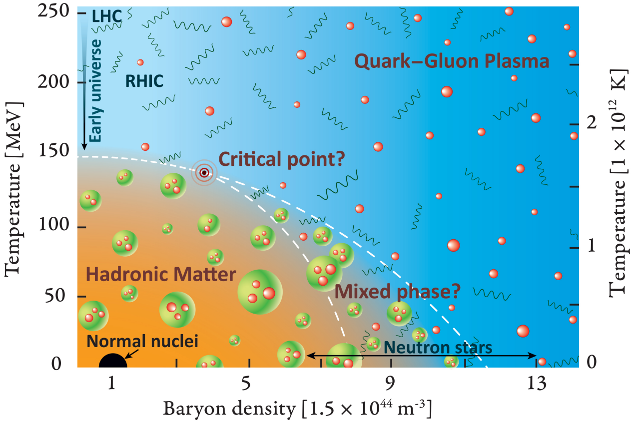
Lawrence Berkeley National Laboratory

Exact block encoding of imaginary time evolution with universal quantum neural networks

Ermal Rrapaj

Nuclear Phase Diagram

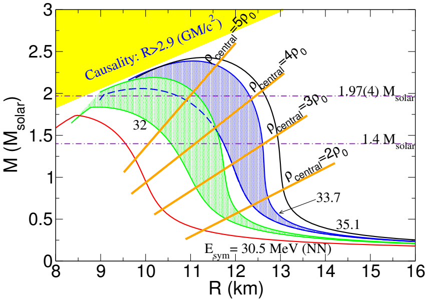


Nuclear potential

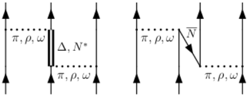
S. Gandolfi, J. Carlson, and Sanjay Reddy, PRC 85, 032801(R), (2012)
S.K. Bogner, R.J. Furnstahl, A. Schwenk Prog.Part.Nucl.Phys.65:94-147,2010

$$V(\vec{r}) = \sum_i V_i(\vec{r}) + \sum_{i<j} V_{ij}(\vec{r}) + \sum_{i<j<k} V_{ijk}(\vec{r}) + \ldots$$

Neutron Star Mass-Radius .

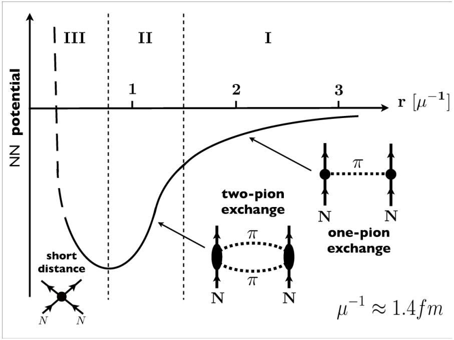


Three body interactions



Nuclear Forces

J .W. Holt, N. Kaiser, W. Weise PPNP 73 (2013)



Nuclear Forces

- Phenomenological treatment: Mean-Field Theory , Interaction Models
- Ab-initio: Chiral Effective Field Theory (χEFT)

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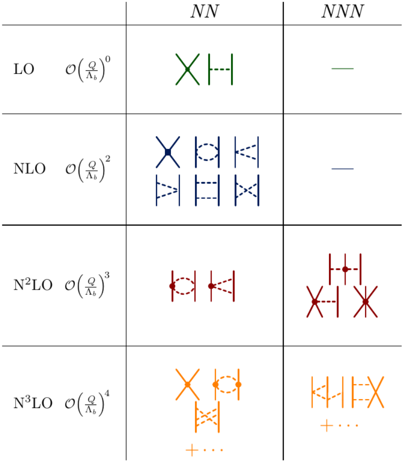
χEFT

"Chiral effective field theory and nuclear forces" by Machleidt, Entem in Physics Reports Volume 503, Issue 1



- χEFT expansion in Q/Λ_b:
  - $Q \sim m_\pi \sim 100$ MeV (soft scale)
  - $\Lambda_b \sim m_\rho \sim 800$ MeV (hard scale)
- Long range physics given by pion exchanges
- Short range physics parametrized by low energy constants (LEC) fit to low energy data
- Many body forces systematically organized and related via the same LECs

Quantum Monte Carlo

Expectation of observables

$$\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta H} O\right]}{\mathrm{Tr}\left[e^{-\beta H}\right]}$$

$$= \sum_{\mathbf{s}} \left(\frac{\langle \mathbf{s} | e^{-\beta H} | \mathbf{s} \rangle}{\sum_{\mathbf{s}} \langle \mathbf{s} | e^{-\beta H} | \mathbf{s} \rangle} \right) O(\mathbf{s})$$

$$= \sum_{\mathbf{s}} P(\mathbf{s}) O(\mathbf{s})$$

$$\langle O \rangle \approx \frac{1}{M} \sum_{n=1}^{M} O(\mathbf{s}_n), \ \mathbf{s}_n \sim P(\mathbf{s})$$

$$e^{-i\tau H} = e^{\beta H} \longrightarrow \tau = i\beta \text{ (Imaginary Time!)}$$

Auxiliary fields

R. L. Stratonovich, Soviet Physics Doklady 2, 416 (1957)
J. Hubbard, Phys. Rev. Lett. 3, 77 (1959)

Hubbard-Stratonovich

$$\exp\left(-\frac{\tau}{2}\hat{O}^2\right) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dh\ \exp\left[-\left(\frac{h^2}{2}+\sqrt{-\tau}h\hat{O}\right)\right], \tau < 0$$

J. E. Hirsch, Phys. Rev. B 28, 4059 (1983)

Hirsch .

$$\exp\left(-\tau\hat{\rho}_\mu\hat{\rho}_\nu\right) = \sum_{h=\pm1} P(h) e^{h(A_\mu\hat{\rho}_\mu + A_\nu\hat{\rho}_\nu)}$$
$$\tau \in R$$

Higher order interactions are hard to represent!

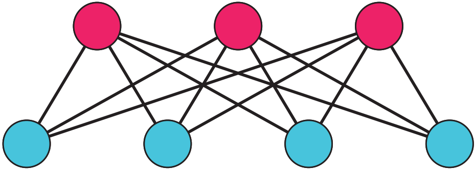
Hamiltonian terms as RBM Layers

Neural Layers $\longleftrightarrow$ Physical + Auxiliary fields

- Quantum + Classical $\Longrightarrow$ QMC + Classical Computing
  E. Rrapaj, A. Roggero, PRE 103, 013302 (2021)
- Quantum + Quantum $\Longrightarrow$ Imaginary time + Quantum Computing
  E. Rrapaj, E.Rule, arxiv 2403.17273

Restricted Boltzmann Machine (RBM)

P. Smolensky, Explorations in the Microstructure of Cognition, Volume 1: Foundations. MIT Press. pp. 194–281. (1986)
N. LE Roux, Y. Bengio Neural Computation, Vol. 20, Issue: 6, June 2008
G. Hinton, Momentum vol. 9, 1, pages 296 (2010)
E. Rrapaj, A. Roggero, PRE 103, 013302 (2021)



- Energy Based Model $F_{\rm rbm}\left(\hat{\rho}, \mathbf{h}\right) = \mathbf{B}\cdot\hat{\rho} + \mathbf{C}\cdot\mathbf{h} + \sum_{\mu=1}^{M}\sum_{j=1}^{N_h} W_{ij}\hat{\rho}_\mu h_j$
- Universal approximator $H_{\rm rbm}\left(\hat{\rho}\right) = -\log\left(\mathrm{Tr}_{\mathbf{h}}\exp\left(-F_{\rm RBM}\left(\hat{\rho}, \mathbf{h}\right)\right)\right) \xrightarrow{N_h\to\infty} H_{\rm physical}\left(\hat{\rho}\right)$

E. Rrapaj, A. Roggero, PRE 103, 013302 (2021)

Algorithm

for $(n = 2,\ n < N,\ n += 1)$ **do**

Require: $H_{\text{rbm}}(\hat{\rho}) = H_n(\hat{\rho})$

(1 hidden unit $\leftrightarrow$ n visible ones $\equiv$ couplings up to order n)

Pick a reference configuration $\hat{\rho}_0$

$$\ln\left(\frac{H_{\text{rbm}}(\hat{\rho})}{H_{\text{rbm}}(\hat{\rho}_0)}\right) = \ln\left(\frac{H_n(\hat{\rho})}{H_n(\hat{\rho}_0)}\right)$$

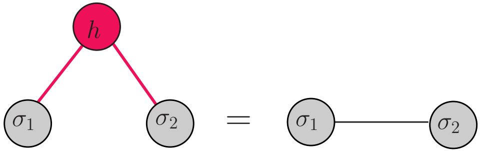
Solve system of $2^n - 1$ linear equations for $2^n - 1$ couplings

Invert the equation for the highest coupling (order n)

set all lower order couplings of same order equal

end for

E. Rrapaj, A. Roggero, PRE 103, 013302 (2021)



Repulsive Spin Pair Interactions

$$e^{-U\alpha_t(\vec{\sigma}_1\cdot\vec{\sigma}_2)} = \frac{e^{-3U\alpha_t}}{8}\prod_{d=1}^{3}\sum_{h_d=0}^{1} e^{a(2h_d-1)(\sigma_d\otimes\mathbb{1}-\mathbb{1}\otimes\sigma_d)}$$

where $\tanh(a)^2 = \tanh\left(\frac{A^{(2)}}{4}\right)$

Nuclear effective field theory on the lattice

J.-W. Chen, D. Lee, and T. Schäfer, Phys. Rev. Lett. 93, 242302 (2004)

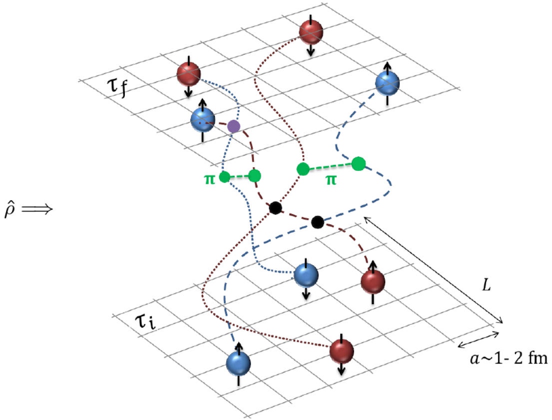


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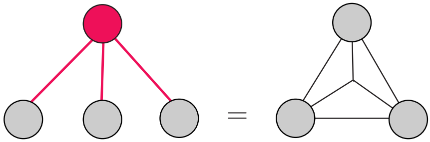
figure from Serdar Elhatisari

Three Body Interaction on the Lattice

J.-W. Chen, D. Lee, and T. Schaefer, PRL. 93, 242302 (2004).

$$Z_{int} = \exp\left(-\frac{U\alpha_t}{2}\sum_{a,b}\hat{\rho}_a\hat{\rho}_b - \frac{V\alpha_t}{6}\sum_{a,b,c}\hat{\rho}_a\hat{\rho}_b\hat{\rho}_c\right) = \int_{-\infty}^{\infty} dhP(h)\exp\left(h\sum_a\hat{\rho}_a\right)$$

Condition: $V^2 < -2\alpha_t U^3$, $\longrightarrow$ Impossible for Repulsive Interactions, $U > 0$



$$\exp\left(-\frac{U\alpha_t}{2}\sum_{a,b}\hat{\rho}_a\hat{\rho}_b - \frac{V\alpha_t}{6}\sum_{a,b,c}\hat{\rho}_a\hat{\rho}_b\hat{\rho}_c\right) = \mathcal{N}\sum_h e^{Ch+h\sum_{\mu=1}^{3}W_\mu\hat{\rho}_\mu}$$

No Conditions on U, V

*

Qubits: Introduction

- Qubit $\equiv$ spin $1/2$, two state system
- n qubits $\equiv$ 2^n states of n spin $1/2$ particle system
- Gate $\equiv$ unitary operator acting on qubits
- Only certain gates are available

  1. One qubit gates $\longrightarrow$ rotations in $SU(2)$
  2. Two qubit gates $\longrightarrow$ controlled rotations

- every other gate can be obtained from them

The state of one qubit

Generic State

$$|\Psi\rangle = \cos(\tfrac{\theta}{2})|0\rangle + e^{-i\phi}\sin(\tfrac{\theta}{2})|1\rangle$$

Z gate (phase flip)

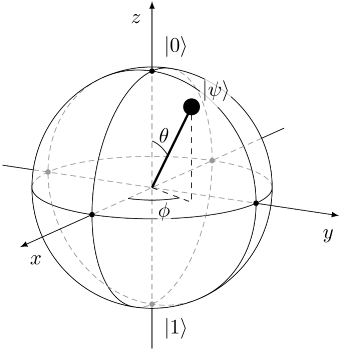
$$\hat{Z}\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

X gate (NOT)

$$\hat{X}|0\rangle = |1\rangle,\ \hat{X}|1\rangle = |0\rangle$$

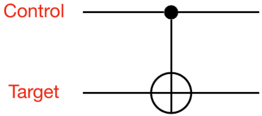
RY gate

$$e^{-i\alpha/2\hat{Y}} = \cos(\tfrac{\alpha}{2})\hat{I} - i\sin(\tfrac{\alpha}{2})\hat{Y}$$



Modifying the state of two qubits

Controled X Gate (CNOT)



Target ↘ ↙ Control

$$|00\rangle \leftrightarrow |00\rangle$$

$$|01\rangle \leftrightarrow |11\rangle$$

$$|10\rangle \leftrightarrow |10\rangle$$

$$|11\rangle \leftrightarrow |01\rangle$$

Gate Based Quantum Computing

- Initial state $|\Psi_0\rangle = |0, 0....\rangle$
- Apply unitary operators, e.g:
  - Single qubit — rotation $(e^{-i\sigma^{x,y,z}\alpha})$
  - Two qubit — controlled operation (CNOT)
- Measure

Encode arbitrary operators

Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of ComputingJune 2019Pages 193–204

Block Encoding

$$U_B = \begin{pmatrix} B/\alpha & * \\ * & * \end{pmatrix} \Rightarrow B = \alpha \left(\langle 1 | \otimes \mathbb{1} \right) U_B \left(|1\rangle \otimes \mathbb{1} \right)$$

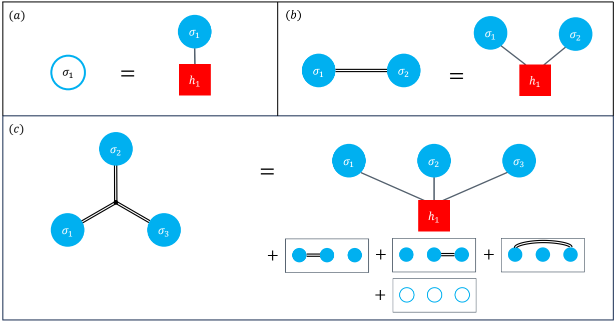
- B is an arbitrary matrix embedded into a larger unitary matrix U_B.
- It requires post-selection on the ancilla qubit.
- The application is probabilistic.

Unitary RBM: Imaginary time propagator

E. Rrapaj, E.Rule, arxiv 2403.17273

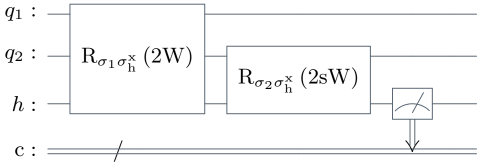
Two body term

$$
\begin{aligned}
e^{-K\sigma_1\sigma_2} =& A\sum_{h=\pm 1} e^{-iW(\sigma_1+s\sigma_2)h}, \\
=& 2A\ \left(\mathbb{1}\otimes\langle\pm 1|\right) e^{-iW(\sigma_1+s\sigma_2)\sigma_h^x}\left(\mathbb{1}\otimes|\pm 1\rangle\right), \text{(block encoding)}
\end{aligned}
$$



Unitary RBM: Quantum circuit

E. Rrapaj, E.Rule, arxiv 2403.17273



Success probability: $P = 1 - (1 - e^{-4|K|})\alpha,\ \alpha \equiv P(q_1 = sq_2), s = \text{sign}(K)$

- Ground state: unaffected, $P = 1$
- Excited state: decreases exponentially, $P = e^{-4|K|}$

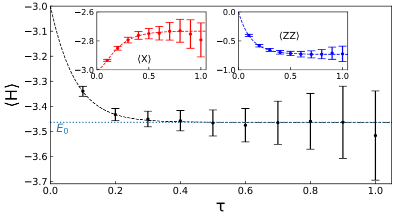
Higher order operator

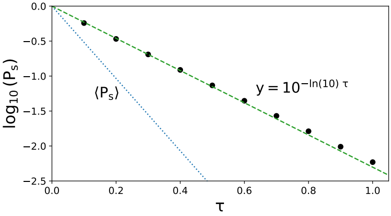
$$e^{-K \prod_i^n \sigma_i} = A\ U \left[\sum_h e^{-iW(\sigma_n^z + s\mathbb{1})h}\right] U^\dagger$$

Example: Transverse Ising model

E. Rrapaj, E.Rule, arxiv 2403.17273

- $H = \sum_i \sigma_i^z \sigma_{i+1}^z - \sum_i \sigma_i^x$
- $|\Psi_0\rangle = |+1_x\rangle\, |+1_x\rangle\, |+1_x\rangle$
- $U^{(2)}(d\tau) = e^{d\tau/2 \sum_i \sigma_i^x} e^{-d\tau \sum_i \sigma_i^z \sigma_{i+1}^z} e^{d\tau/2 \sum_i \sigma_i^x}$



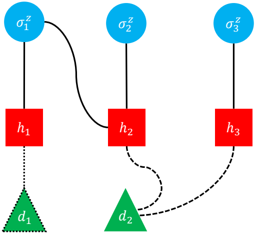


Deep Boltzmann Machines

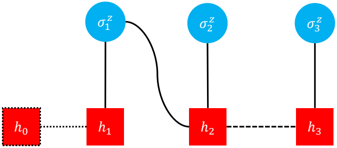
E. Rrapaj, E.Rule, arxiv 2403.17273

DBM : $\Psi_{\mathcal{D}}(\vec{z}) = \sum_{\vec{h},\vec{d}} \exp\left[i\left(\sum_i a_i z_i + \sum_{i,j} z_i W_{ij} h_j + \sum_{i,j} h_i W'_{ij} d_j + \sum_i b_i h_i + \sum_i b'_i d_i\right)\right]$

L-DBM: $\Psi_{\mathcal{L}}(\vec{z}) = \sum_{\vec{h}} \exp\left[i\left(\sum_i a_i z_i + \sum_{i,j} z_i W_{ij} h_j + \sum_{i<j} h_i L_{ij} h_j + \sum_i b_i h_i\right)\right]$



(a)

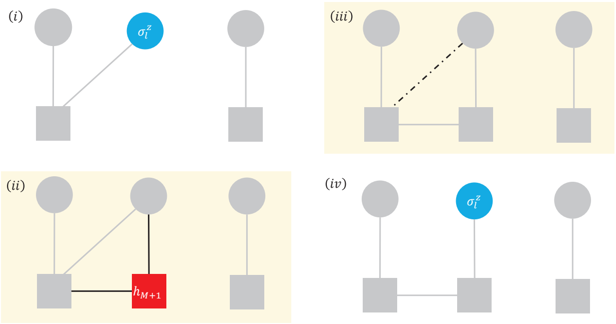


(b)

L-DBM is universal!

E. Rrapaj, E.Rule, arxiv 2403.17273

Example: Action of Hadamard Gate



Summary

RBM Propagator

Real Couplings	$\longrightarrow$	Imaginary Time (Classical Computer)
Imaginary Couplings	$\longrightarrow$	Imaginary Time (Quantum Computer)
Complex Couplings	$\longrightarrow$	Complex Time (Quantum Computer)

L-DBM Wavefunction

Real Couplings	$\longrightarrow$	Classical
Imaginary Couplings	$\longrightarrow$	Quantum

Thank You