

Breaking through the quantum barrier

Thorsten B. Wahl

Rudolf Peierls Centre for Theoretical Physics

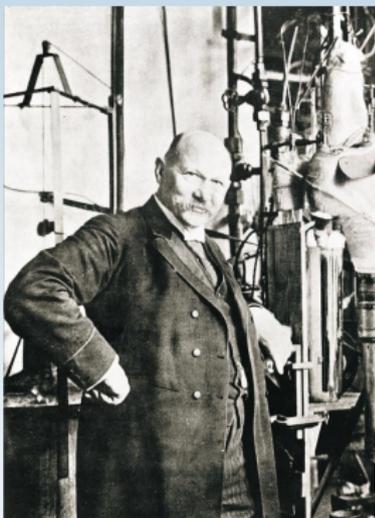
6 February 2016



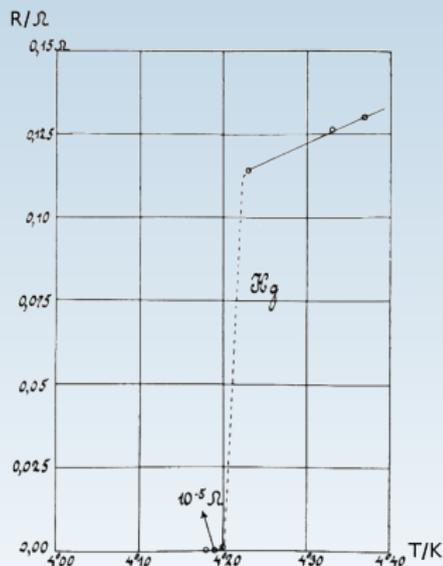
Why should we want to break through the “quantum barrier” and what is it in the first place?

Superconductivity

- 1911 Discovery of superconductivity  1913



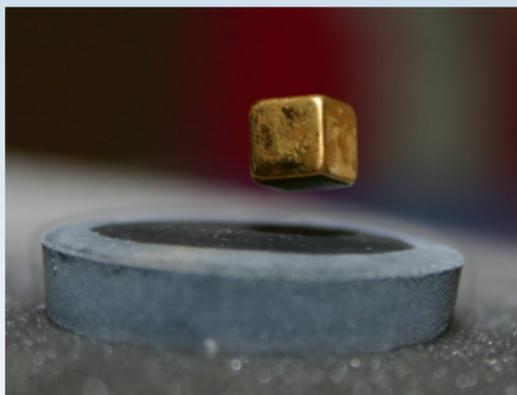
Heike Kamerlingh Onnes



- 1920s and 30s: quantum mechanics, Schrödinger equation  1933
- 1957 explanation given by Bardeen, Cooper and Schrieffer  1972

High-temperature Superconductivity

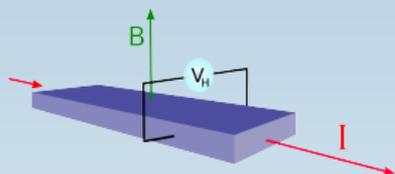
- 1986 High temperature superconductivity in $\text{La}_{1.85}\text{Ba}_{0.15}\text{CuO}_4$ (Bednorz and Müller 🏆 1987)



World record:
138 K (-135 °C)

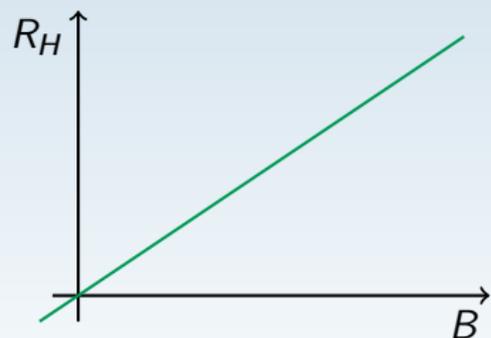
- 20?? explanation 🏆

Quantum Hall Effect

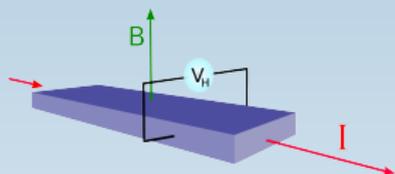


$$R_H \propto B$$

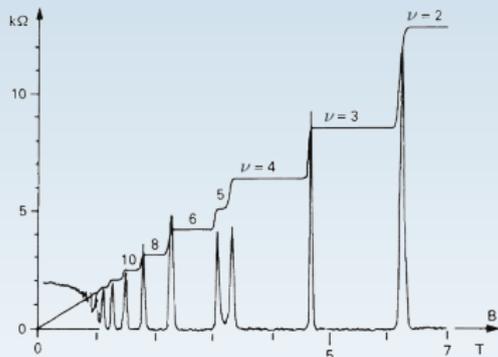
classical case:



Quantum Hall Effect



$$R_H = \frac{h}{\nu e^2}$$



K. v. Klitzing, G. Dorda, M. Pepper, Phys. Rev. Lett. 45, 494 (1980)

1980 Integer Quantum Hall Effect



1985

Why such effects are incredibly hard to describe

The Schrödinger Equation

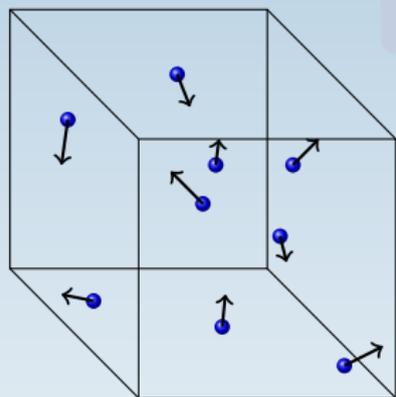
$$\left(-\sum_{i=1}^M \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{i>j=1}^M V_{\text{int}}(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i=1}^M V_{\text{ext}}(\mathbf{r}_i) \right) \psi_n(\mathbf{r}_1, \dots, \mathbf{r}_M) = E_n \psi_n(\mathbf{r}_1, \dots, \mathbf{r}_M)$$

Why such effects are incredibly hard to describe

The Schrödinger Equation

$$\underbrace{\left(-\sum_{i=1}^M \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{i>j=1}^M V_{\text{int}}(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i=1}^M V_{\text{ext}}(\mathbf{r}_i) \right)}_{\text{Hamiltonian } \hat{H}} \psi_n(\mathbf{r}_1, \dots, \mathbf{r}_M) = E_n \psi_n(\mathbf{r}_1, \dots, \mathbf{r}_M)$$

The quantum barrier



M identical particles in a box

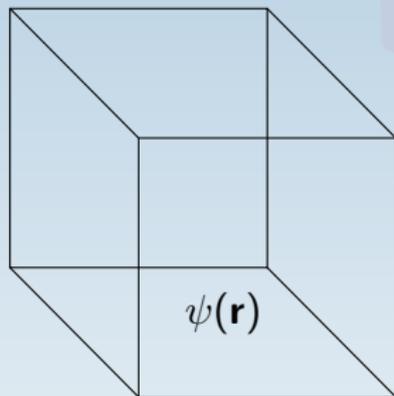
Classical system

$$\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M\}$$

$$\{\dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \dots, \dot{\mathbf{r}}_M\}$$

$\rightarrow 6M$ numbers $\in \mathbb{R}$

The quantum barrier



M identical particles in a box

Classical system

$$\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M\}$$

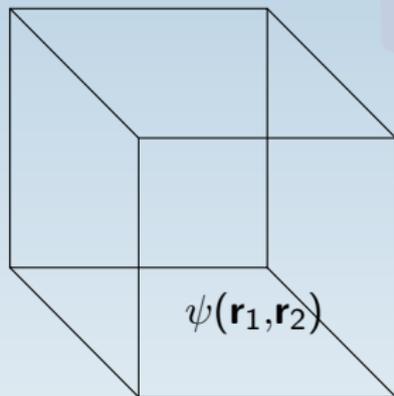
$$\{\dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \dots, \dot{\mathbf{r}}_M\}$$

$\rightarrow 6M$ numbers $\in \mathbb{R}$

Quantum mechanical problem, $M = 1$

$$\psi(\mathbf{r}) \in \mathbb{C}, \rho(\mathbf{r}) = |\psi(\mathbf{r})|^2$$

The quantum barrier



M identical particles in a box

Classical system

$$\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M\}$$

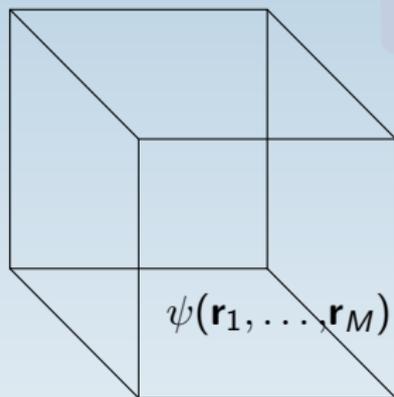
$$\{\dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \dots, \dot{\mathbf{r}}_M\}$$

$\rightarrow 6M$ numbers $\in \mathbb{R}$

Quantum mechanical problem, $M = 2$

$$\psi(\mathbf{r}_1, \mathbf{r}_2) \in \mathbb{C}, p(\mathbf{r}_1, \mathbf{r}_2) = |\psi(\mathbf{r}_1, \mathbf{r}_2)|^2$$

The quantum barrier



M identical particles in a box

Classical system

$$\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M\}$$

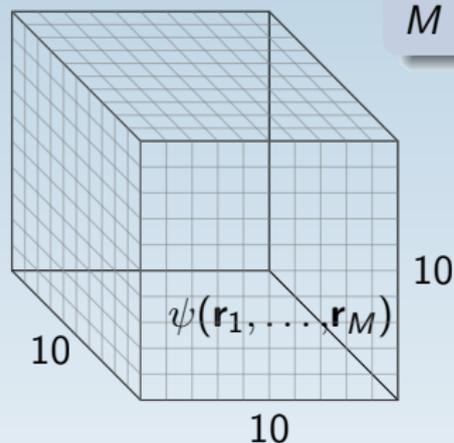
$$\{\dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \dots, \dot{\mathbf{r}}_M\}$$

$\rightarrow 6M$ numbers $\in \mathbb{R}$

Quantum mechanical problem, M arbitrary

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_M) \in \mathbb{C}, p(\mathbf{r}_1, \dots, \mathbf{r}_M) = |\psi(\mathbf{r}_1, \dots, \mathbf{r}_M)|^2$$

The quantum barrier



M identical particles in a box

Classical system

$$\{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M\}$$

$$\{\dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \dots, \dot{\mathbf{r}}_M\}$$

$\rightarrow 6M$ numbers $\in \mathbb{R}$

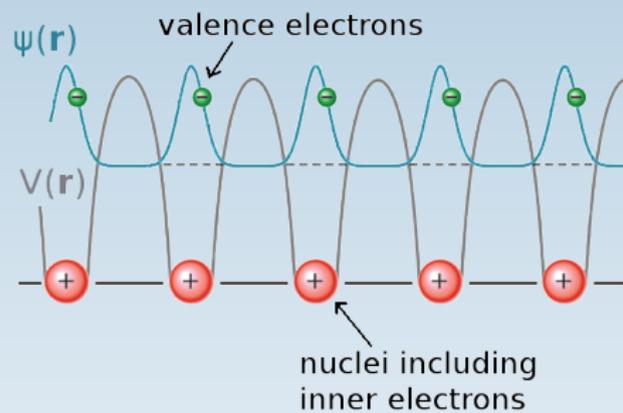
$$10 \times 10 \times 10 = 1000$$

Quantum mechanical problem

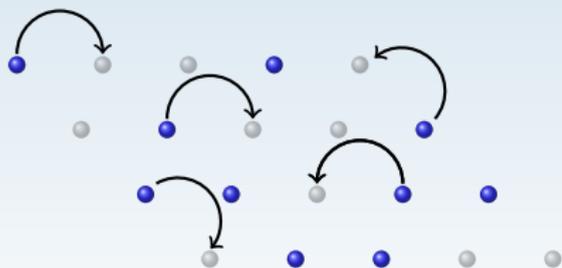
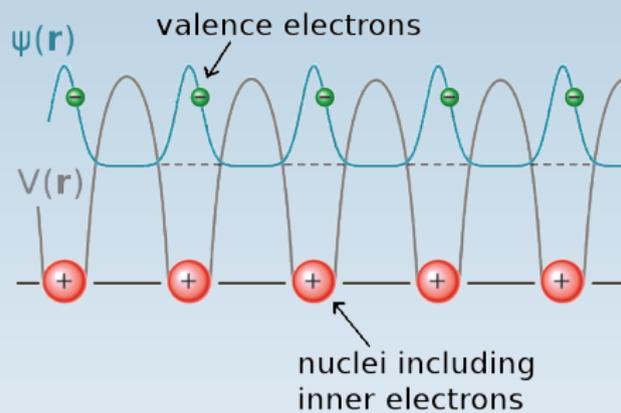
$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_M) \in \mathbb{C}, p(\mathbf{r}_1, \dots, \mathbf{r}_M) = |\psi(\mathbf{r}_1, \dots, \mathbf{r}_M)|^2$$

1000^M numbers $\in \mathbb{C}$ (impossible for $M > 4$)

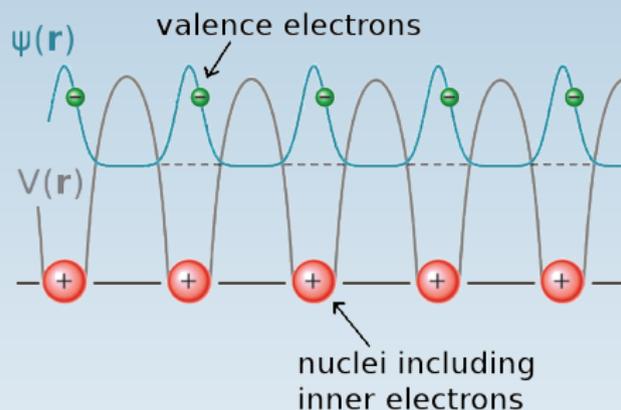
Physical motivation for a lattice model



Physical motivation for a lattice model



Physical motivation for a lattice model



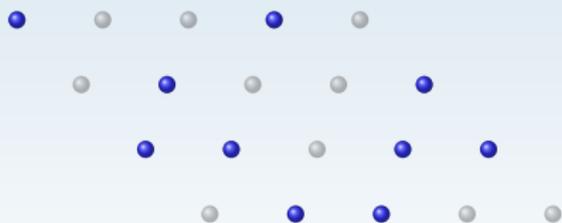
Representation of a state

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M) \rightarrow |\psi\rangle$$

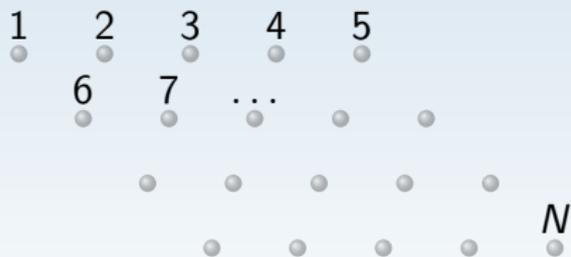
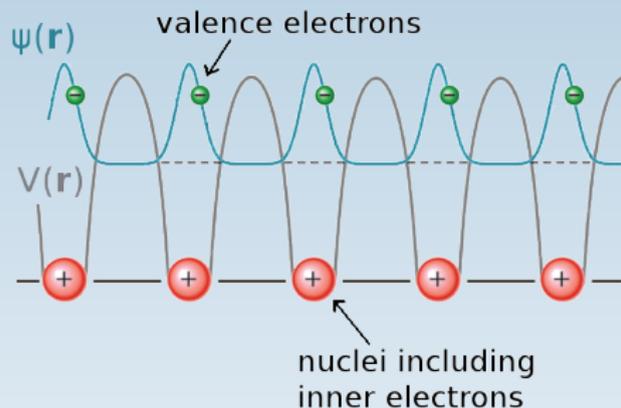
Orthonormal basis:

$$\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, \dots\}$$

$$|\psi\rangle = \sum_k c_k |\varphi_k\rangle$$



Physical motivation for a lattice model



Representation of a state

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M) \rightarrow |\psi\rangle$$

Orthonormal basis:

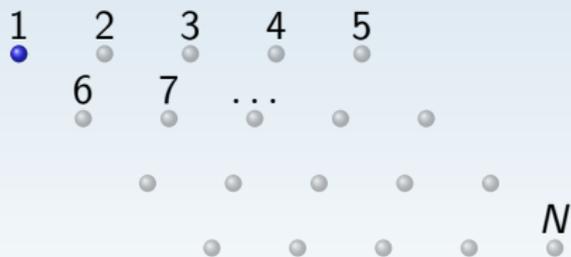
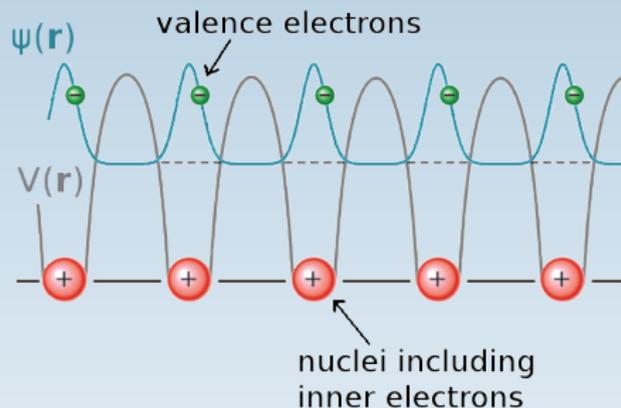
$$\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, \dots\}$$

$$|\psi\rangle = \sum_k c_k |\varphi_k\rangle$$

possible configurations:

$$|000\dots 0\rangle$$

Physical motivation for a lattice model



Representation of a state

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M) \rightarrow |\psi\rangle$$

Orthonormal basis:

$$\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, \dots\}$$

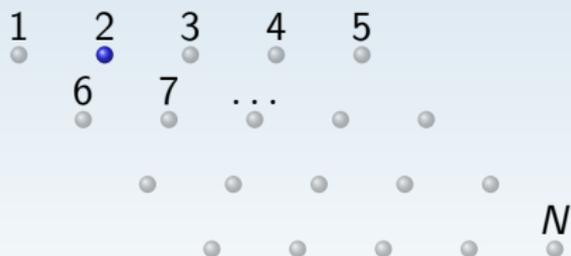
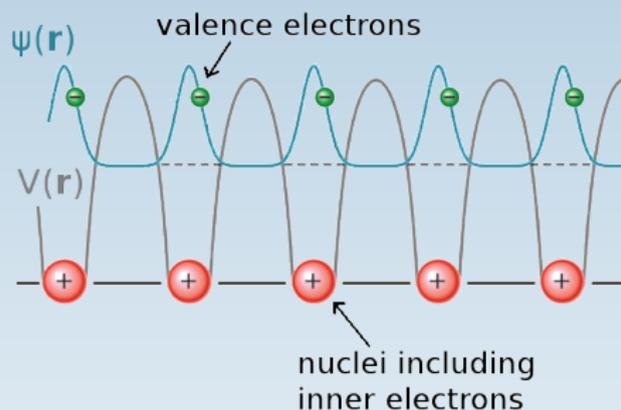
$$|\psi\rangle = \sum_k c_k |\varphi_k\rangle$$

possible configurations:

$$|000\dots 0\rangle$$

$$|100\dots 0\rangle$$

Physical motivation for a lattice model



Representation of a state

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M) \rightarrow |\psi\rangle$$

Orthonormal basis:

$$\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, \dots\}$$

$$|\psi\rangle = \sum_k c_k |\varphi_k\rangle$$

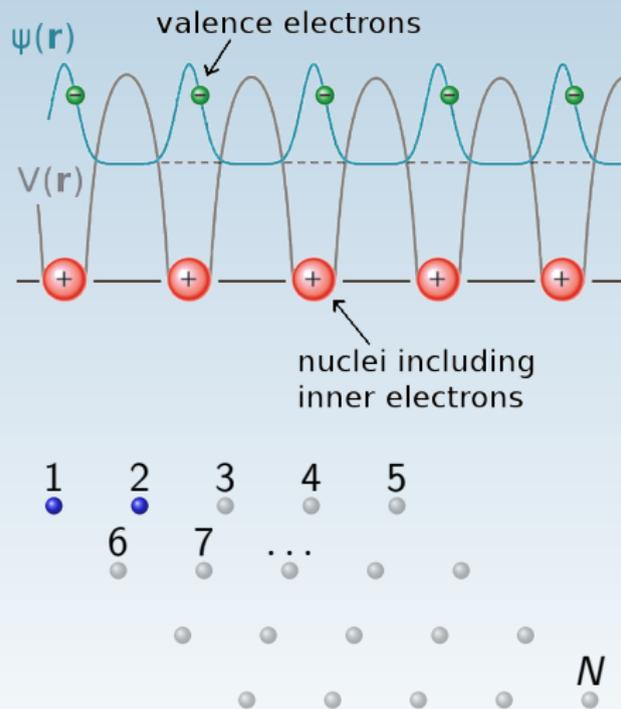
possible configurations:

$$|000\dots 0\rangle$$

$$|100\dots 0\rangle$$

$$|010\dots 0\rangle$$

Physical motivation for a lattice model



Representation of a state

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M) \rightarrow |\psi\rangle$$

Orthonormal basis:

$$\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, \dots\}$$

$$|\psi\rangle = \sum_k c_k |\varphi_k\rangle$$

possible configurations:

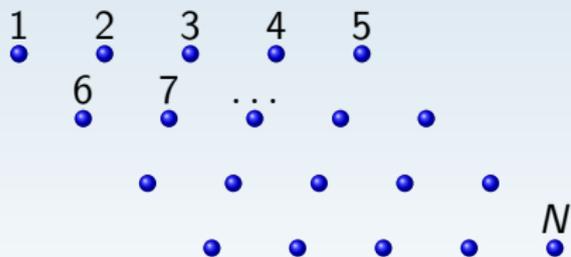
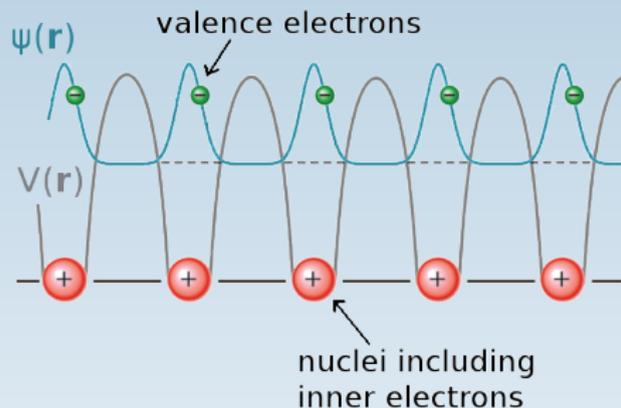
$$|000\dots 0\rangle$$

$$|100\dots 0\rangle$$

$$|010\dots 0\rangle$$

$$|110\dots 0\rangle$$

Physical motivation for a lattice model



Representation of a state

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M) \rightarrow |\psi\rangle$$

Orthonormal basis:

$$\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, \dots\}$$

$$|\psi\rangle = \sum_k c_k |\varphi_k\rangle$$

possible configurations:

$$|000\dots 0\rangle$$

$$|100\dots 0\rangle$$

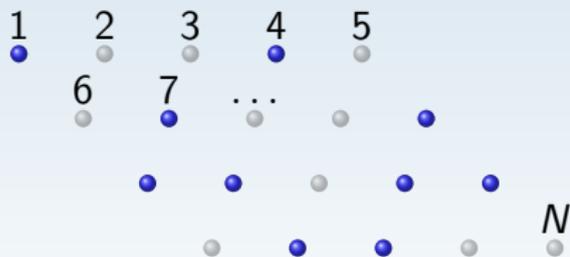
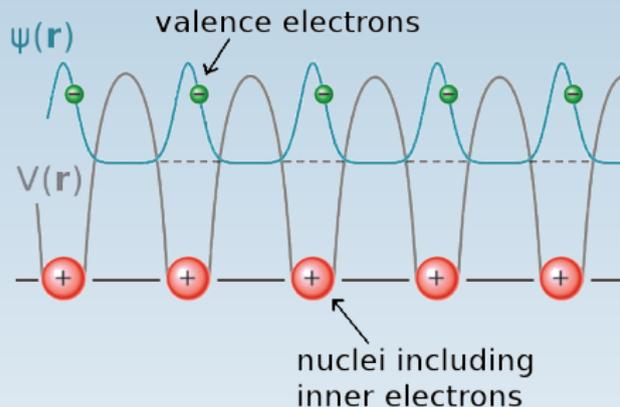
$$|010\dots 0\rangle$$

$$|110\dots 0\rangle$$

...

$$|111\dots 1\rangle$$

Physical motivation for a lattice model



usually $\frac{M}{N} = \text{const.}$

Representation of a state

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_M) \rightarrow |\psi\rangle$$

Orthonormal basis:

$$\{|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, \dots\}$$

$$|\psi\rangle = \sum_k c_k |\varphi_k\rangle$$

possible configurations:

$$|000\dots 0\rangle \quad |\varphi_1\rangle$$

$$|100\dots 0\rangle \quad |\varphi_2\rangle$$

$$|010\dots 0\rangle \quad |\varphi_3\rangle$$

$$|110\dots 0\rangle \quad |\varphi_4\rangle$$

...

$$|111\dots 1\rangle \quad |\varphi_{2N}\rangle$$

$$|\psi\rangle = \sum_{i_1, i_2, \dots, i_N=0}^1 c_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$

Problem

Calculations exponentially hard

- both in the continuum and on the lattice!

Reduction to polynomial scaling:

- 1 naïve ansatz: Hartree-Fock
- 2 Quantum Monte Carlo

Based on physical insight

- 3 sophisticated ansatz:
Tensor Network States

Idea 1: Naïve approximation ansatz - Hartree-Fock

Idea: no correlations

wave function is built of independent states for the individual electrons (= orbitals)

- exact solution for **non-interacting** electrons
- otherwise approximation of the true ground state

Idea 1: Naïve approximation ansatz - Hartree-Fock

Idea: no correlations

wave function is built of independent states for the individual electrons (= orbitals)

- exact solution for **non-interacting** electrons
- otherwise approximation of the true ground state

Advantage: easy to use

explains

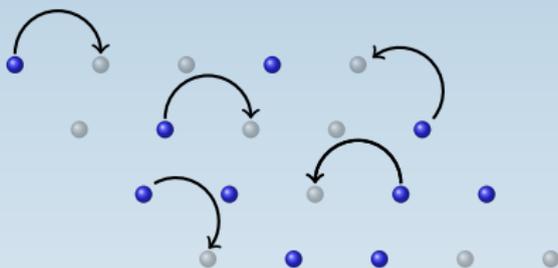
- low temperature superconductivity
- integer Quantum Hall Effect

Disdvantage: bad approximation

fails at

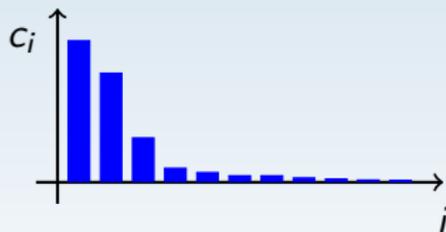
- high temperature superconductivity
- fractional Quantum Hall Effect

Idea 2: Quantum Monte Carlo



$$|\psi\rangle = \sum_{i_1, i_2, \dots, i_N=0}^1 c_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$

importance sampling



- does not work for fermionic systems (sign problem)

Idea 3 based on profound physical insight

Ground states of realistic Hamiltonians fulfil the
Area Law of Entanglement.

Idea 3 based on profound physical insight

Ground states of realistic Hamiltonians fulfil the
Area Law of Entanglement.

Entanglement

Consider the state $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

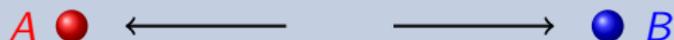


Idea 3 based on profound physical insight

Ground states of realistic Hamiltonians fulfil the **Area Law of Entanglement**.

Entanglement

Consider the state $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$



Idea 3 based on profound physical insight

Ground states of realistic Hamiltonians fulfil the **Area Law of Entanglement**.

Entanglement

Consider the state $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$



50%



Idea 3 based on profound physical insight

Ground states of realistic Hamiltonians fulfil the
Area Law of Entanglement.

Entanglement

Consider the state $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$



50%

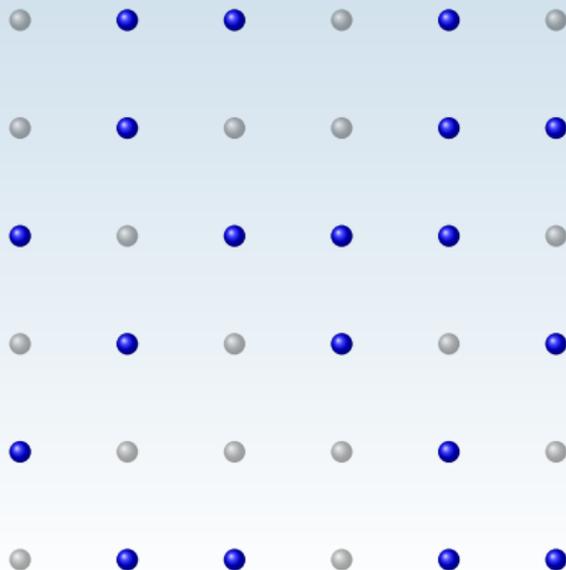


Entanglement!

No such effect for $|\psi'\rangle = |\uparrow\uparrow\rangle$.

Idea 3 based on profound physical insight

$$|\psi\rangle = \sum_{i_1, i_2, \dots, i_N=0}^1 c_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$



Idea 3 based on profound physical insight

Area Law (realistic Hamiltonians)

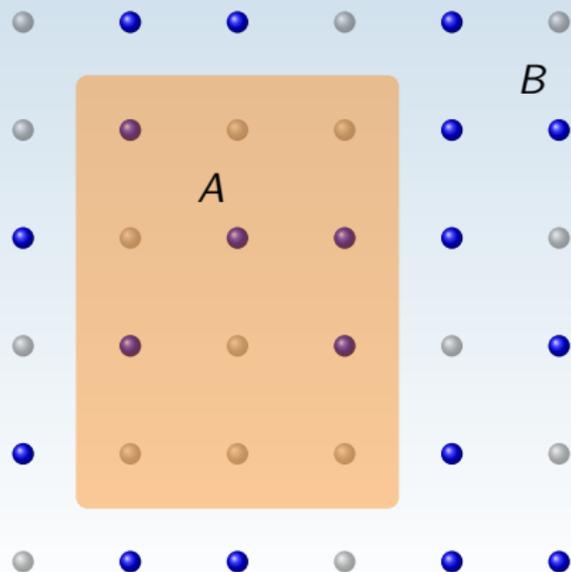
$$\text{Entanglement}(A, B) \propto \partial A$$

generic state:

$$\text{Entanglement}(A, B) \propto \text{num}(A)$$

exp. scaling $\xrightarrow{\text{Area Law}}$ poly. scaling

$$|\psi\rangle = \sum_{i_1, i_2, \dots, i_N=0}^1 c_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$



Idea 3 based on profound physical insight

Area Law (realistic Hamiltonians)

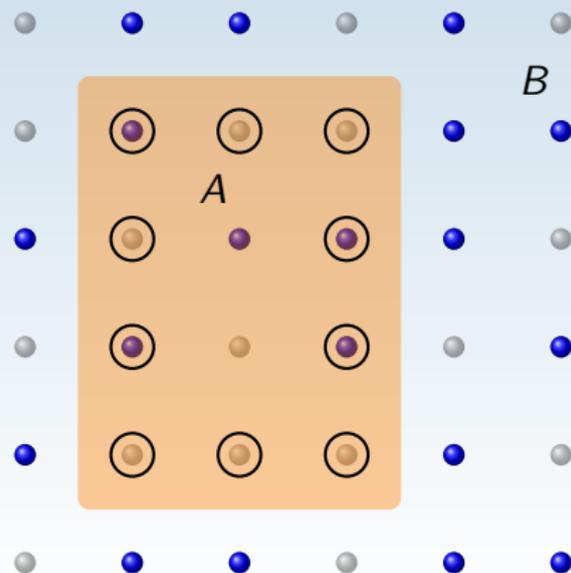
$$\text{Entanglement}(A, B) \propto \partial A$$

generic state:

$$\text{Entanglement}(A, B) \propto \text{num}(A)$$

exp. scaling $\xrightarrow{\text{Area Law}}$ poly. scaling

$$|\psi\rangle = \sum_{i_1, i_2, \dots, i_N=0}^1 c_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$



Idea 3 based on profound physical insight

Area Law (realistic Hamiltonians)

$$\text{Entanglement}(A, B) \propto \partial A$$

generic state:

$$\text{Entanglement}(A, B) \propto \text{num}(A)$$

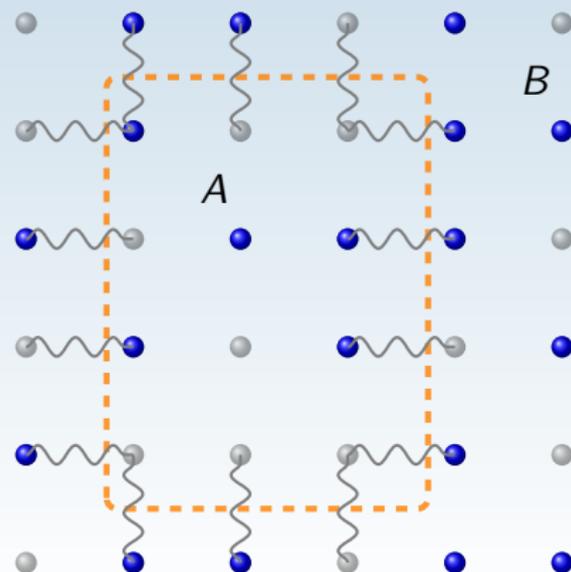
exp. scaling $\xrightarrow{\text{Area Law}}$ poly. scaling

Idea 3

Construct states that fulfil the Area Law:

Tensor Network States

$$|\psi\rangle = \sum_{i_1, i_2, \dots, i_N=0}^1 c_{i_1 i_2 \dots i_N} |i_1 i_2 \dots i_N\rangle$$



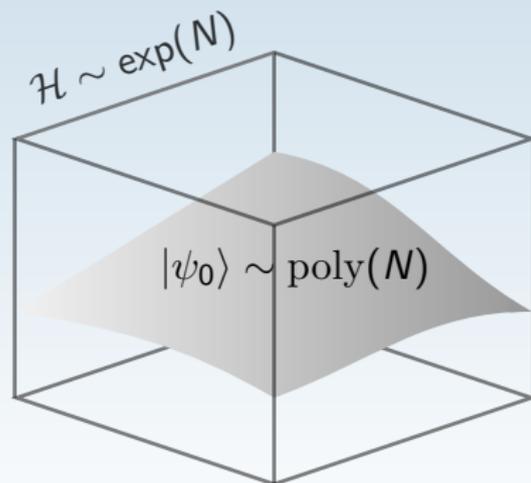
Overcoming the exponential scaling problem

Problems of previous approximation schemes

- 1 Hartree-Fock: Limited applicability
- 2 Quantum Monte Carlo: sign problem

Area Law

- strong restriction on physical ground states
- Tensor Network States



Construction of Tensor Network States

Theorem

Tensor Network States fulfil the Area Law:

- every site gets a tensor $A_{\alpha_1 \alpha_2 \dots \alpha_z}^i$
- **bond dimension:** $\alpha = 1, \dots, D, i = 0, 1$

Construction of Tensor Network States

Theorem

Tensor Network States fulfil the Area Law:

- every site gets a tensor $A_{\alpha_1 \alpha_2 \dots \alpha_z}^i$
- bond dimension:** $\alpha = 1, \dots, D, i = 0, 1$

In 1D:



Construction of Tensor Network States

Theorem

Tensor Network States fulfil the Area Law:

- every site gets a tensor $A_{\alpha_1 \alpha_2 \dots \alpha_z}^i$
- bond dimension:** $\alpha = 1, \dots, D, i = 0, 1$

In 1D:



Matrix Product States

$$|\psi\rangle = \sum_{i_1, \dots, i_N=0}^1 \underbrace{A_{\alpha\beta}^{i_1} B_{\beta\gamma}^{i_2} C_{\gamma\delta}^{i_3} \dots Z_{\omega\alpha}^{i_N}}_{c_{i_1 i_2 i_3 \dots i_N}} |i_1 i_2 i_3 \dots i_N\rangle$$

- number of parameters = $2D^2N$

Performance of Matrix Product States

Ground state energies

- extremely high accuracies
e.g., spin-1/2 anti-ferromagnetic Heisenberg chain:

	exact	numerical
E_0	-0.4431471806	-0.4431471825

Time Evolution

- optical lattice
- time-dependent Schrödinger equation

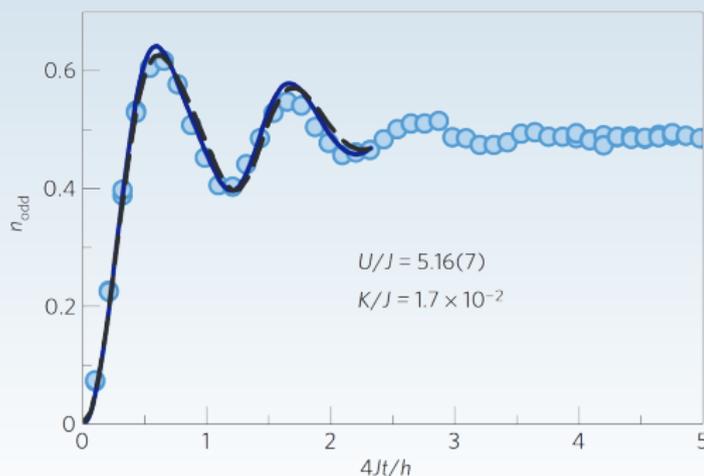
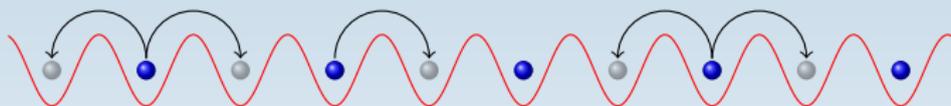
$$|\psi_{\text{init}}\rangle = |0101010101\rangle$$



Time Evolution

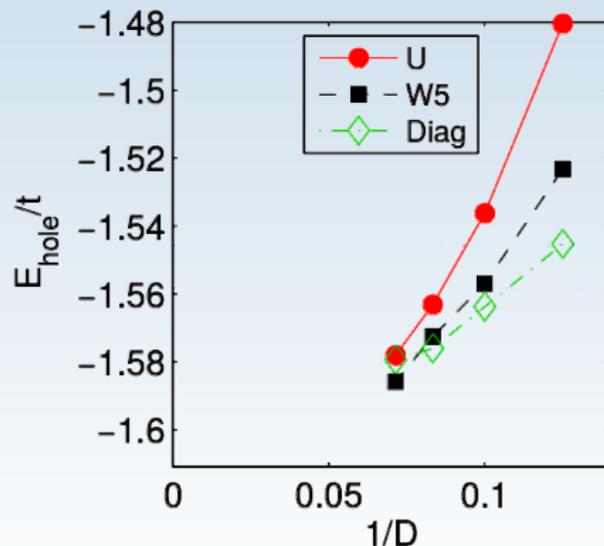
- optical lattice
- time-dependent Schrödinger equation

$$|\psi_{\text{init}}\rangle = |0101010101\rangle$$



Two dimensional Tensor Network States

- given by tensors $A^i_{\alpha\beta\gamma\delta}$, $\alpha = 1, \dots, D$
- efficient algorithms are being developed
- promising results for the Hubbard model (high temperature superconductivity):



P. Corboz, T. M. Rice, and M. Troyer, PRL 2014

2D Tensor Network States in High Energy Physics

1. Simulation with

- classical quarks
- quantum fields

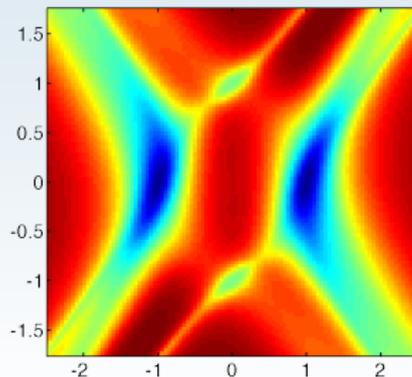
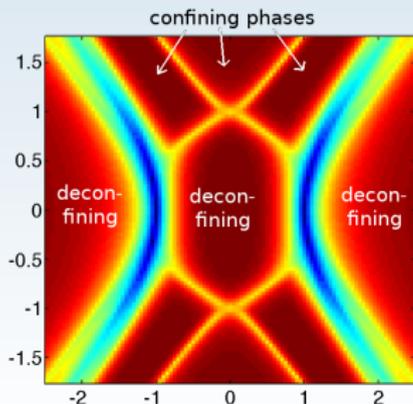
2. Simulation with

- quantum quarks (no sign problem!)
- quantum fields

Confinement:



$$E = \infty$$



Summary

Description of Quantum Matter

solving the Schrödinger equation:
exponentially hard

Tensor Network States: use Area Law \Rightarrow polynomial overhead

- no sign problem
- huge successes in 1D
- first impressive results in 2D

