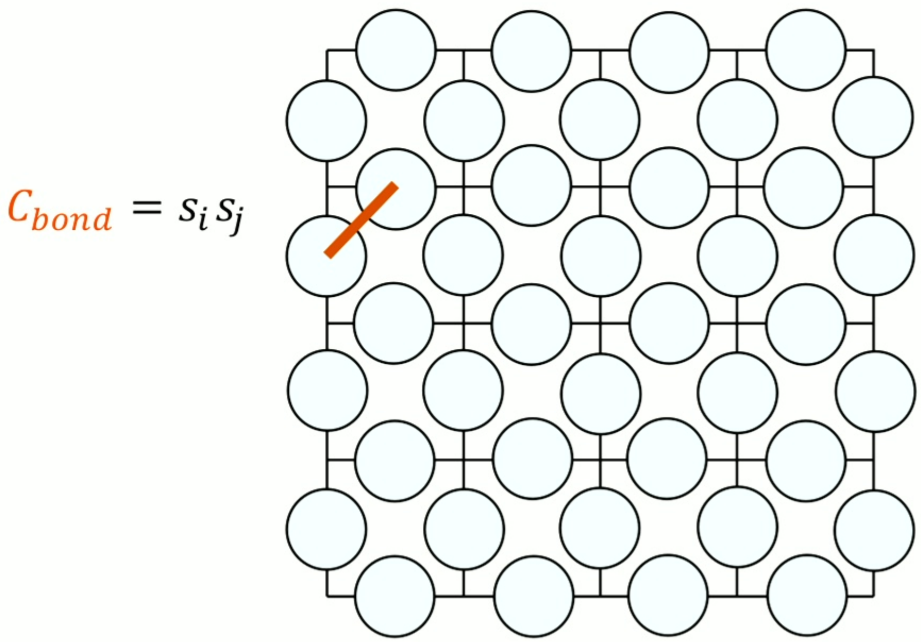

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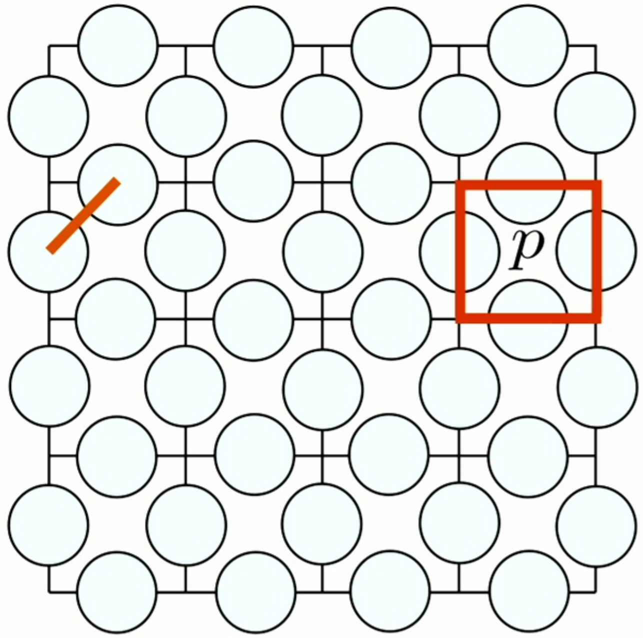
Toric code, magnetic fields and correlated RBMs (I)

$C_{bond} = s_i s_j$



$C_{plaquette} = \prod_{i \in p} s_i$

- cRBM ansatz: $\Psi_W(S) = \sum_h \exp(E_{cRBM})$, $\quad E_{cRBM} = E_{RBM} + \sum_i a_i^{corr} C_i + \sum_{i,j} W_{i,j}^{corr} C_i h_j$

Toric code, magnetic fields and correlated RBMs (I)

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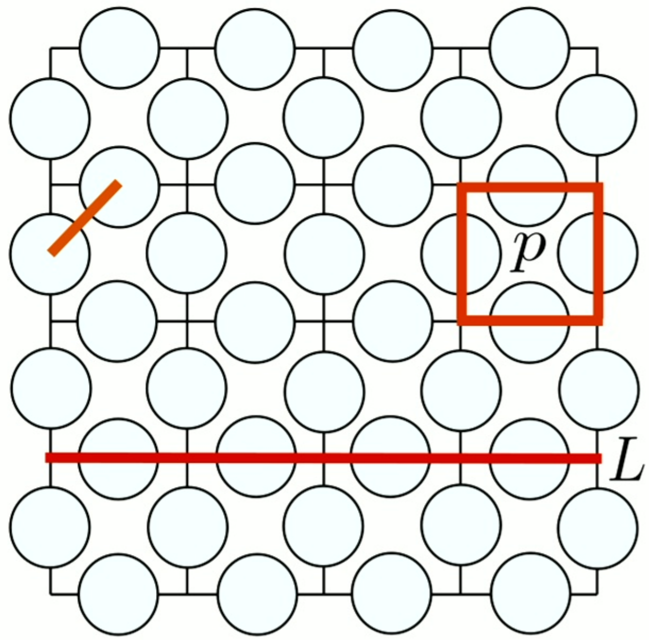
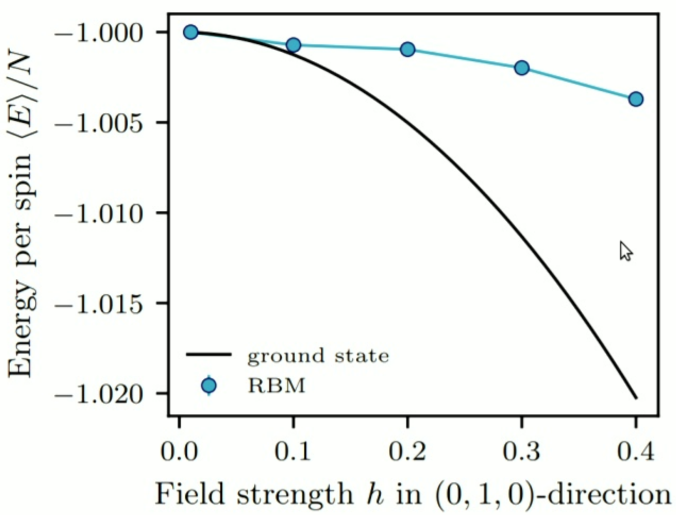


$C_{plaquette} = \prod_{i \in p} s_i$

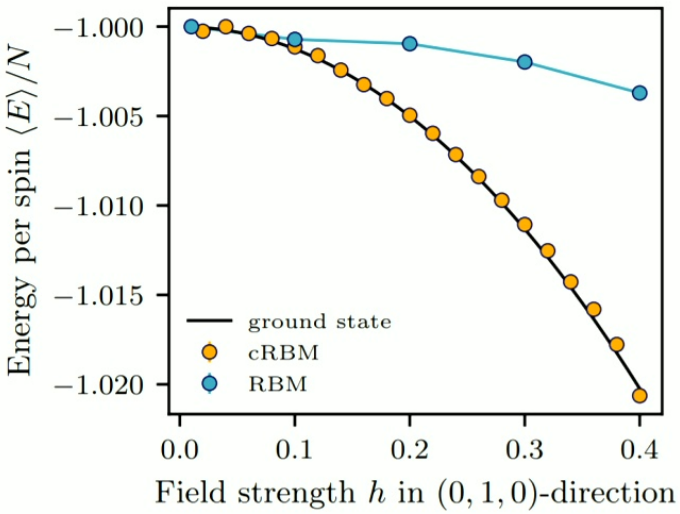
$C_{loop} = \prod_{i \in L} s_i$

- cRBM ansatz: $\Psi_W(S) = \sum_h \exp(E_{cRBM})\,, \qquad E_{cRBM} = E_{RBM} + \sum_i a_i^{corr} C_i + \sum_{i,j} W_{i,j}^{corr} C_i h_j$

Toric code, magnetic fields and correlated RBMs (II)



Toric code, magnetic fields and correlated RBMs (II)



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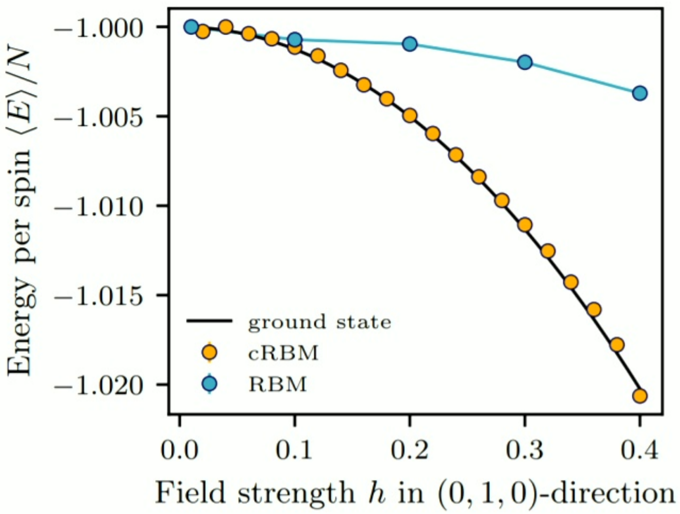
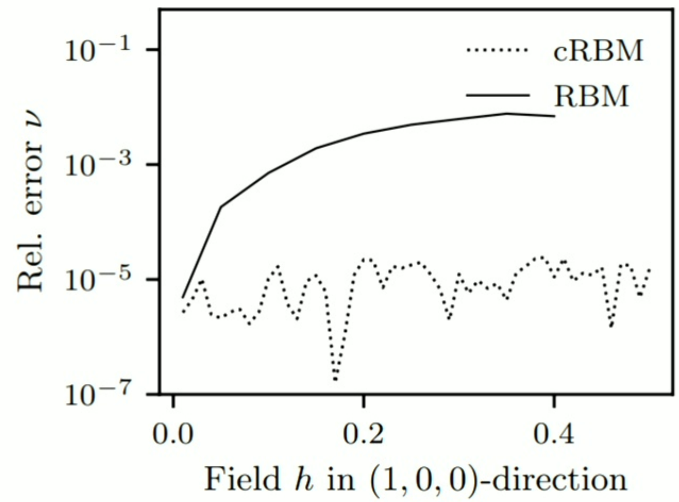
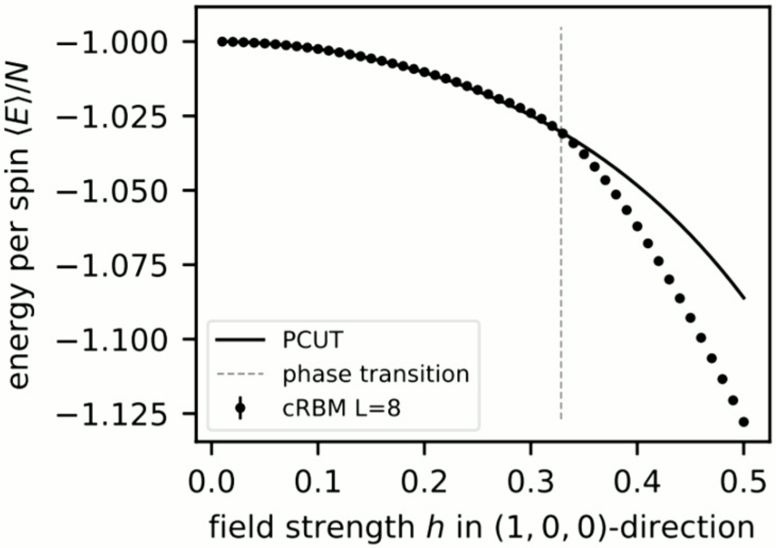




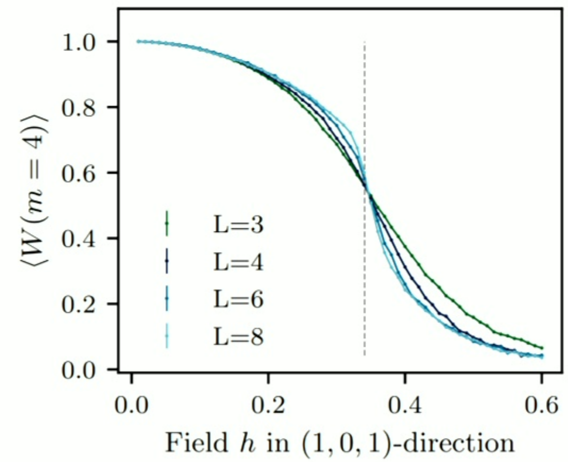
⟹ Introducing correlators improves precision by **several orders of magnitude**

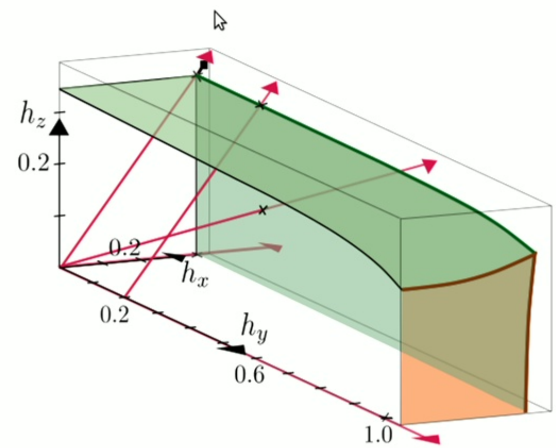
Scaling and topological phases

Wilson loops: $\langle W \rangle = \langle \prod_{i \in loop} \sigma_i^z \rangle$



probe phase diagram





- Beyond exact diagonalization:
  Compare with perturbation theory

Testing correlated RBMs on

- *Topological phases*: Toric code with magnetic fields
- *Frustrated magnetism*: Heisenberg model (triangular lattice)

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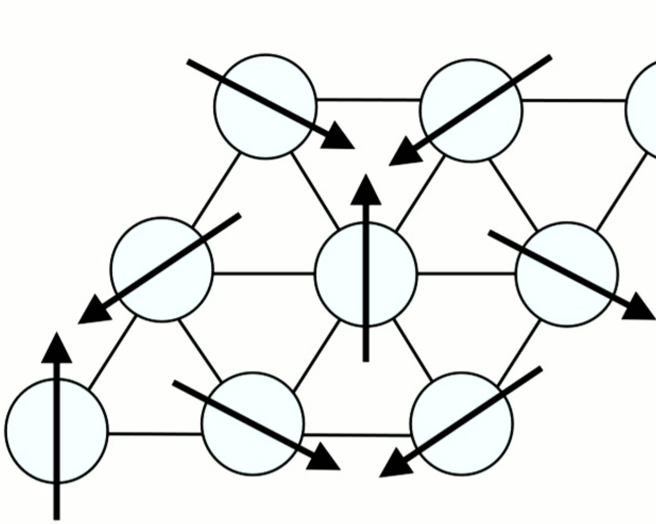
Heisenberg model on the triangular lattice

$H = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j,$ antiferromagnetic coupling: $J > 0$

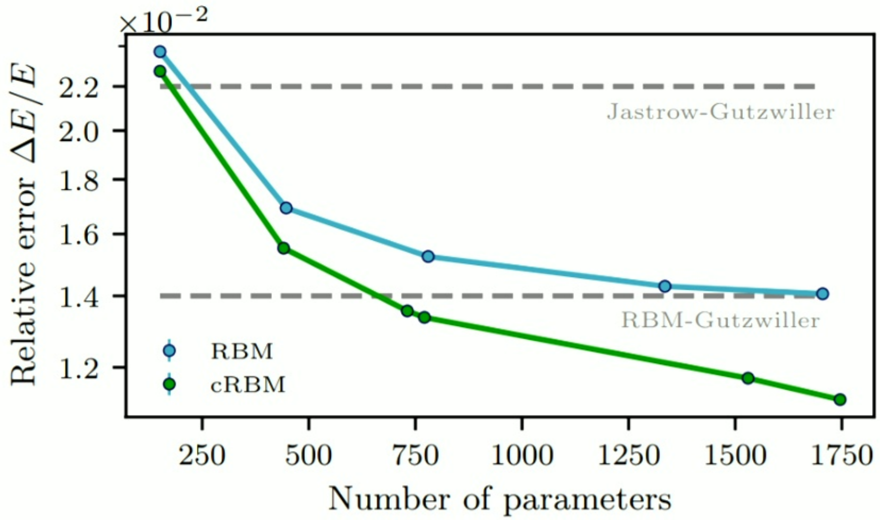


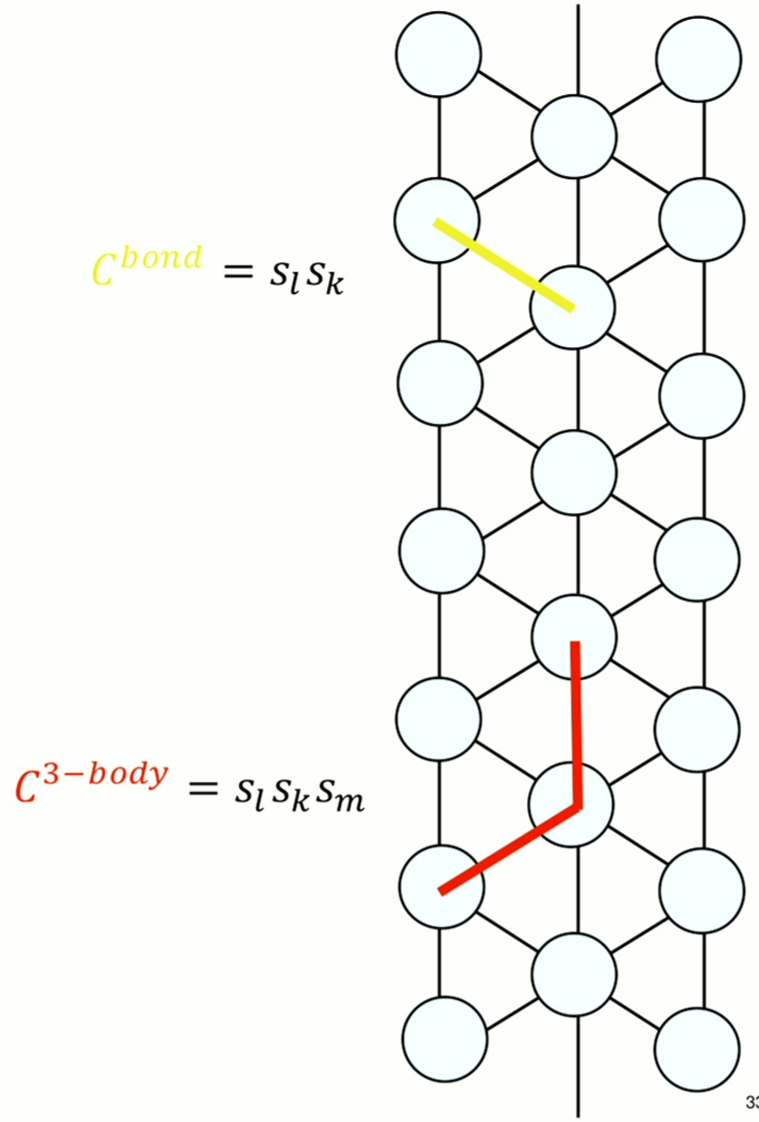
- Frustrated: classical Neel order unstable
  quantum fluctuations

- "Two types" of sign problem

[L Capriotti *et al.*, PRL (1999), [L Capriotti, IJMP B (2001)]

cRBMs for the Heisenberg model



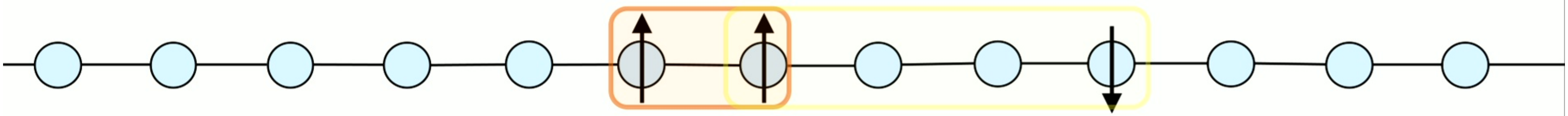


→ Including bond correlators C^{bond} and 3-body correlators C^{3-body} improves precision!

Summary and Outlook: Part I

[AV, E Greplova, NH Lindner and SD Huber, **PRR 4 (2022)**]

- Capitalizing on physical intuition: including correlators
- Obtain highly accurate ground- and excited states
- Applicable to further models: Frustrated Heisenberg, transverse-field Ising...



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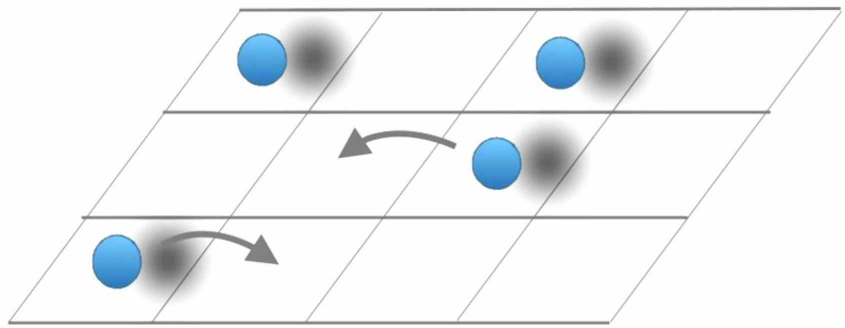
Part I: Variational wave-functions: Neural Networks and physical intuition

Part II: Variational wave-functions: Physical insights beyond lattice models

Fermionic systems



[J Robledo Moreno et al, PNAS 119 (2022)]
[K Choo et al, nature comm. 11 (2020)]

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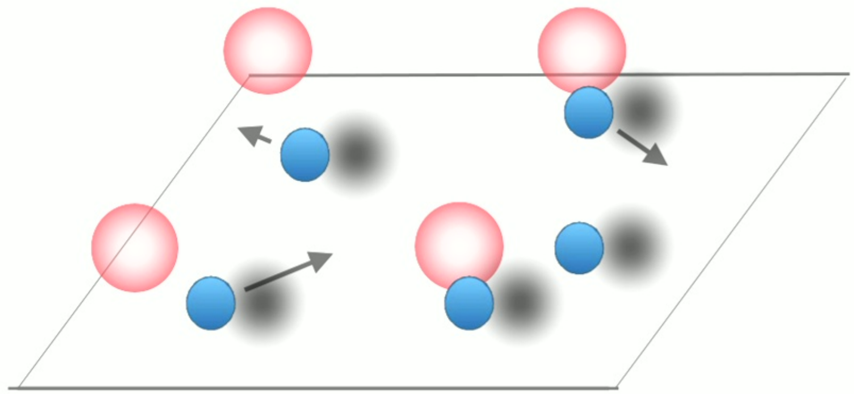
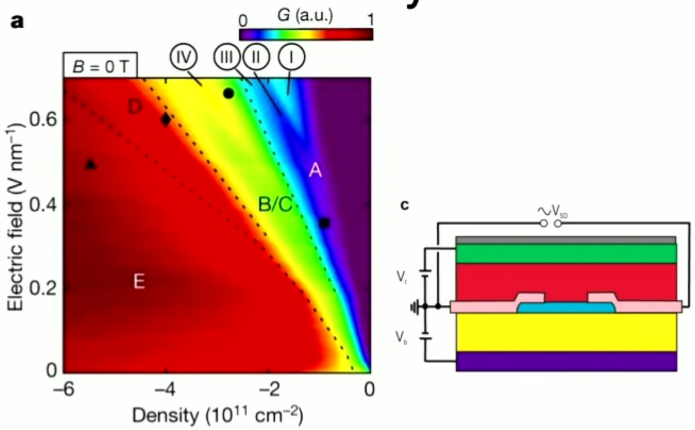
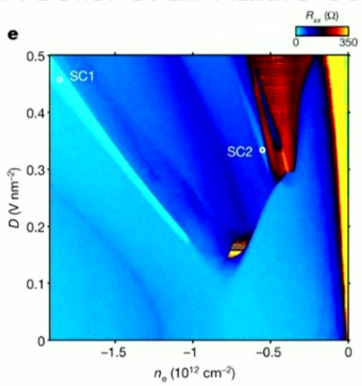
Fermionic systems



Fermionic systems

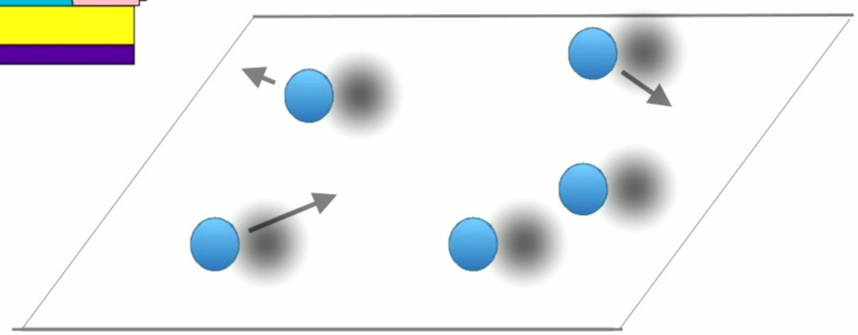


[A Seiler et al. Nature 608 (2022)]

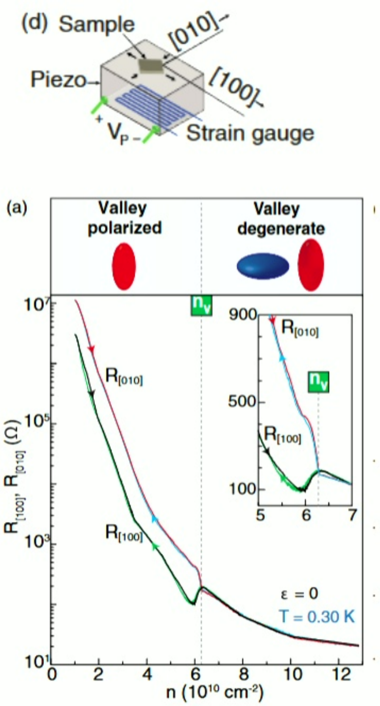


[H Zhou et al, Nature 598 (2021)]

Low-energy description: 2D Electron gas



Fermionic systems



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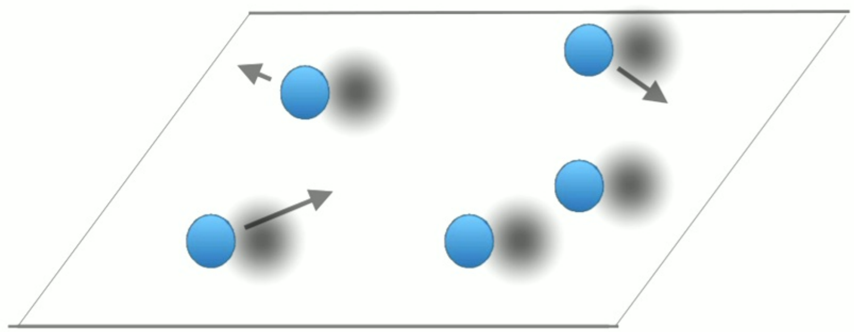
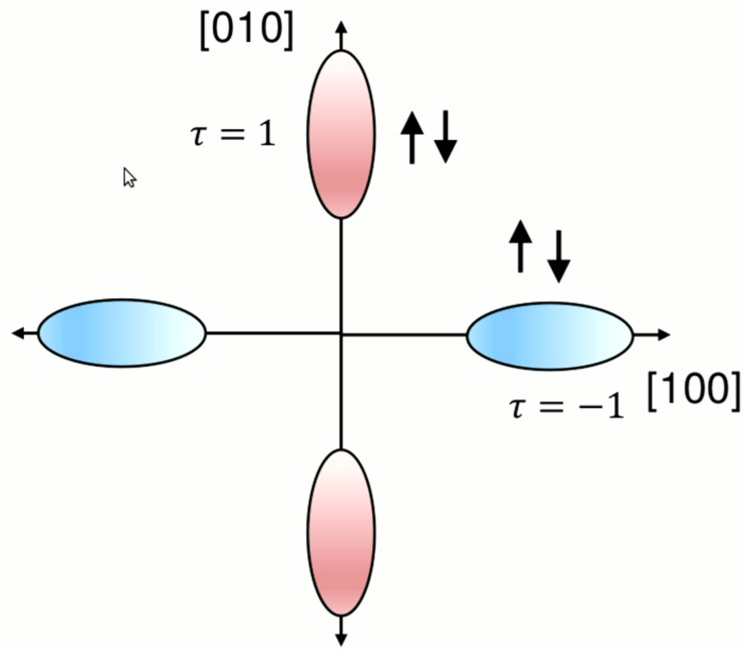


[Md S Hossain et al, PRL 127 (2021)]

AlAs quantum well



GaAs: $m^* = 0.067\ m_e$

AlAs: $m^* = 0.49\ m_e$

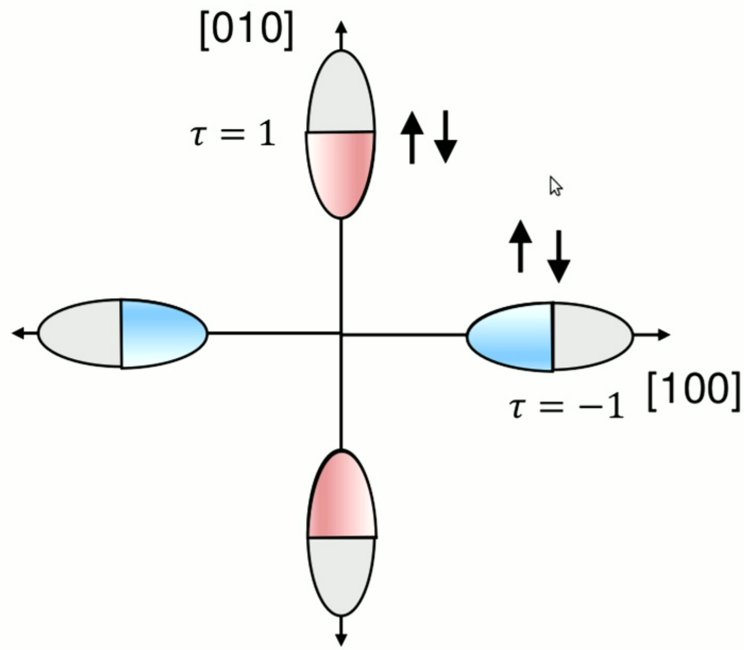
$$\frac{E_C}{E_{kin}} \sim e^2 m^* r_0 / \hbar^2$$

⇩

Strong correlations at accessible densities

$$H \approx \sum_{\sigma,\tau} \int d\,\vec{r}\,\Psi^\dagger_{\tau,\sigma}(\vec{r})\,\frac{\hbar^2}{2m^*}\,\left(-\eta^{\frac{\tau}{2}}\partial_x^2 - \eta^{-\frac{\tau}{2}}\partial_y^2\right)\,\Psi_{\tau,\sigma}(\vec{r}) + \sum_{\sigma,\sigma',\tau,\tau'} \int d\vec{r}\,d\vec{r}'\,V(\vec{r}-\vec{r}')\Psi^\dagger_{\sigma\tau}(\vec{r})\Psi^\dagger_{\sigma'\tau'}(\vec{r}')\Psi_{\sigma'\tau'}(\vec{r}')\Psi_{\sigma\tau}(\vec{r})$$

AlAs quantum well



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AlAs: $m^* = 0.49\, m_e$

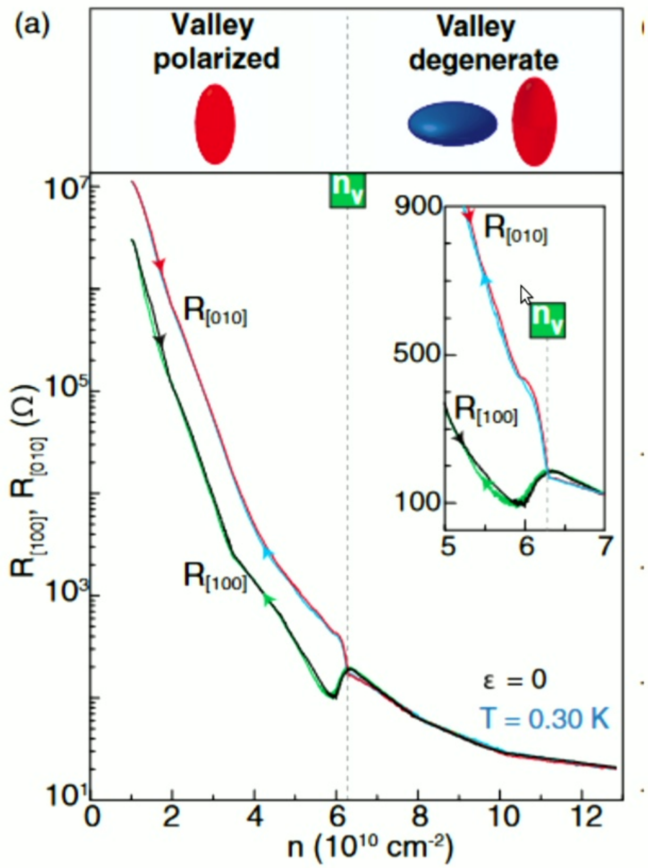
$$\frac{E_C}{E_{kin}} \sim e^2 m^* r_0/\hbar^2; \quad r_0^2 \sim \frac{1}{n}$$

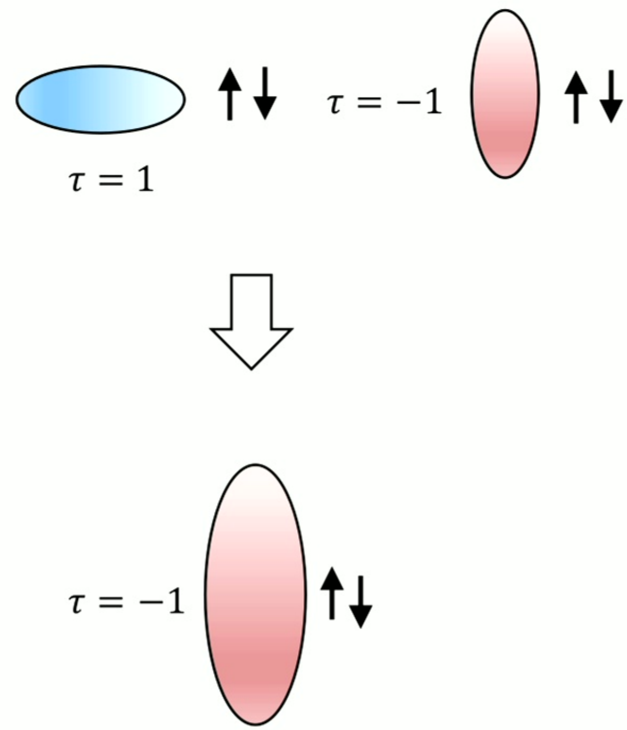
⇩

Strong correlations at accessible densities

$$H \approx \sum_{\sigma,\tau} \int d\,\vec{r}\, \Psi^{\dagger}_{\tau,\sigma}(\vec{r})\, \frac{\hbar^2}{2m^*} \left(-\eta^{\frac{\tau}{2}}\partial_x^2 - \eta^{-\frac{\tau}{2}}\partial_y^2\right)\, \Psi_{\tau,\sigma}(\vec{r}) + \sum_{\sigma,\sigma',\tau,\tau'} \int d\vec{r}d\vec{r}'V(\vec{r}-\vec{r}')\Psi^{\dagger}_{\sigma\tau}(\vec{r})\Psi^{\dagger}_{\sigma'\tau'}(\vec{r}')\Psi_{\sigma'\tau'}(\vec{r}')\Psi_{\sigma\tau}(\vec{r})$$

Spontaneous valley-polarization in AlAs





[Md S Hossain et al, PRL 127 (2021)]

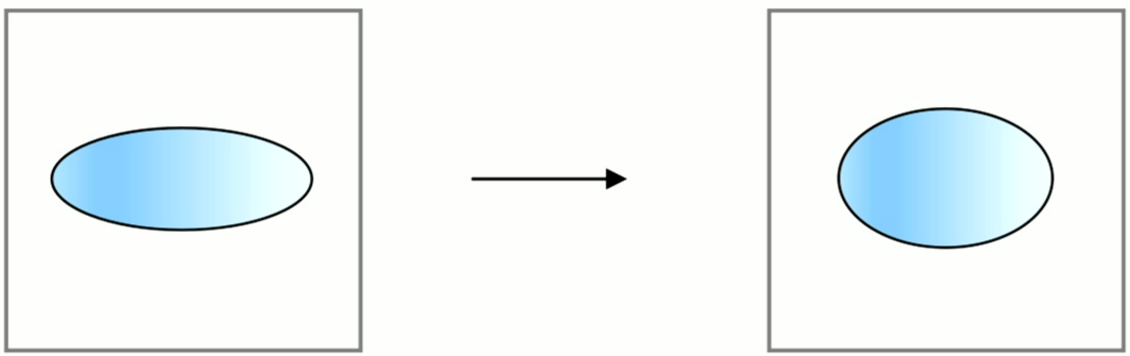
ETH zürich D-PHYS

Hartree-Fock approach

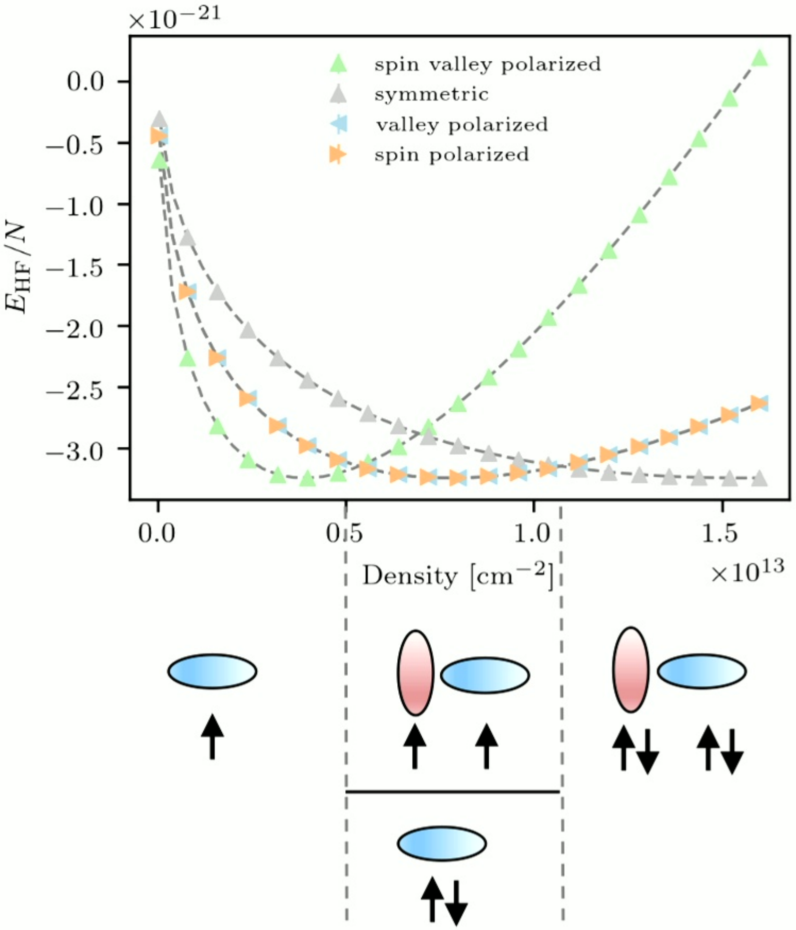
- Non-interacting ground state
- Fluid phase: $\Phi_i(r_j) = e^{ik_i r_j}$

$$\Psi(r_1, \ldots r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Phi_1(r_1) & \cdots & \Phi_1(r_N) \\ \vdots & \ddots & \vdots \\ \Phi_N(r_1) & \cdots & \Phi_N(r_N) \end{vmatrix}$$

$$E_{var} = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = E_{kin} + E_{Hartree} - E_{exchange}$$

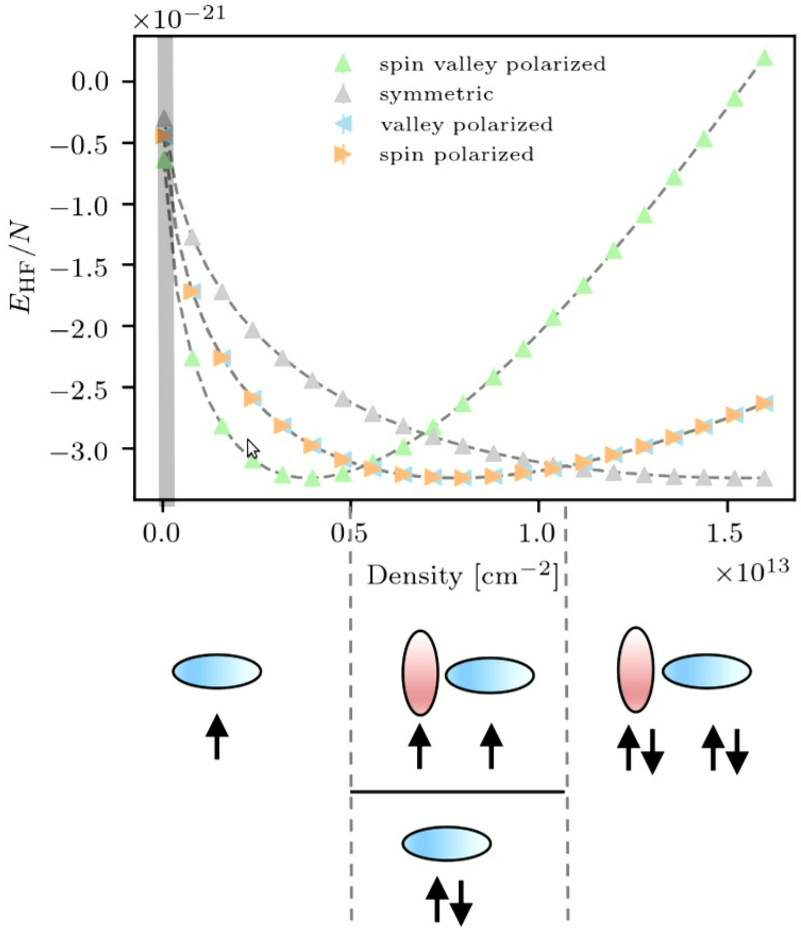


Hartree-Fock approach



$$\Psi(r_1, \ldots r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Phi_1(r_1) & \cdots & \Phi_1(r_N) \\ \vdots & \ddots & \vdots \\ \Phi_N(r_1) & \cdots & \Phi_N(r_N) \end{vmatrix}$$

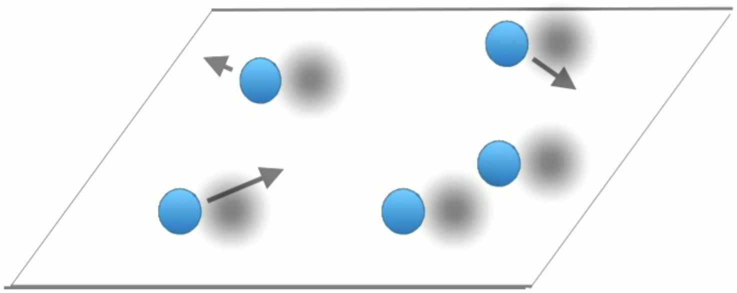
Hartree-Fock approach



$$\Psi(r_1, \ldots r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \Phi_1(r_1) & \cdots & \Phi_1(r_N) \\ \vdots & \ddots & \vdots \\ \Phi_N(r_1) & \cdots & \Phi_N(r_N) \end{vmatrix}$$

⇨ Need approach beyond mean-field!

Real-space variational Monte Carlo in the continuum



$$\Psi(r_1, \ldots r_N) = e^{-J(r_1,..r_N)} \frac{1}{\sqrt{N!}} \begin{vmatrix} \Phi_1(r_1) & \cdots & \Phi_1(r_N) \\ \vdots & \ddots & \vdots \\ \Phi_N(r_1) & \cdots & \Phi_N(r_N) \end{vmatrix}$$

exchange/ correlation hole

$$H(r_1, \ldots r_N) = \sum_i \frac{1}{2m_i} \nabla_i^2 + \sum_{i \neq j} U(|r_i - r_j|)$$

- Jastrow factor: $J(r_1, \ldots r_N) = \sum_{i<j} u_{\sigma_i \tau_i \sigma_j \tau_j}(|r_i - r_j|) + \cdots$

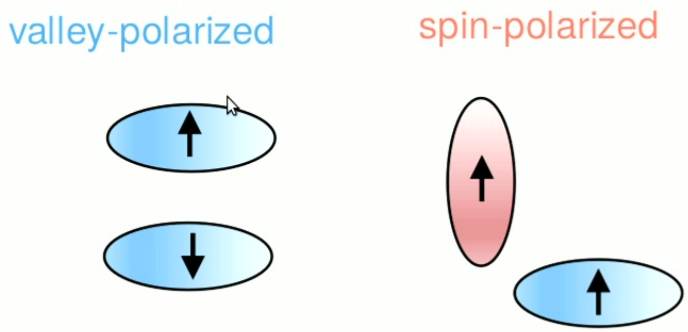
↓

parametrization

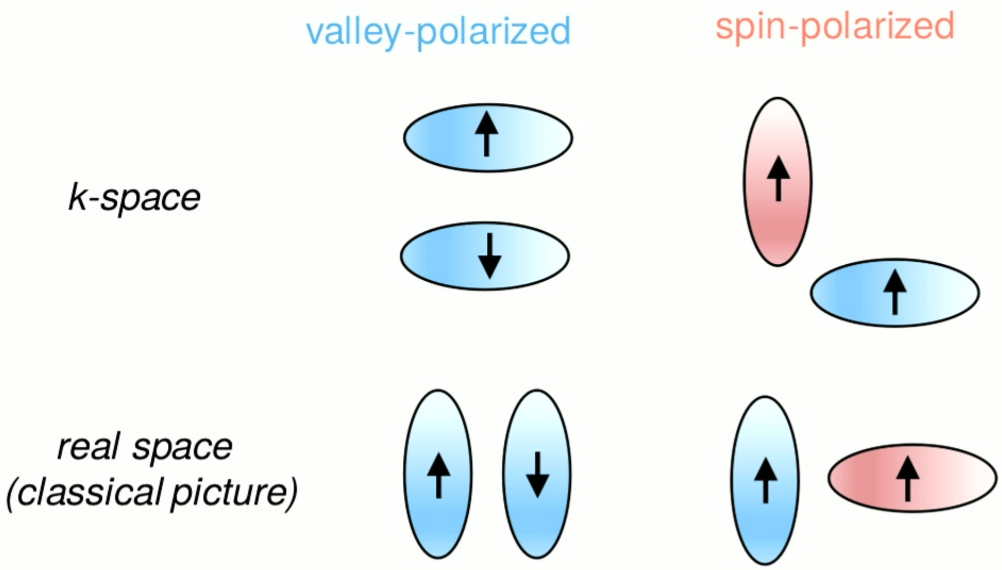
optimize using VMC

Valley-polarization with VMC (preliminary results)

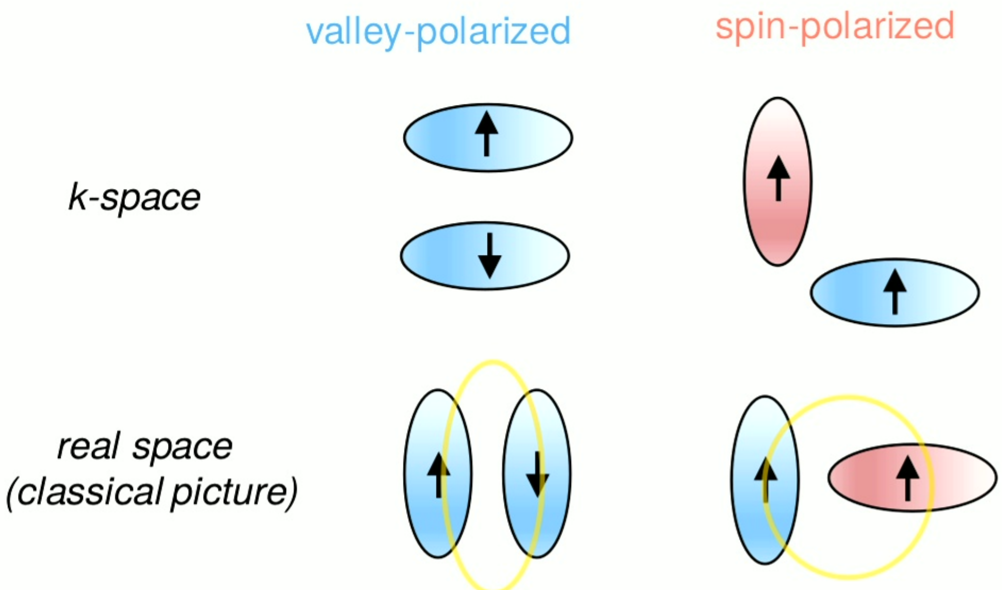
k-space



Valley-polarization with VMC (preliminary results)



Valley-polarization with VMC (preliminary results)



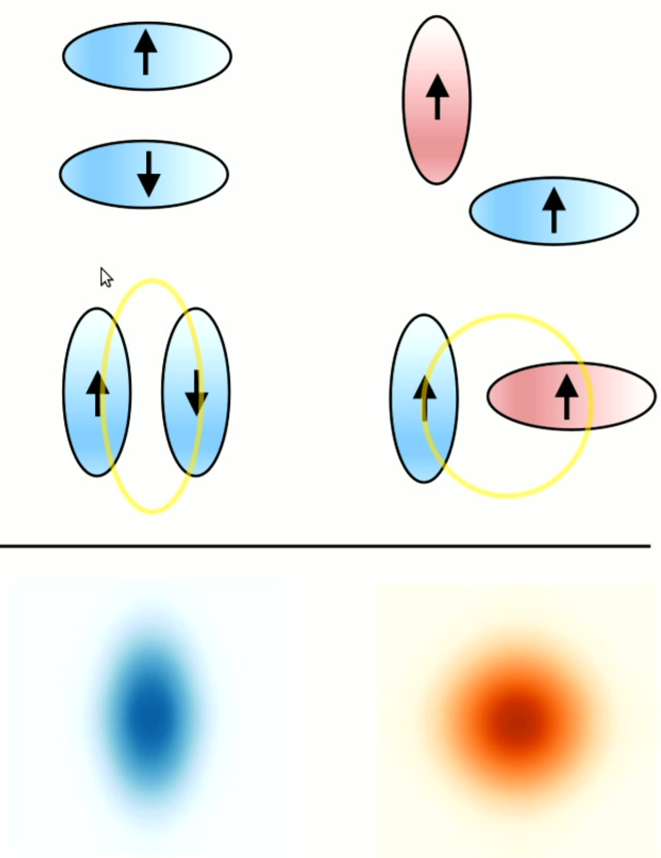
Valley-polarization with VMC (preliminary results)

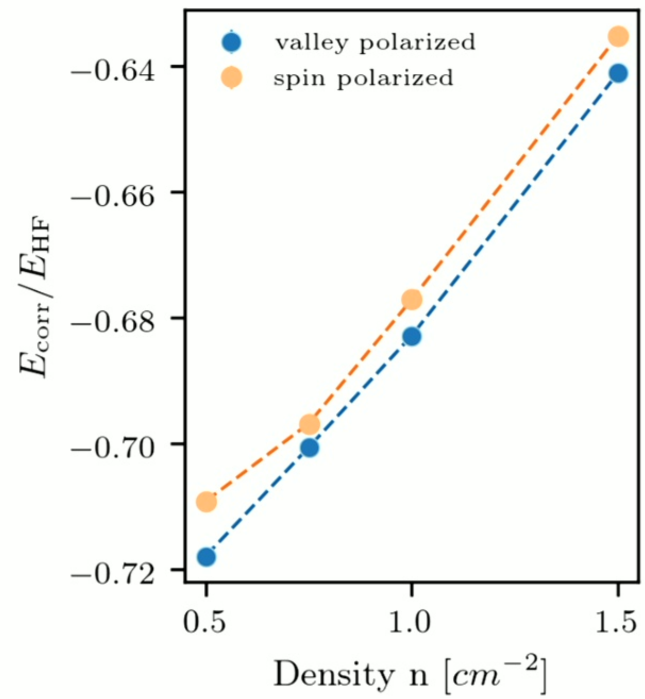
valley-polarized | spin-polarized

k-space

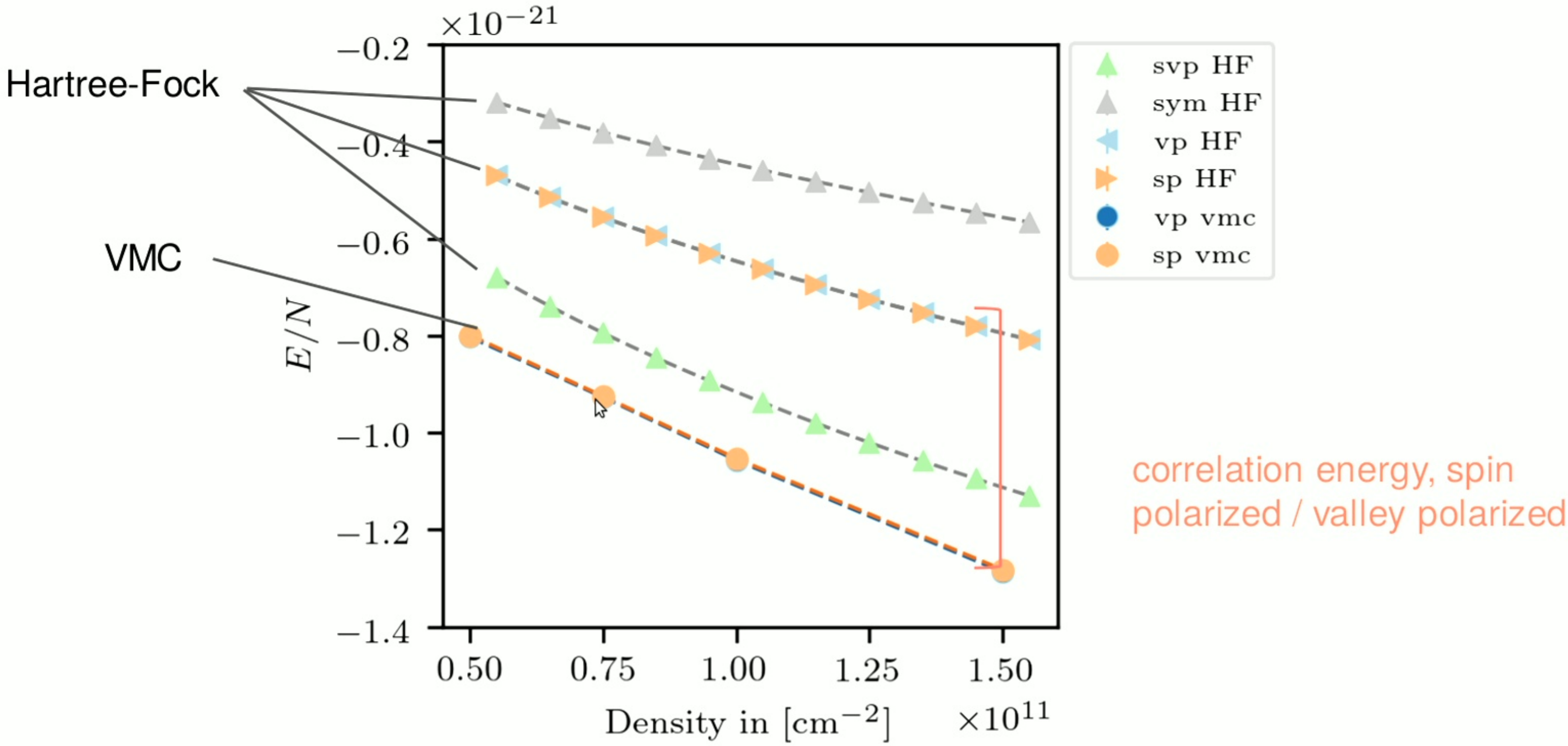
real space (classical picture)

correlation hole using VMC (Jastrow factor)

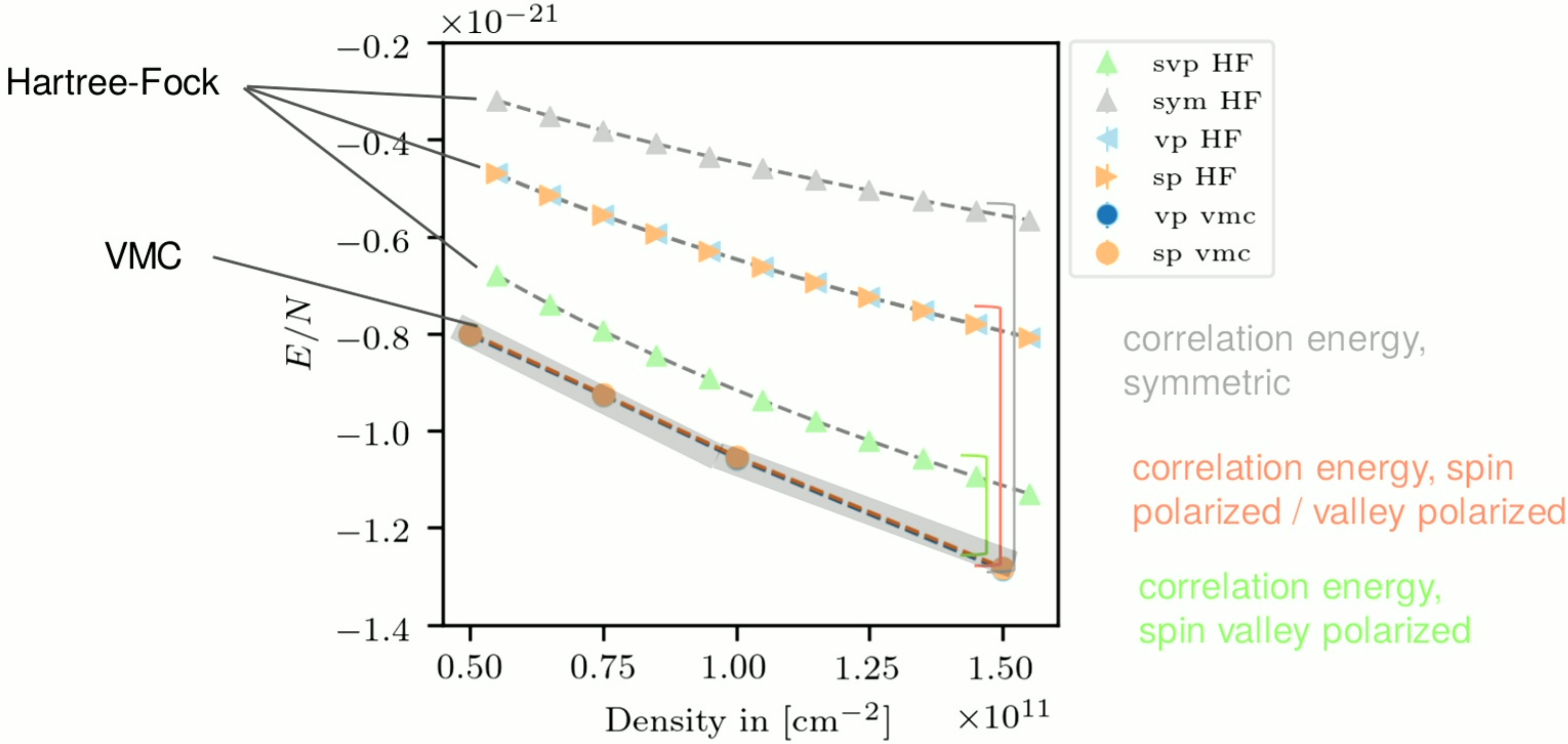




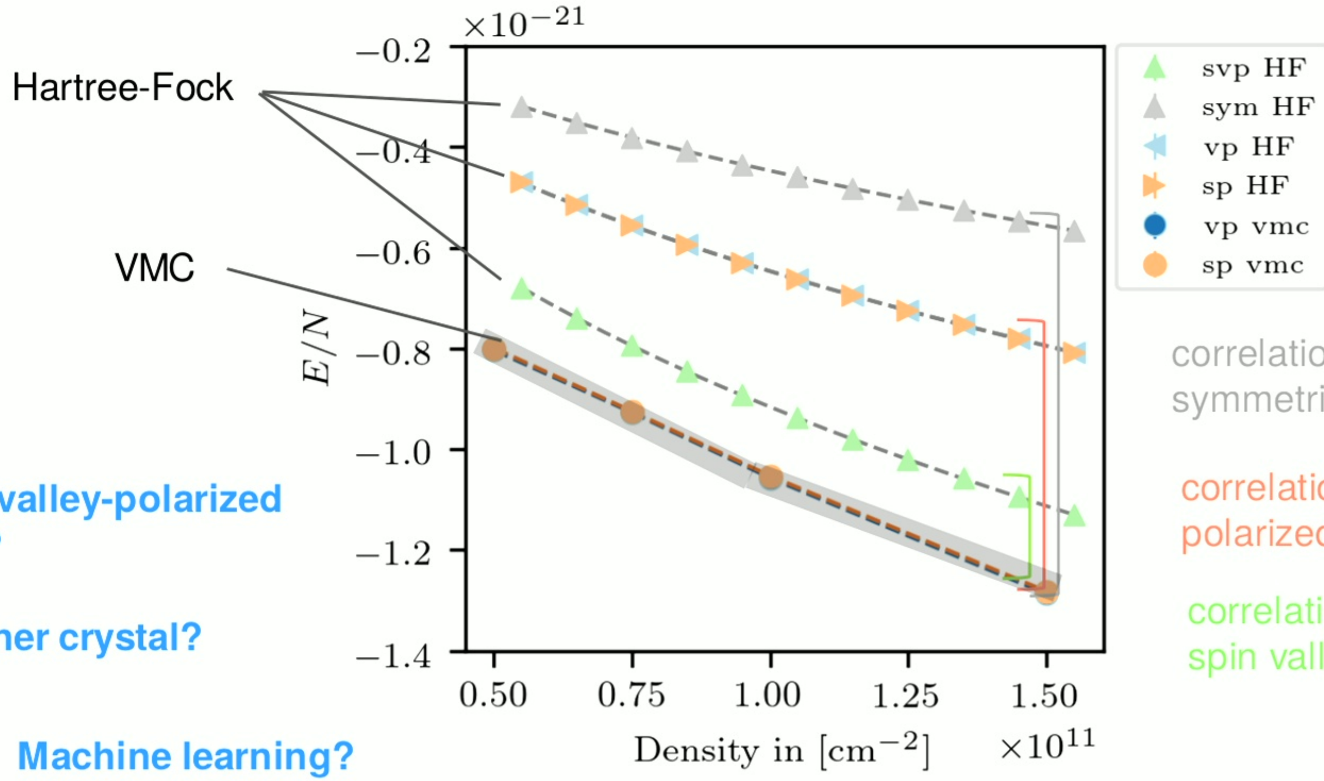
Phase diagram?



Phase diagram?



Phase diagram?



correlation energy, symmetric

correlation energy, spin polarized / valley polarized

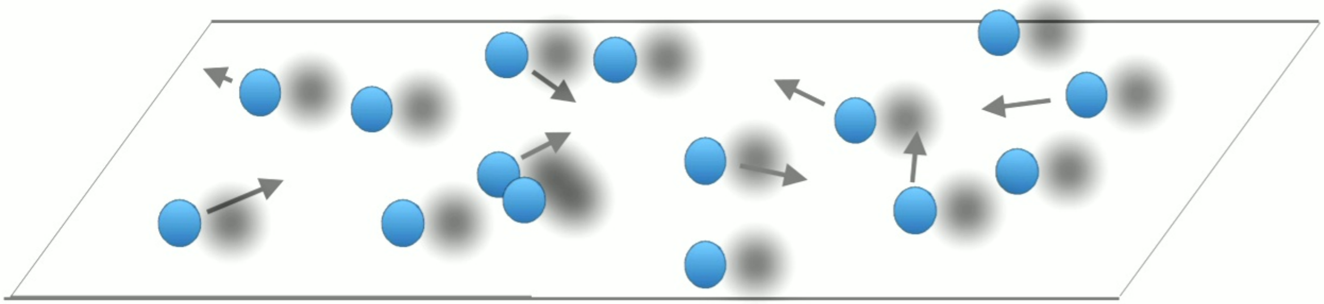
correlation energy, spin valley polarized

Stable valley-polarized phase?

Wigner crystal?

Machine learning?

Summary and Outlook: Part II



- Strongly correlated systems: Methods beyond mean-field required
- Valley polarization explainable through correlation effects
- Complete phase diagram: Machine learning?