# 强关联电子系统的数值方法简介


杨义峰

中国科学院物理研究所



http://hf.iphy.ac.cn


中国科学院物理研究所 Institute of Physics CAS

中国科学院 CHINESE ACADEMY OF SCIENCES

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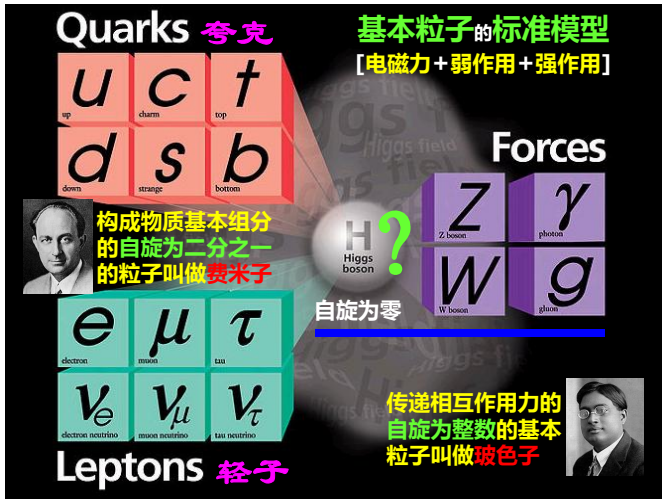
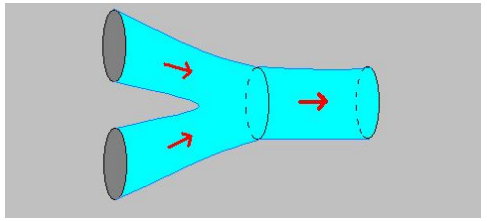
# What is Condensed Matter Physics?

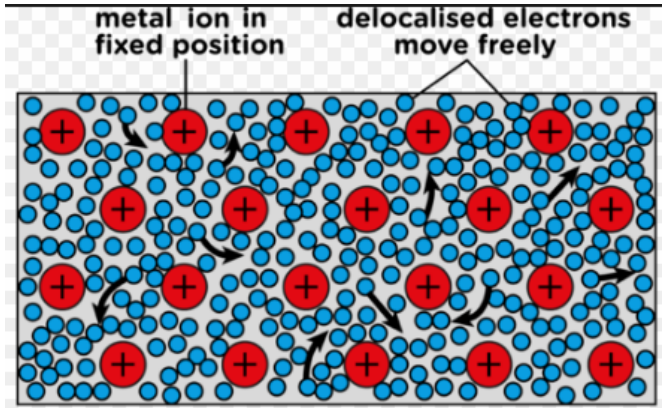
## High energy/particle physics



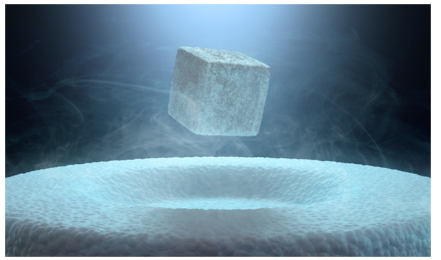

- 高能物理本质上是低能物理，从低能走向高能
- 借助加速器，观测身边“低能”世界的结构单元
- 寻找更底层 / 高能的理论，解释这些单元的成因



## Condensed matter physics



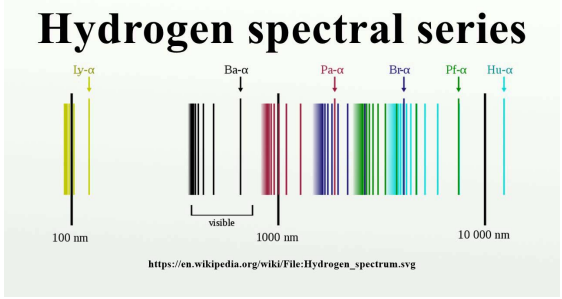

- 凝聚态物理本质上是高能物理，从高能走向低能
- 借助实验，观测电子等已知结构单元因相互作用而产生的复杂低能现象
- 已知电子模型，寻找这些现象的有效描述及其组织原则



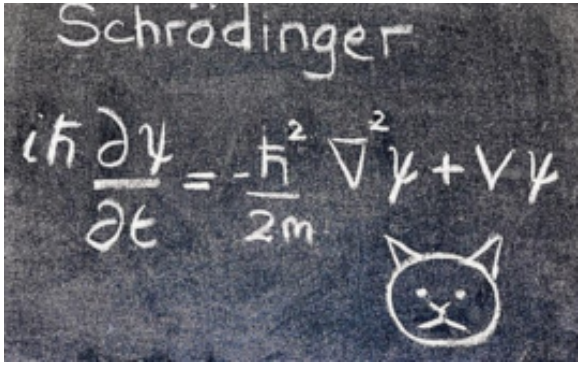
*Also known as “solid state physics” in 50s*

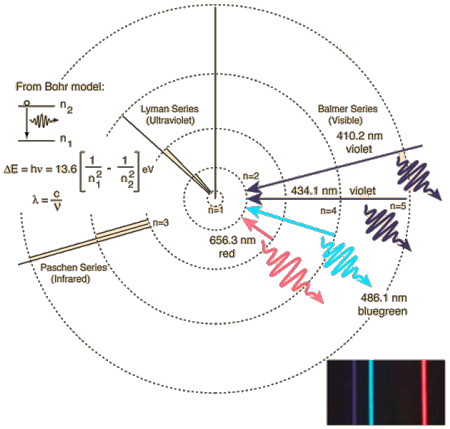
# It all begins with Quantum Mechanics/Statistics

## Quantum Mechanics



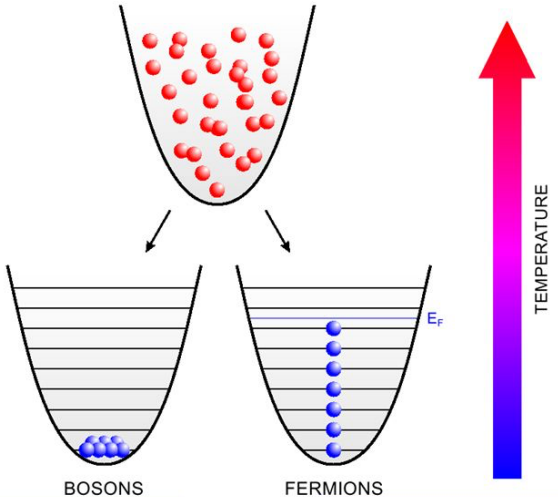

薛定谔方程的本征值$H\psi=E\psi$即为电子轨道能量




## Quantum Statistics

电子为费米子，满足Pauli不相容原理




- 零温下 $\psi(r_1,\ldots,r_N)$ 满足反对易关系，无相互作用时可写为Slater行列式

$$\Psi_{(x_1,x_2,\cdots,x_n)}=\frac{1}{\sqrt{N!}}\begin{vmatrix}\chi_{i(x_1)} & \chi_{j(x_1)} & \cdots & \chi_{k(x_1)}\\ \chi_{i(x_2)} & \chi_{j(x_2)} & \cdots & \chi_{k(x_2)}\\ \vdots & \vdots & \ddots & \vdots\\ \chi_{i(x_n)} & \chi_{j(x_n)} & \cdots & \chi_{k(x_n)}\end{vmatrix}$$

$$\psi(\ldots,x_i,\ldots,x_j,\ldots)=-\psi(\ldots,x_j,\ldots,x_i,\ldots)$$

- 有限温度下用量子统计系综描述，引入配分函数

$$Z=\mathrm{Tr}\exp(-H/k_BT)=\sum\exp(-E_i/k_BT)$$

$$\langle O\rangle=Z^{-1}\mathrm{Tr}[O\exp(-H/k_BT)]$$

# Real materials: the density functional theory (DFT)

## The Hohenberg-Kohn theorem (1964)

$$\hat{H}^{el} = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla_{r_i}^2 - \frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{n}\sum_{\alpha}\frac{Z_\alpha e^2}{|R_\alpha - r_i|} + \frac{1}{4\pi\varepsilon_0}\sum_{i=1}^{n}\sum_{j>i}\frac{e^2}{|r_i - r_j|}$$

The Ground-State properties of any system of n-interacting particles are rigourously deduced from the electron density distribution ρ(r).

$$E_n[\psi_n] = \frac{\langle \psi_n(x_1,\cdots,x_n)|\hat{H}^{el}|\psi_n(x_1,\cdots,x_n)\rangle}{\langle \psi_n(x_1,\cdots,x_n)|\psi_n(x_1,\cdots,x_n)\rangle}$$

$$E_v[\rho] = \min_{\rho}\left\{F_{HK}[\rho] + \int \rho(r)v(r)\right\}$$

Walter Kohn was awarded with the Nobel Prize in Chemistry in 1998

**把对复杂多变量波函数的变分简化为对电子空间密度分布的变分**

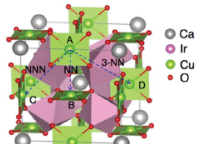
## The Kohn-Sham equation

$$\rho_s(r) = \sum_{i=1}^{n}|\phi_i(r)^2|$$

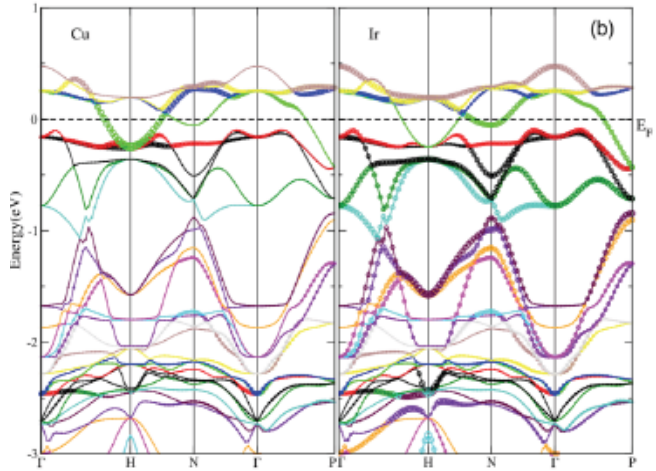
$$\sum_{i=1}^{n}\left\{-\frac{1}{2m_e}\nabla_i^2 + V_{eff}(r)\right\}\phi_i(r) = \sum_{i=1}^{n}\varepsilon_i\phi_i(r)$$

**其中有效势场 $V_{eff}$ 只存在近似公式，依赖于密度分布函数 ρ**

**或其空间梯度等，以上方程需自洽求解！**




$CaCu_3Ir_4O_{12}$

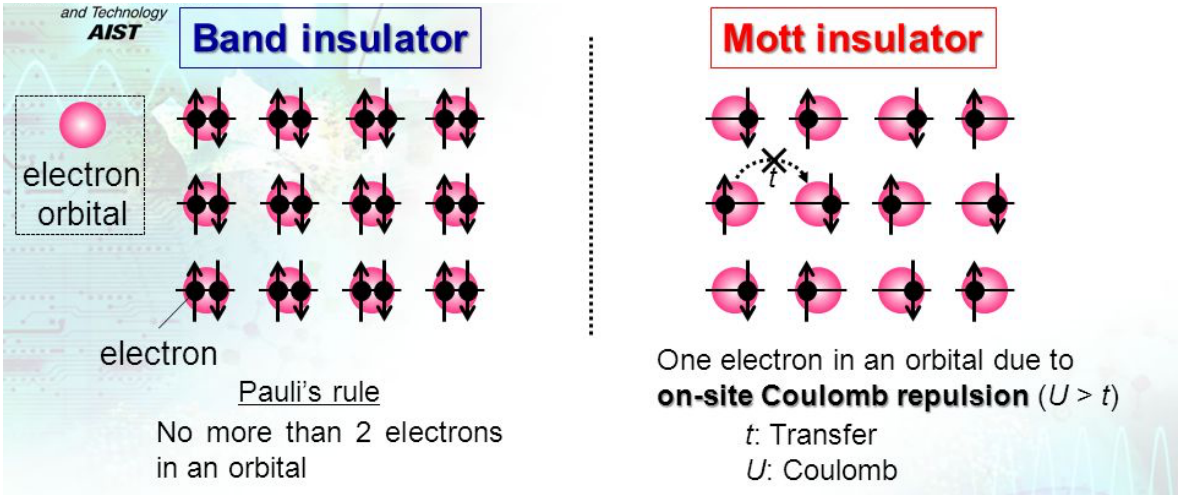


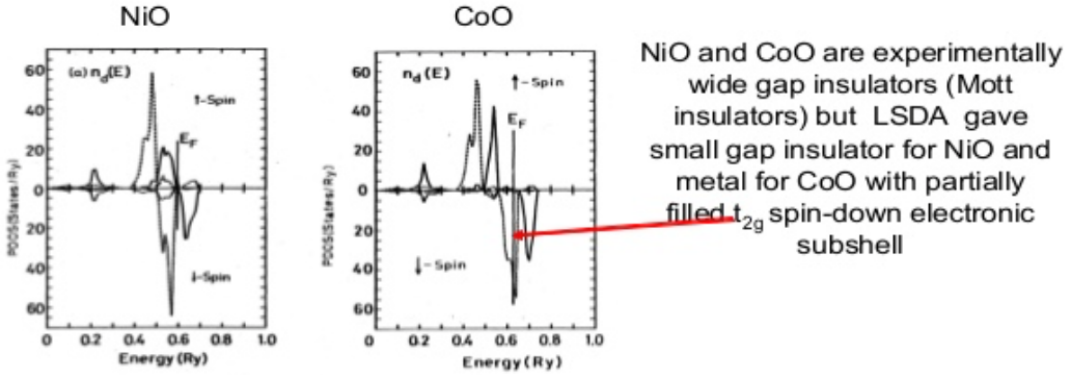

**Very successful in explaning metal and semiconductor !!!**

*Physical Review Lett.* ***111,*** *176403 (2013)*
*arXiv: 1705.00846 (2017)*

# Breakdown of the density functional theory (DFT)

## The role of electronic correlations: localization versus itinerancy

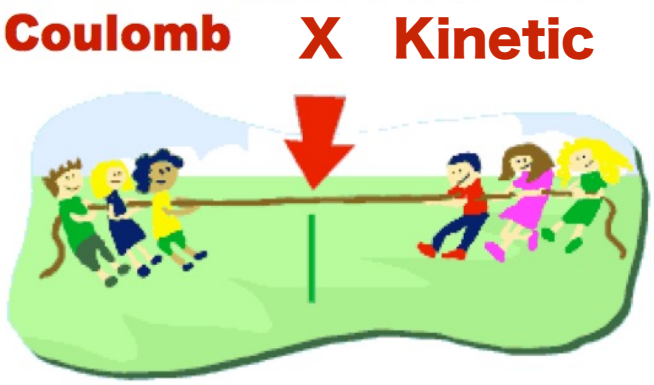



NiO and CoO are experimentally wide gap insulators (Mott insulators) but LSDA gave small gap insulator for NiO and metal for CoO with partially filled $t_{2g}$ spin-down electronic subshell

多体关联效应

$$H = H_{kinetic} + H_U$$




局域 versus 巡游

**有趣的物理往往都发生在两者交界， 如 高温超导 等等**

**缺乏共识，需要进行严格的数值求解以进行裁决！**

# There are several roads to Rome

- **Renormalization group approach**

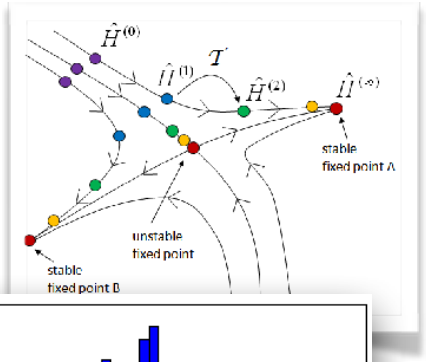
  ED/NRG/DMRG/TNRG/…

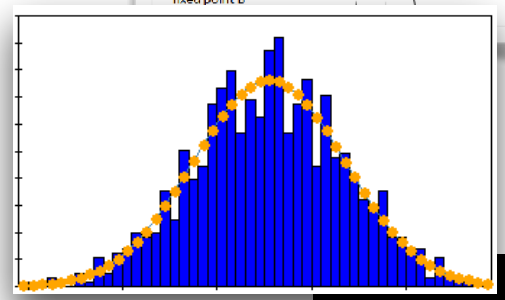
- **Monte Carlo sampling**

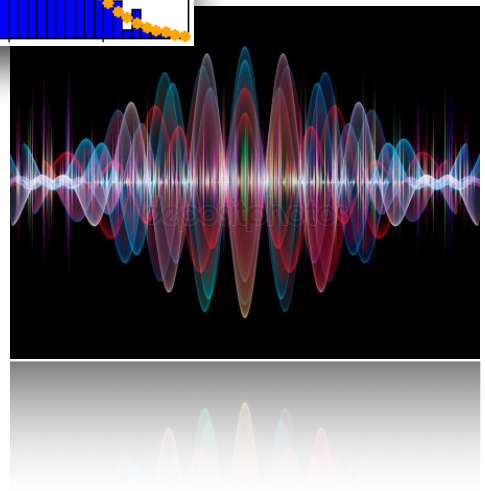
  MC/QMC/DQMC/CTQMC/…

- **Trial wave-function/variational method**

  Gutzwiller/BCS/Laughlin/…



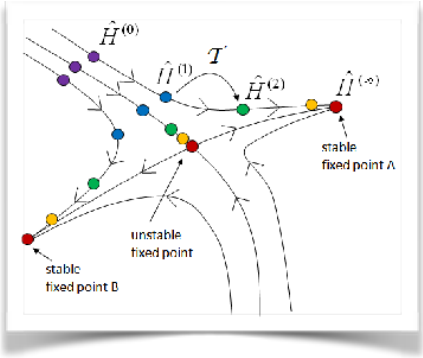


每一种方法都有其优势，但又有一定的限制范围！

很不幸的是，这些范围都没能涵盖我们最关心的实际材料中的强关联物理！

# Renormalization group approach

ED/NRG/DMRG/TNRG/…



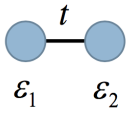
# Let's start with the exact diagonalization (ED)

## The ultimate problem is the eigenproblem

$$H|\varphi\rangle = E|\varphi\rangle$$

$$|\varphi\rangle = \sum_{\{n_i\}} \varphi(n_1, n_2, \ldots, n_N)|n_1, n_2, \ldots, n_N\rangle$$

$\varphi$为Hilbert态空间上的一个矢量；
其自然基底为每个格点上电子占据态的直积


$$\{|0\rangle_1, |1\rangle_1\} \otimes \{|0\rangle_2, |1\rangle_2\}$$

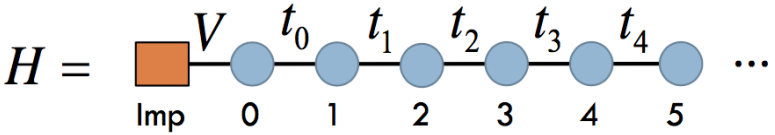
$$\underline{\underline{H}} = \begin{array}{c} \\ \langle 0,0| \\ \langle 1,0| \\ \langle 0,1| \\ \langle 1,1| \end{array} \begin{array}{c} \begin{array}{cccc} |0,0\rangle & |1,0\rangle & |0,1\rangle & |1,1\rangle \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon_1 & t & 0 \\ 0 & t & \varepsilon_2 & 0 \\ 0 & 0 & 0 & \varepsilon_1 + \varepsilon_2 \end{pmatrix} \end{array}$$

- ☑ Size of Hilbert space rise as $M = s^N$
- ☑ Computational time scales as $M^3$
- ☑ Typically only for N ≲ 10

求解基态可以采用Lanczos方法，求解激发态需要进行严格对角化，
但存在所谓的"指数墙"问题！！！

# Numerical renormalization group (NRG)

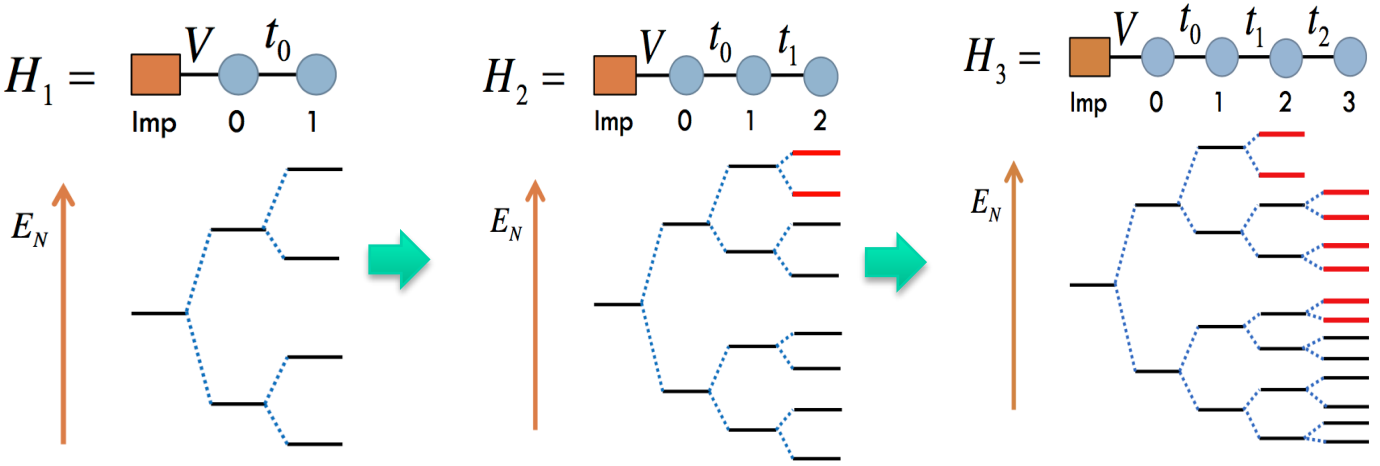
**Reduce the Hilbert space by throwing away high energy states**

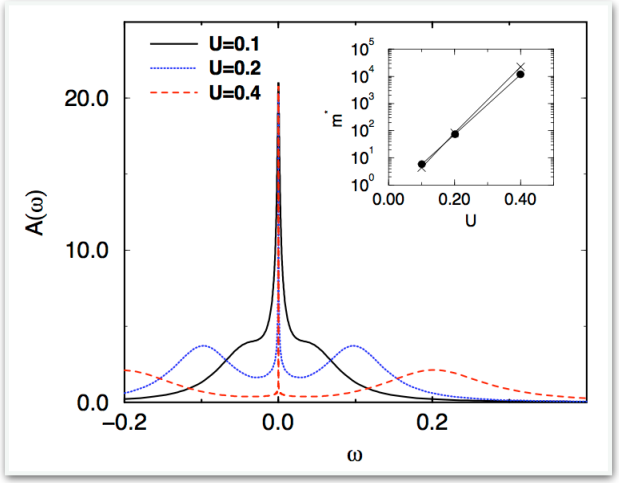



$$H_{N+1} = H_N + H^{hop}_{N+1}$$
$$H^{hop}_{N+1} = \sum_\sigma t_N c^\dagger_{N\sigma} c_{(N+1)\sigma} + \text{H.c.}$$

K. G. Wilson
Nobel prize 1982

***Iterative diagonalization & Truncation (keep fixed number of low energy states)***




*require separation of energy scales ($t_{N+1}/t_N \sim \Lambda < 1$)*

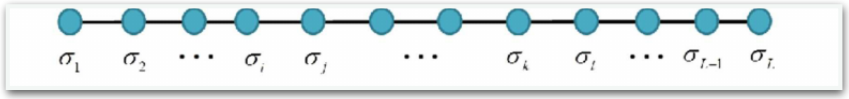
这解决了强关联物理的一大问题，即单格点（0维）的Kondo问题！

NRG方法的背后，是重整化群的思想，亦即系统随尺寸flow到固定点！

NRG方法给出了Kondo基态，但局限于较小的s（≤6），且无法处理lattice体系！

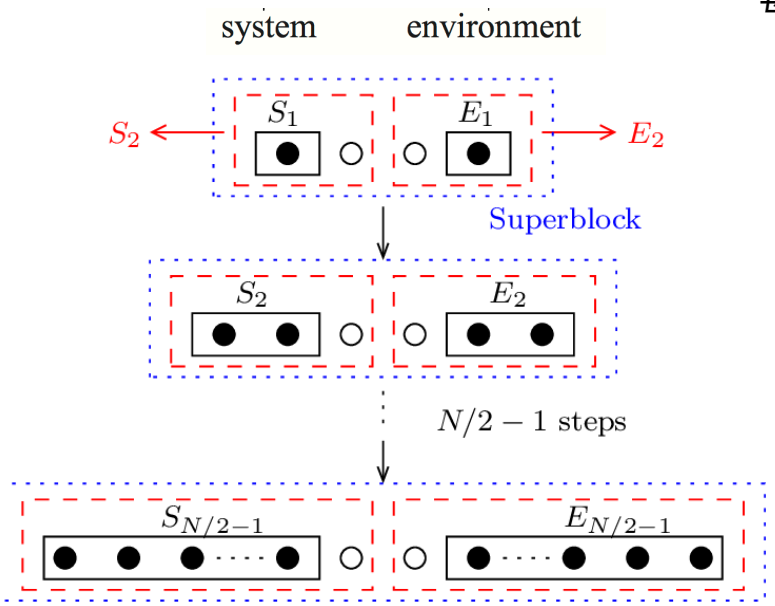
# Density matrix renormalization group (DMRG)

## Reduce the Hilbert space by keeping only states with higher weights



DMRG能够比较好地处理一维系统！

***Iterative diagonalization & Truncation (keep states of higher weights)***




每次增加格点后，计算基态，积掉环境的自由度，对得到的系统密度矩阵$\rho_{ii'}$对角化，保留固定数目的具有最大本征值的态作为系统（和环境）的基底。

求解Ms²维系统基态：

$$|\psi\rangle = \sum_{i,j} \psi_{i,j} |i\rangle |j\rangle$$

增加格点，循环

计算Ms x Ms维密度矩阵：

$$\hat{\rho} = \mathrm{Tr}_E |\psi\rangle\langle\psi|, \quad \rho_{i,i'} = \sum_j \psi_{i,j}\psi^*_{i',j}$$

对角化密度矩阵：

$$\rho = \sum_l w_l |\phi_l\rangle\langle\phi_l|$$

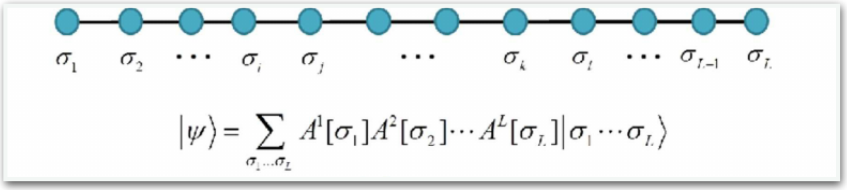
保留最大权重的M个态作为新的态空间基底

DMRG是处理一维问题的最好数值方法！

但在处理激发态与高维体系时比较困难，而现实材料很多都是2或3维的!

# Tensor network renormalization group (TNRG)

## DMRG state is a matrix-product-state (MPS)




first and last tensors have one fewer auxiliary index

$$\Psi^{n_1 n_2 n_3 \ldots n_l} = \sum_i A^{n_1}_{i_1} A^{n_2}_{i_1 i_2} A^{n_3}_{i_2 i_3} \cdots A^{n_l}_{i_l}$$

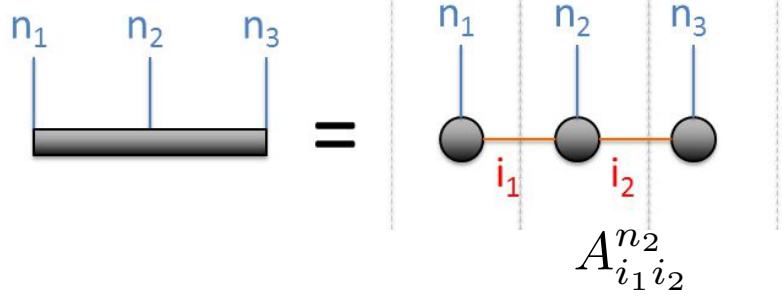
"bond" or "auxiliary" dimension
"M" or "D" or "χ"

1D structure of entanglement

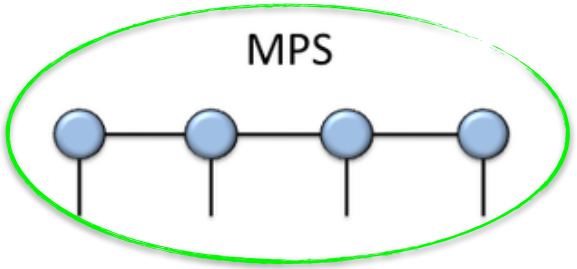
$$= \mathbf{A}^{n_1} \mathbf{A}^{n_2} \ldots \mathbf{A}^{n_l}$$

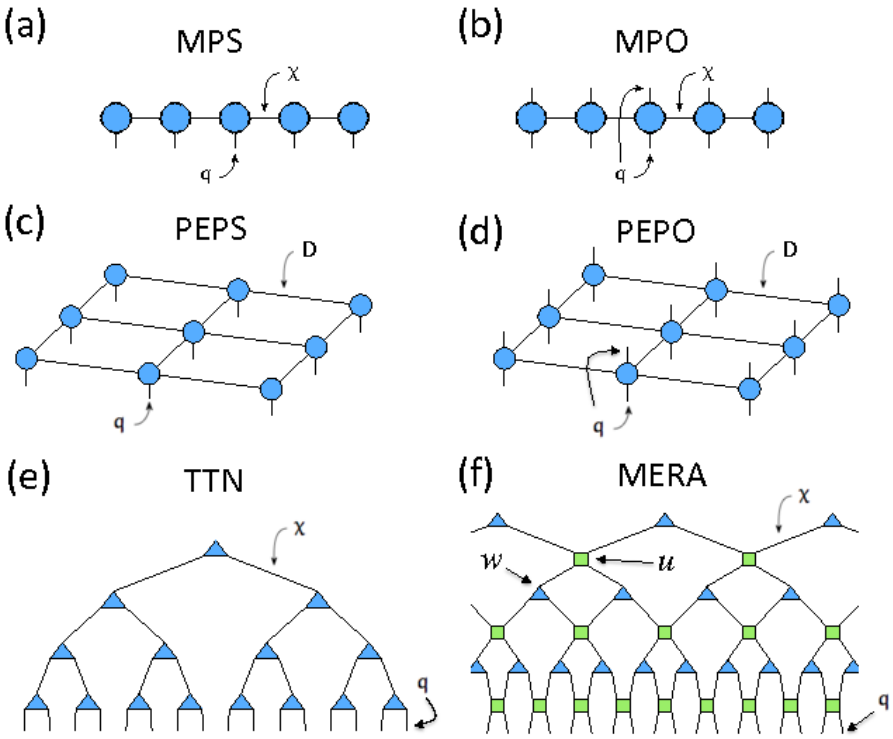
amplitude is obtained as a product of matrices

General state




MPS



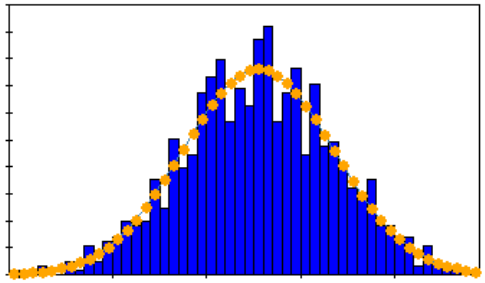

TNRG可处理高维问题，近10年正快速发展！

MPS与TNRG背后是量子多体纠缠的物理！

直观上，TNRG与机器学习方法相关！

# Monte Carlo simulation

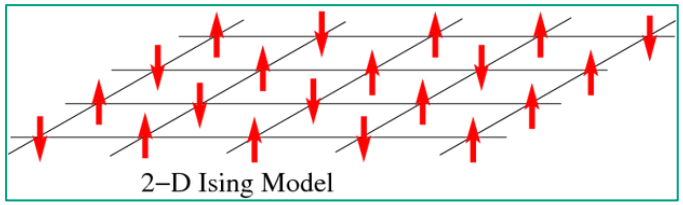
MC/QMC/DQMC/CTQMC/…



# Classical versus quantum Monte Carlo

## Classical Monte Carlo

$$H = -J\sum_{<i,j>} S_i S_j - h\sum_i S_i$$




对任一位形，H({Si})为一数

对自旋空间的所有位形按照权重取样

$$Z = \sum_{\{S_i\}} e^{-\beta H(\{S_i\})}, \quad \langle m\rangle = \sum_{\{S_i\}} \frac{1}{Z} e^{-\beta H(\{S_i\})} m(\{S_i\}) = \sum_{\{S_i\}} w(\{S_i\}) m(\{S_i\})$$

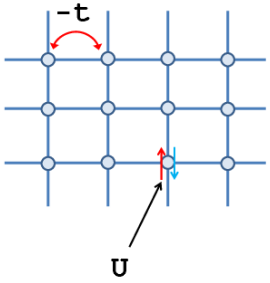
*Metropolis algorithm*

- 随机选择z，翻转自旋：$\{\overline{S}_i\} = (S_1^k, S_2^k, \ldots, -S_z^k, \ldots, S_N^k)$
- 计算前后权重的比值：$\alpha = \frac{w(\{\overline{S}_i\})}{w(\{S_i\}_k)} = e^{-\beta(H(\{\overline{S}_i\}) - H(\{S_i\}_k))} = e^{-\beta\Delta E}$
- 选择随机数$\gamma$，若$\alpha \geq \gamma$，接受新位形，否则拒绝！

---

## Quantum Monte Carlo (QMC)

$$H = U\sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} - t\sum_{<ij>\sigma} c_{i\sigma}^\dagger c_{j\sigma}$$




对任一状态，H({Si})不是数，需要构造新的位形空间！

### 多种处理方法

☑ 辅助场QMC：引入合适的经典辅助场，将费米子态积掉，得到辅助场的有效作用量，在辅助场的位形空间进行取样。

Hubbard-Stratonovich变换：

$$\exp\left[-\Delta\tau U(n_\uparrow n_\downarrow - \frac{1}{2}(n_\uparrow + n_\downarrow))\right] = \frac{1}{2}\mathrm{Tr}_\sigma[\exp[\lambda\sigma(n_\uparrow - n_\downarrow)]$$

$$Z = \sum_{\{\sigma_i\}} D(\{\sigma_i\})$$

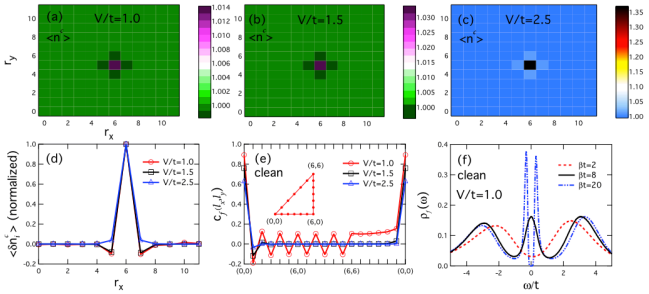
*After integrate out the "free" fermions, sample {σ} with the Metropolis algorithm*

☑ 连续时间QMC：在配分函数中将动能t项或相互作用U项做微扰展开，以自由电子(t)或孤立原子(U)为背景，对微扰展开项进行取样。

# Comment on quantum Monte Carlo Simulations

☑ **非常成功地处理一大批问题，是强关联主要方法之一**

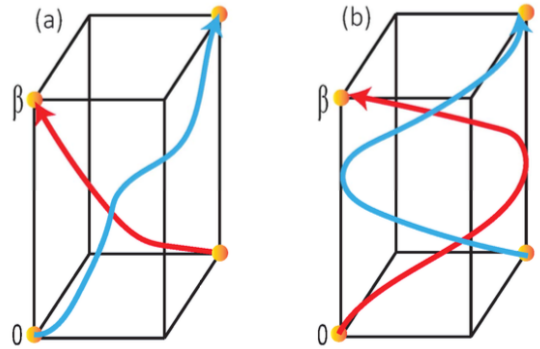
Kondo问题、Mott问题、玻色子系统等等




☑ **在很多重要的问题上，存在难以避免的“符号问题”**

费米子的交换反对称性，导致配分函数权重可能为负

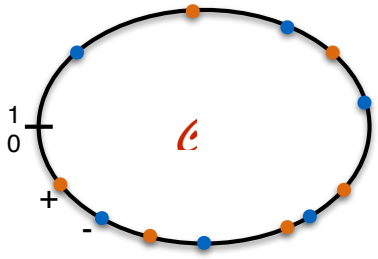
某些情况下，对称性可以抑制“符号问题”

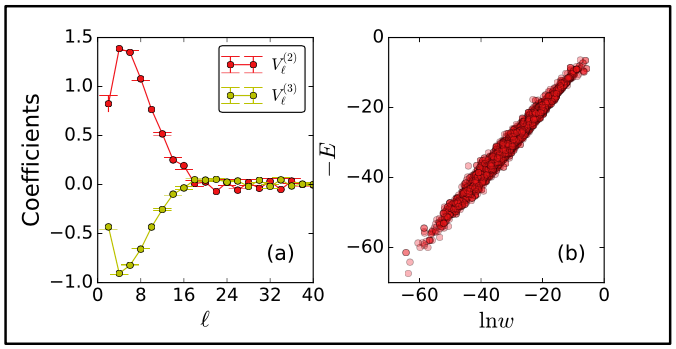



☑ **在低温和自由度较多或体系尺寸大时，计算速度慢**

要寻找可能的加速方法，如结合机器学习寻找推荐系统

$$Z / Z_0 = \sum_C \omega(C)$$



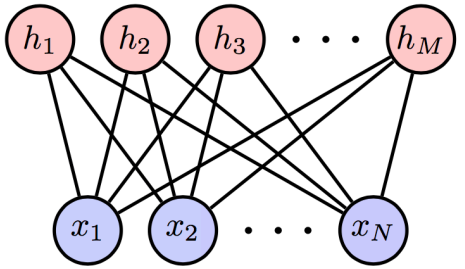




$$E_{\text{eff}}(C) = -\sum_{i,j>i}\sum_{q_i,q_j=\pm} V_{q_i q_j}(x_j^{q_j} - x_i^{q_i}) + \mu k + E_0$$

*Phys. Rev. E 95, 031301 (2017)*

Restricted Boltzmann Machine

$$E(\{x_i\},\{h_j\}) = \sum_i a_i x_i + \sum_j b_j h_j + \sum_{ij} x_i W_{ij} h_j$$




$$e^{-H_{RBM}(h)} \equiv \sum_{\{x_i\}} e^{-E(\{x_i\},\{h_j\})}$$

$$= e^{-\sum_j b_j h_j} \prod_i (1 + e^{a_i + \sum_j W_{ij} h_j})$$

## Trial wave function/variational method

Gutzwiller/BCS/Laughlin/…

# Construct trial wave function using neural network

## An well-known example of the trial wave functions

The goal is to find a good approximation of the ground state wave function

$$E_n[\psi_n] = \frac{\langle \psi_n(x_1,\cdots,x_n) | \hat{H}^{el} | \psi_n(x_1,\cdots,x_n) \rangle}{\langle \psi_n(x_1,\cdots,x_n) | \psi_n(x_1,\cdots,x_n) \rangle}$$

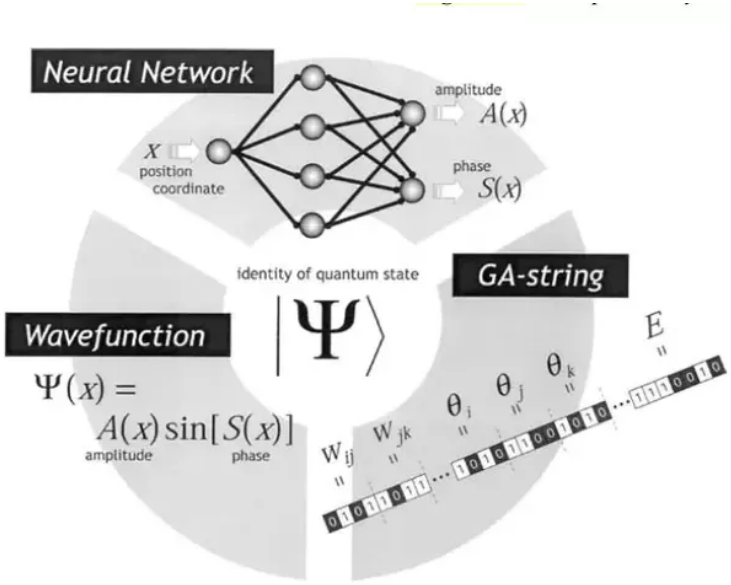
$$\psi_{\mathrm{RVB}} = \mathcal{P}_{\mathrm{N}} \mathcal{P}_{\mathrm{G}} \psi_{\mathrm{BCS}}$$

Jastrow factor
concerning the short-range correlation
due to strong on-site repulsion

Quasi-particle wave function
concerning the long-range correlation
due to the BCS Hamiltonian

**把复杂的求基态多体波函数的问题，转变为对有限几个自由参量求变分的问题**

## The neural network as a trial wave function




**就我目前了解，机器学习方法还没有能够真正帮助解决凝聚态物理的任何困难问题；**

**反过来，凝聚态物理的方法似乎对理解神经网络提供了一些新的视角。**

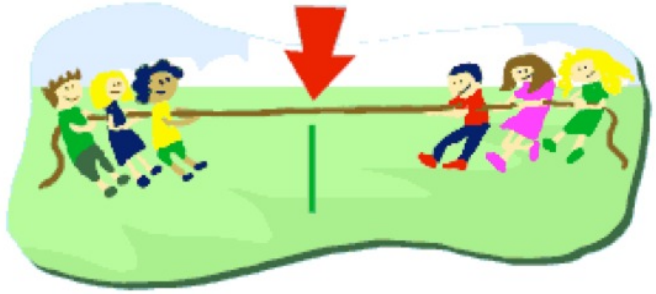
# Summary

- **Various approaches to solve correlated electron systems**
  - ☑ weak correlation: density functional theory (DFT); *extension of DFT?*
  - ☑ strong correlation: NRG/DMRG/*TNRG*; MC/QMC/CTQMC

- **Each method has its own advantages and problems**
  - ☑ computational cost, dimensionality, sign problem, uncontrolled approximation
- **It is demanding in order to settle down the already exhausting debates**
  - ☑ Too many uncertainties, no consensus so far; *is machine learning useful?*


***Unusual richness of strongly correlated materials !!!***

**Coulomb X Kinetic**



局域 versus 巡游