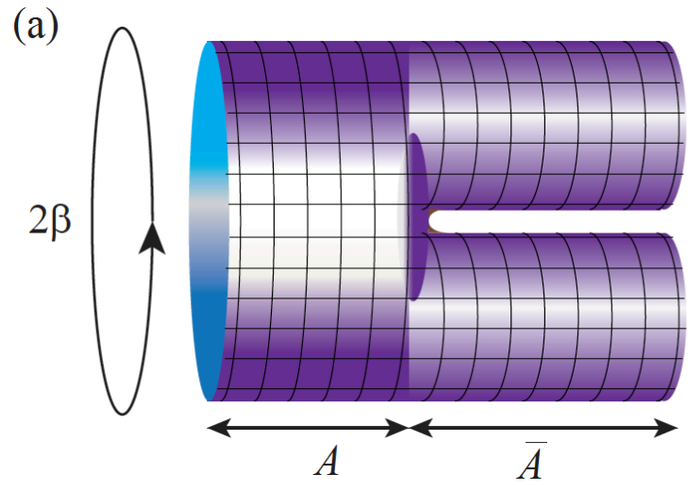
Computational Physics

PHYS4150/8150 (6 credits)

Place: MW T2

Time : Mon 14:30-15:20
Thu 13:30-14:20; 14:30-15:20

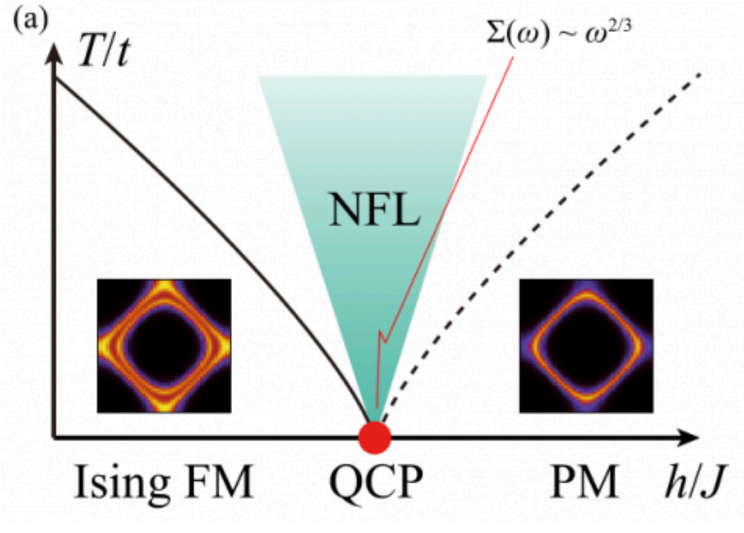




https://quantummc.xyz/teaching/hku-phys4150-8150-2023/

Teacher: Zi Yang Meng (zymeng@hku.hk), HOC 231

Tutor: Min Long (u3009934@connect.hku.hk), HOC 217
Menghan Song (songmh@connect.hku.hk) , HOC 217

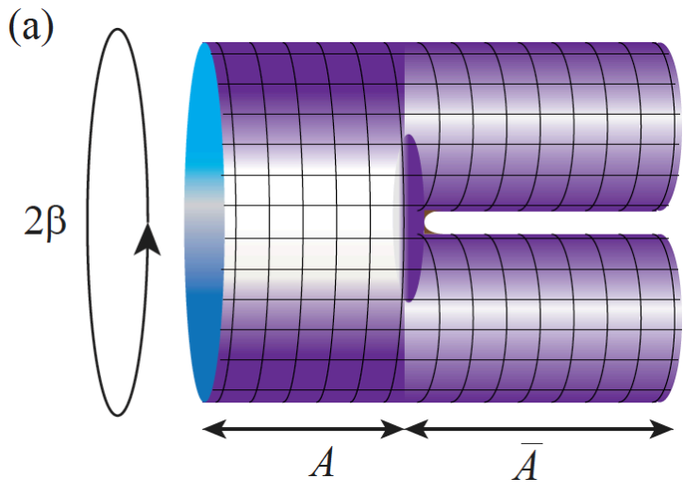


Computational Physics

Teaching Materials:

https://quantummc.xyz/teaching/

Slides
Reading materials
Python Notebooks
Assignments



Literature: Books, there are many, actually too many

- Andi Klein and Alexander Godunov, Introductory Computational Physics, Cambridge 2010
- Tao Pang, An Introduction to Computational Physics, Cambridge University Press 2012
- J.M. Thijssen, Computational Physics, 2nd Edition, Cambridge University Press 2012
- L. Böttcher and H.J. Herrmann, Computational Statistical Physics, Cambridge University Press 2021

Computational Physics

Course Learning outcomes

- demonstrate knowledge in essential methods and techniques for computation in physics
- solve differential equations governing the dynamics of physical systems
- learn matrix methods for eigenvalue problems
- apply Monte Carlo and other simulation methods to solve classical and quantum few-body and many-body problems
- use effective written and verbal communication skills through presentation

Pre-requisites

- MATH3301 or 3401, 3403, 3405
- PHYS3350, 3351, 3450, 3550
- PHYS2160 (Introductory computational physics)
- PHYS3151 (AI & Machine learning in physics)

Assessment Methods and Weighting

- Assignments 30%
- Presentation 20%
- Project report 20%
- Exam 30%

Content



0. Introduction

1. Differential equations
   1.1 Classical equation of motion (classical mechanics, pendulum)
   1.2 Partial differential equation relaxation methods (electromagnetism, diffusion)
   1.3 Partial differential equation in space-time (traffic flow, tsunami)

2. Eigenvalue problem
   2.1 Schrödinger equation and Hamiltonian (Harmonic oscillator, wave package)
   2.2 Quantum lattice model and Hibert space (Heisenberg model)
   2.3 Exact diagonalization of spin chain (Spin wave, Haldane conjecture, topology)
   2.4 Matrix product state and density matrix renormalization group (DMRG)

Content



3. Statistical and many-body physics

3.1 Classical Monte Carlo and phase transitions (Ising model and critical phenomena)

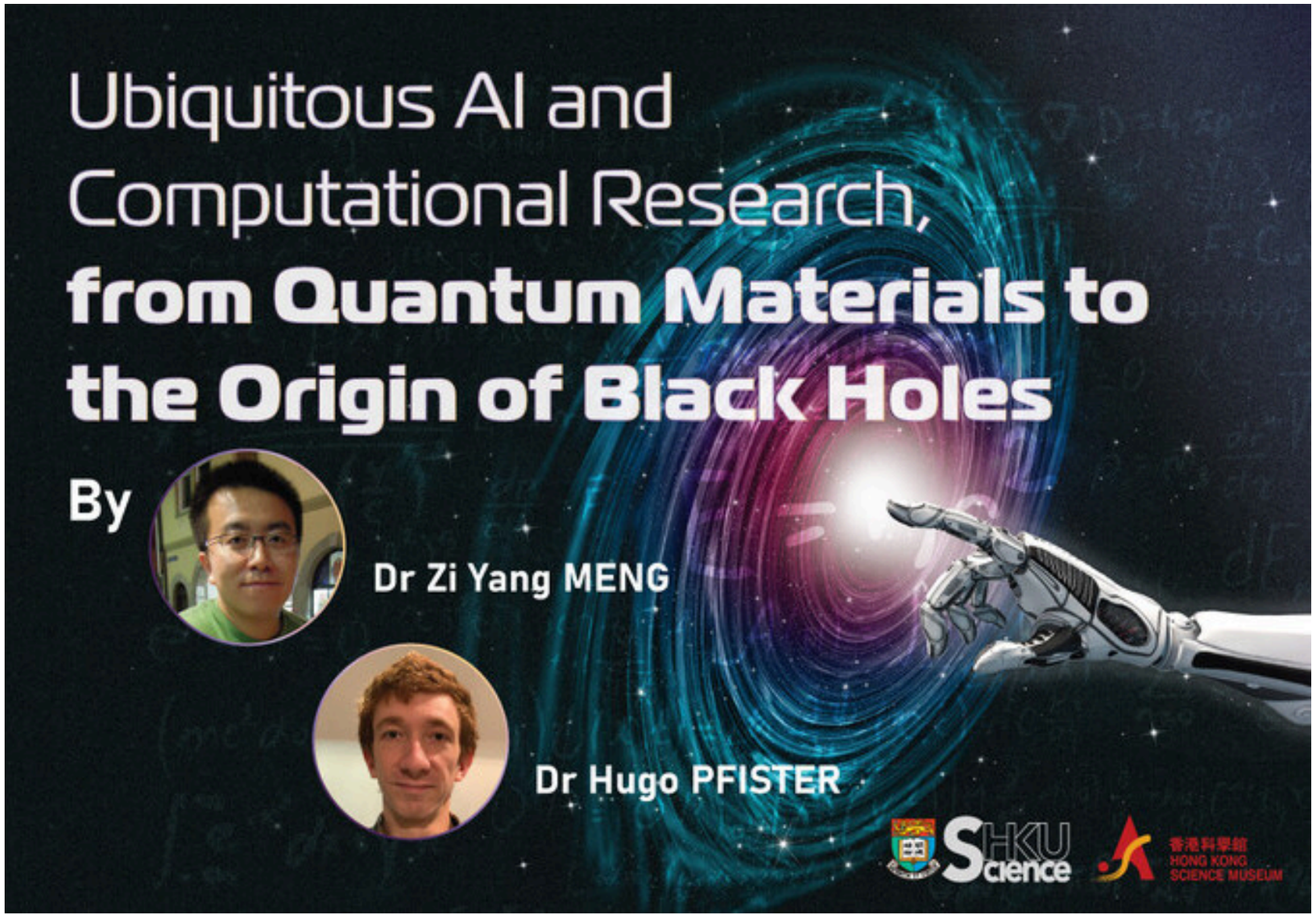
3.2 Quantum Monte Carlo methods (Path-integral and cluster update)

4. Machine learning in physics and High performance computation

4.1 AI in quantum physics

4.2 HPC and parallelism

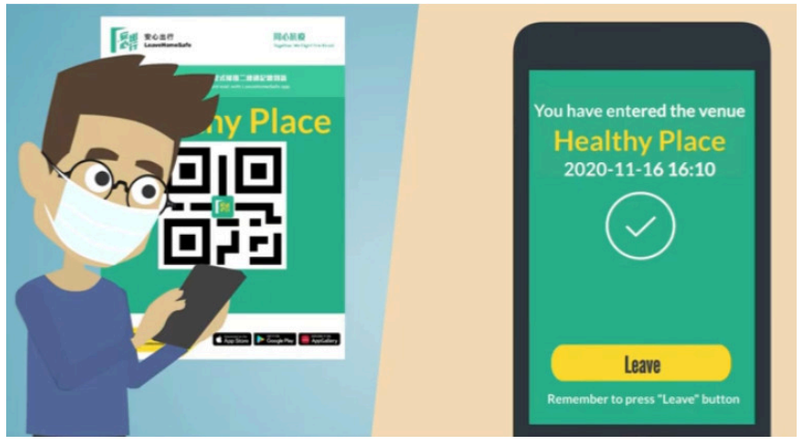
4.3 …



Hong Kong Science Museum 01/15/2022

https://www.scifac.hku.hk/events/ai-computational-research

Computation is everywhere



QR / Face Recognition

In April 2017, AlphaGo vs. Jie Ke





- The machine played perfect…
- I am so behind, unbelievable…
- AlphaGo is not the God, but it is a superior species than human being…

AlphaGo

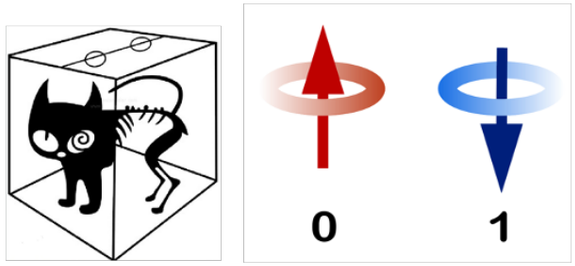


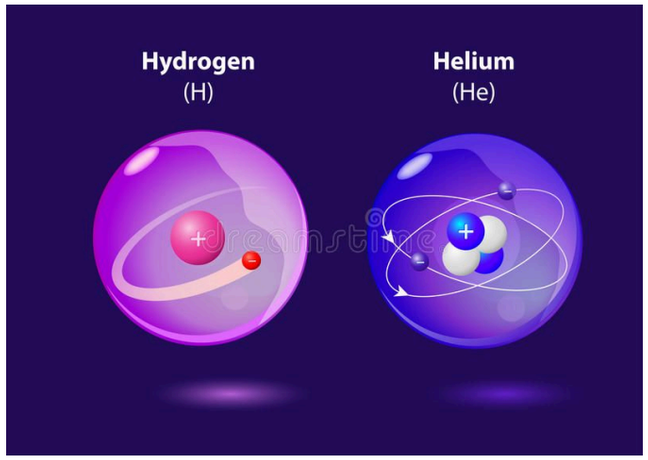
Smart Robots https://www.bostondynamics.com/

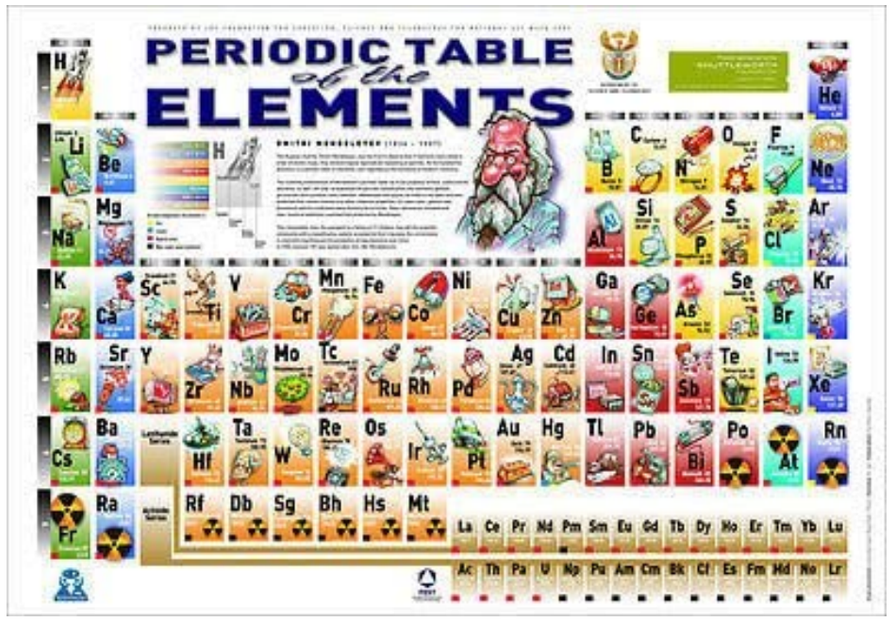


Self-driving Car

Computation on quantum bit and quantum entanglement







Lead to the famous "exponential wall"

Krishna and Radha playing chaturanga

Multi-electron atoms, cannot be solved exactly







2^N

$N = 10 \quad 2^{10} = 1{,}024 \sim 10^3$

$N = 20 \quad 2^{20} = 1{,}048{,}576 \sim 10^6$

$N = 30 \quad 2^{30} = 1{,}073{,}741{,}824 \sim 10^9$ right now

$N = 40 \quad 2^{40} = 1{,}099{,}511{,}627{,}776 \sim 10^{12}$

$N = 50 \quad 2^{50} = 1{,}125{,}899{,}906{,}842{,}624 \sim 10^{15}$

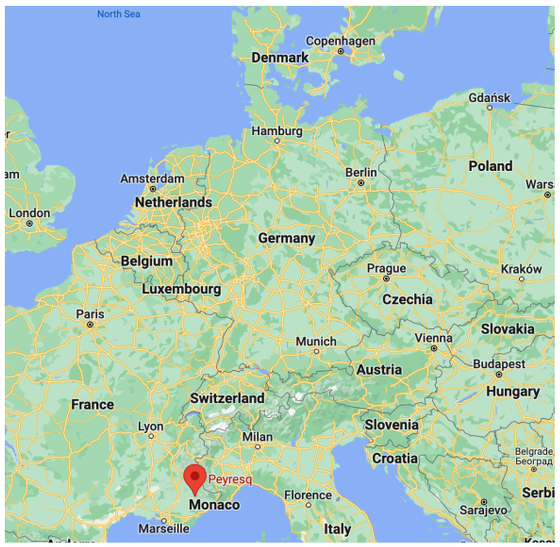
Wheat grains on chessboard — Sissa ibn Dahir, inventor of Chaturanga

$2^{64} - 1 = 18{,}446{,}744{,}073{,}709{,}551{,}615$ grains of wheat,
weighing about 1,199,000,000,000 tons.
About 1,645 times the global production of wheat.

Solving exponentially complex problem in polynomial time

Computation has interesting history

- The relation between the modern quantum Monte Carlo simulation and the Opium war and Hong Kong



Azure Coast
Cannes, Nice, Monaco





Metropolis and Monte Carlo

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

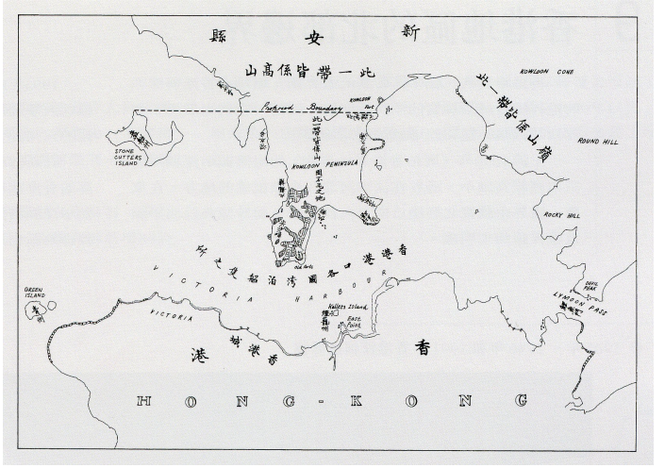
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

Burning of the summer palaces



Late Qing Dynasty
1856-1860 2nd Opium war

Convention of Peking



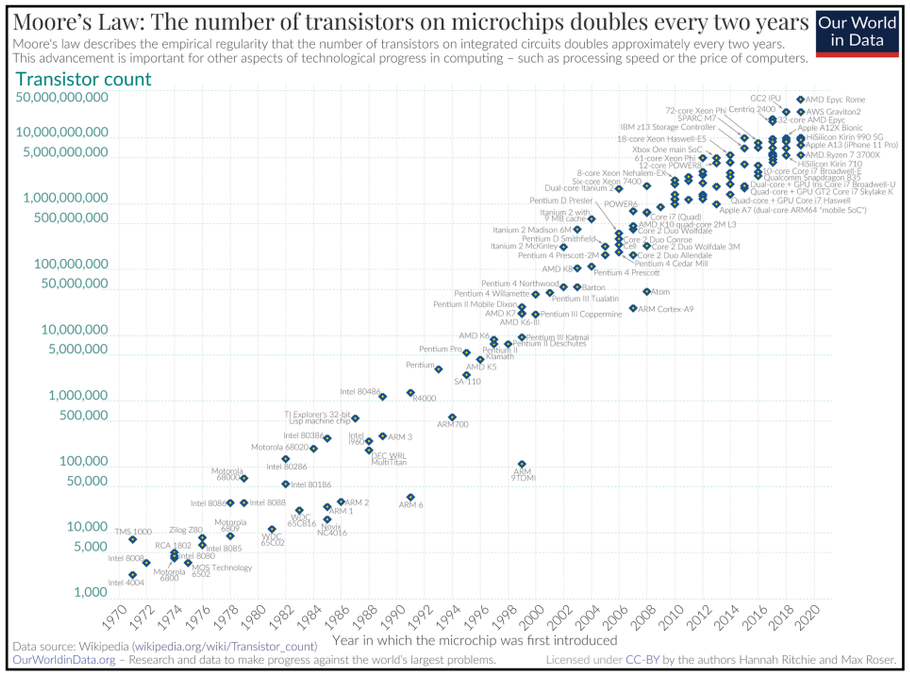
8 million taels of silver apiece

Casino de Monte Carlo
Since 1865

Computation becomes easy

50 years of supercomputer tracks Moore's law

 # transistors doubles every 2 years



Floating-point operations per second: FLOPS

GigaFlOPS: 10^9

TeraFLOPS: 10^12

PetaFLOPS: 10^15

ExaFLOPS: 10^18



国家超级计算天津中心 National SuperComputer Center in Tianjin

Tianhe-1 (天河1号): 5 PetaFLOPS



K-computer (京): 10 PetaFLOPS

国家超级计算广州中心 NATIONAL SUPERCOMPUTER CENTER IN GUANGZHOU

Tianhe-2 (天河2号): 100 PetaFLOPS



	Supercomputer	Personal Computer	Human Brain
Computational Units	32,000 Xeon CPUs 10^12 transistors	4 CPUs, 10^9 transistors	10^11 neurons
Cycle time	10^-9 sec	10^-9 sec	10^-3 sec
Operations/sec	10^15	10^10	10^17
Memory updates/sec	10^14	10^10	10^14
Weight / Space	150 tons / Basketball court	1 Kg / A4 Paper	1.5 Kg / 1/6 basketball
Power consumption	500 megawatt	100 watt	20 watt

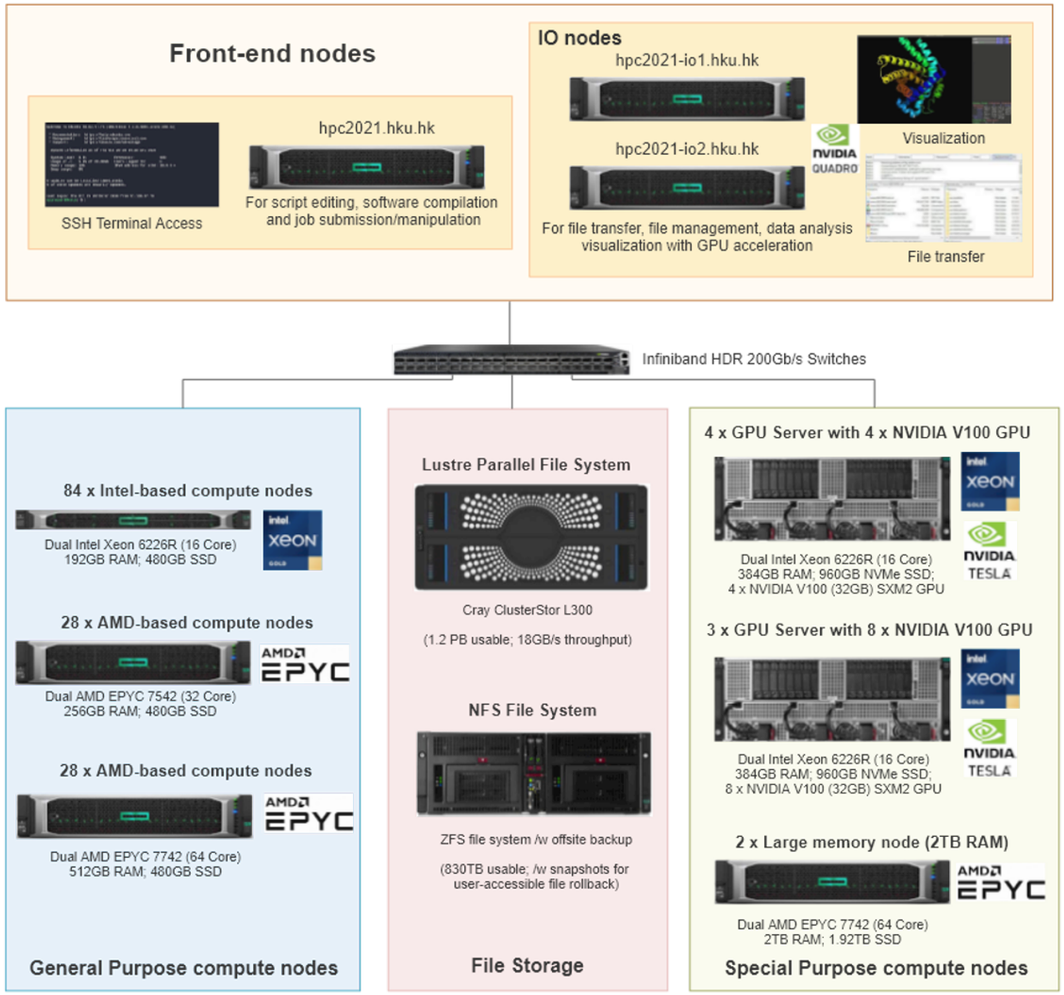




Sunway TaihuLight (神威·太湖之光) Fugaku (富岳)

HPC2021

8064 cpu cores



Tianhe-II: 16,000 node, 24 Intel Xeon E5 core CPU, 384,000 in total

2023/11

AMD 7702P (64 core) x 2 x 10 = 1280 cores
AMD 7573X (32 core) x 2 x 1 = 64 cores
AMD 7763 (64 core) x 2 x 7 = 896 cores
AMD 9654 (96 core) x 2 x 2 = 384 cores

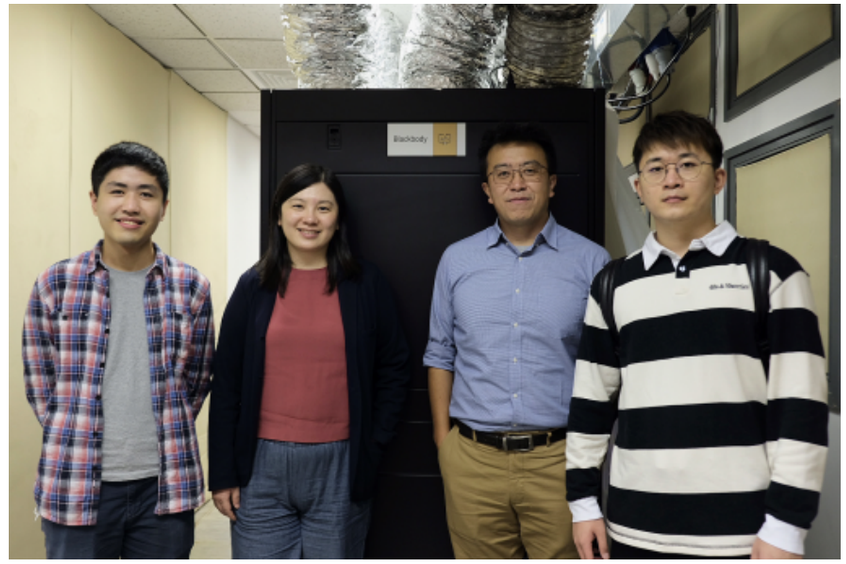
Intel(R) Xeon(R) Gold 6226 (12 cores) 2 x 2 =48 cores (head node)
Intel(R) Xeon(R) Platinum 9242 (48 cores) 2 x 4 = 384 cores (computation node)

3056 CPU cores

Our own Blackbody

1024 cpu cores

2022/09

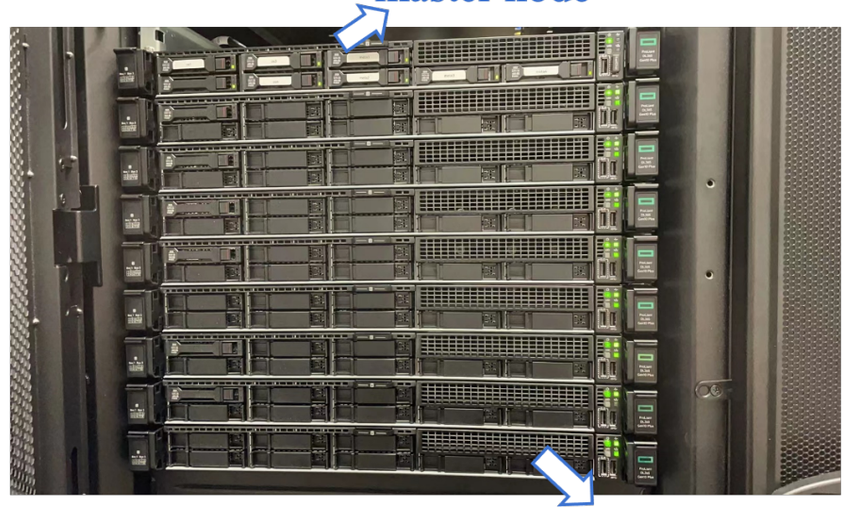




Our Blackbody Cluster in Room 311 of CYM Building



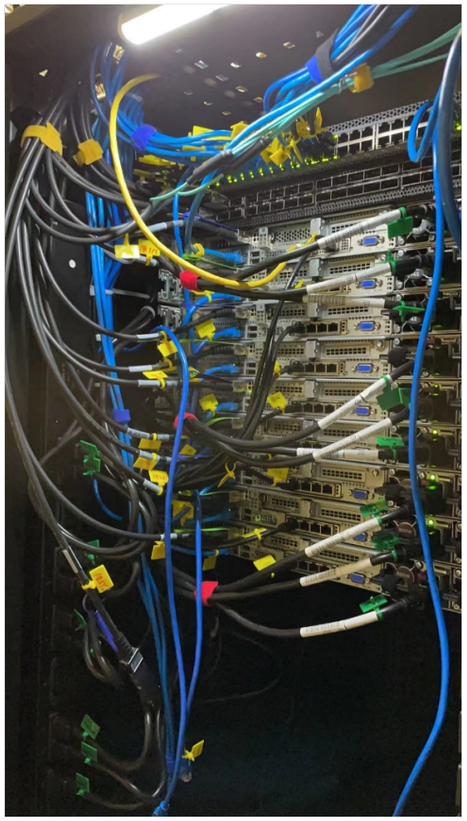




2 x AMD 7702 64C 2.0 GHz
512 GB RAM DDR4-3200
2 x 480 GB RI SSD RAID 1

1024 cpu cores

Cable Management & Labeling



Exhaust Pipes and Inrow Cooling







Electricity

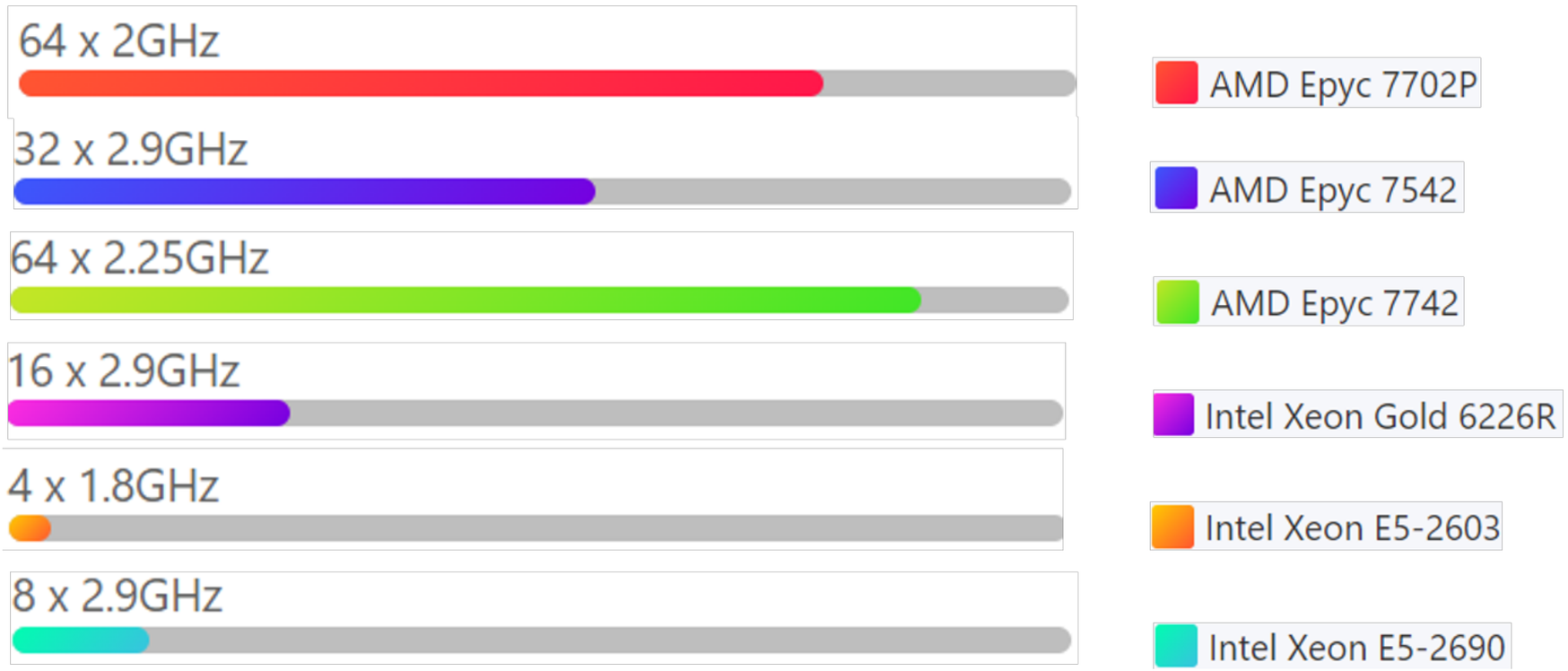


Total Electricity: 24 kW
Current Usage:
cluster ~ 5.4 kW (computing nodes 0.55 kW × 8, head node, storage)
cooling ~ 8 kW (each ~ 2.4 kW)

Around 10 kW electricity for future use.

CPU Comparison

versus data from versus.com



Blackbody: AMD 7702P (64 core) × 2 × 8

HPC2021 (general purpose): AMD 7542 (32 core) × 2 × 28

AMD 7742 (64 core) × 2 ×28

Intel Xeon Gold 6226R (16 core) × 2 × 84

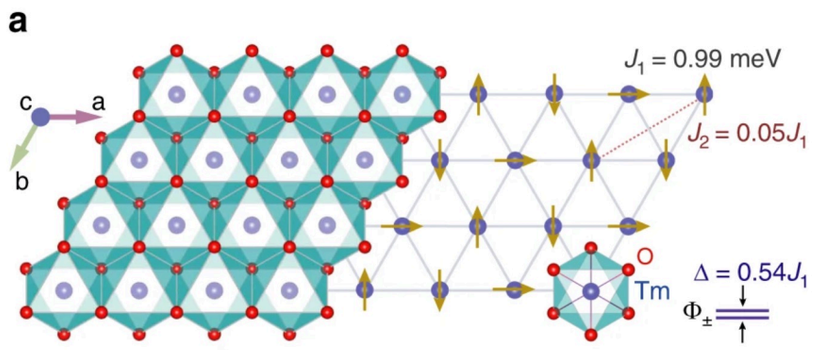
HPC2015 (general) : Intel Xeon E5-2600 v3 (10 core) × 2 × 104

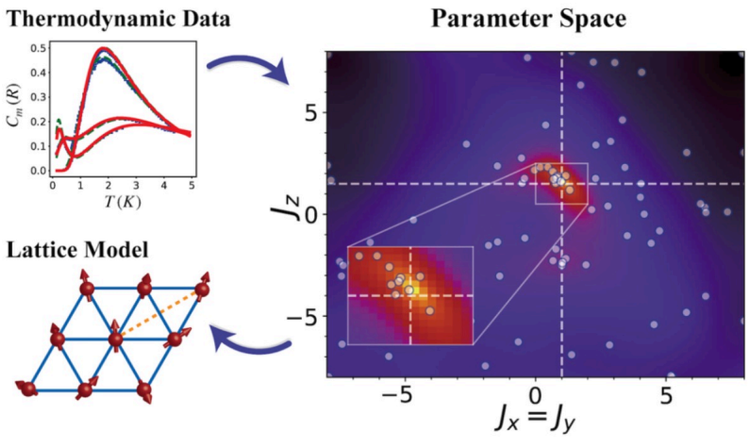
Tianhe II: Intel Xeon E5-2692 (10 core) × 2 × 16000

Computation in Physics

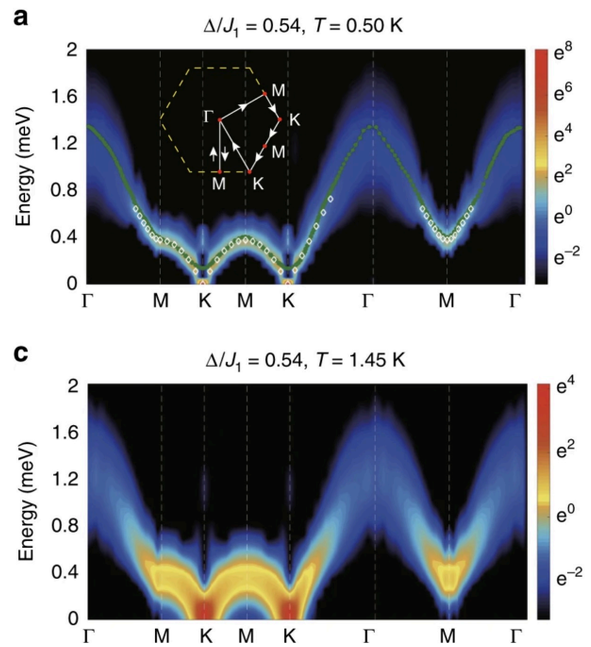
- Quantum material research connecting physicists in Hong Kong, Beijing and Shanghai

Tm (Thulium) Mg (Magneisum) Ga (Gallium) O4 (tetroxide) — TMGO



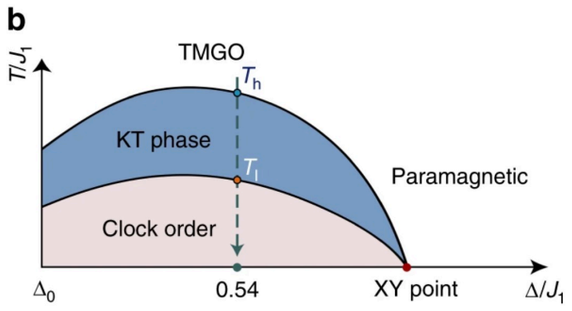


auto-gradient, Bayesian optimization

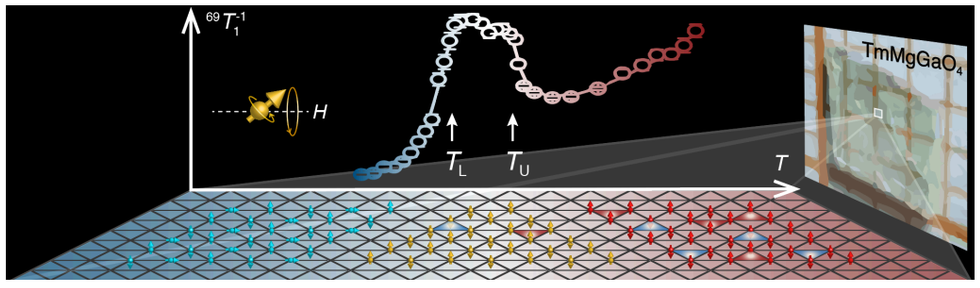


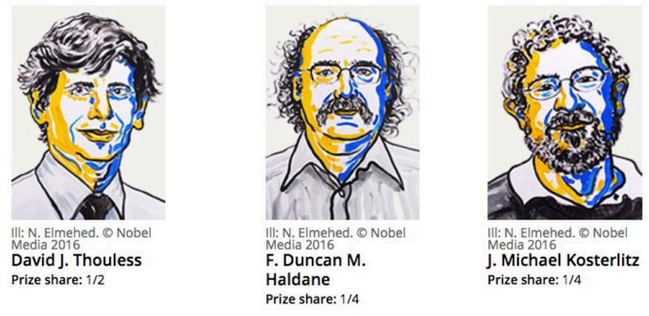
[Nature Communications 11, 1111 (2020)](#)

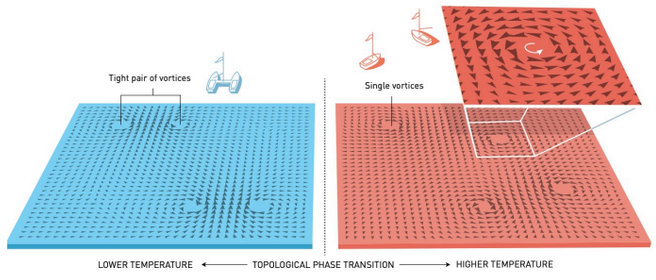
- Confirming simulated calculations, quantum material research reveals topological KT phase



Nuclear magnetic resonance — MRI / CT scans







[Nature Communications 11,5631 (2020)](#)

Computation in Physics

CLP 中電 electric power transmission at high voltage



Maglev (magnetic levitation) bullet train with 600 k/h

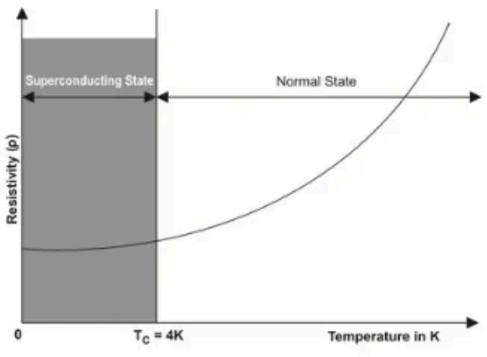


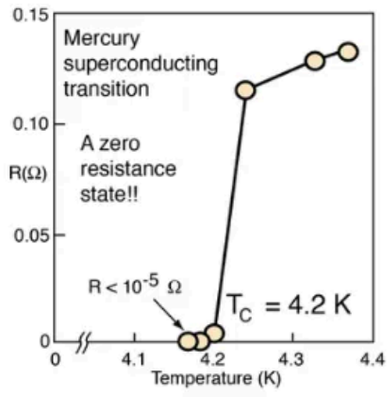
High speed rail



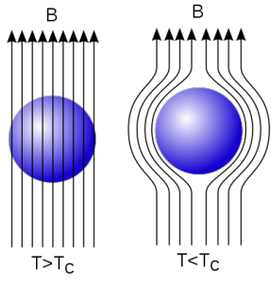
superconductors at ~ -270°C

What is Superconductivity?



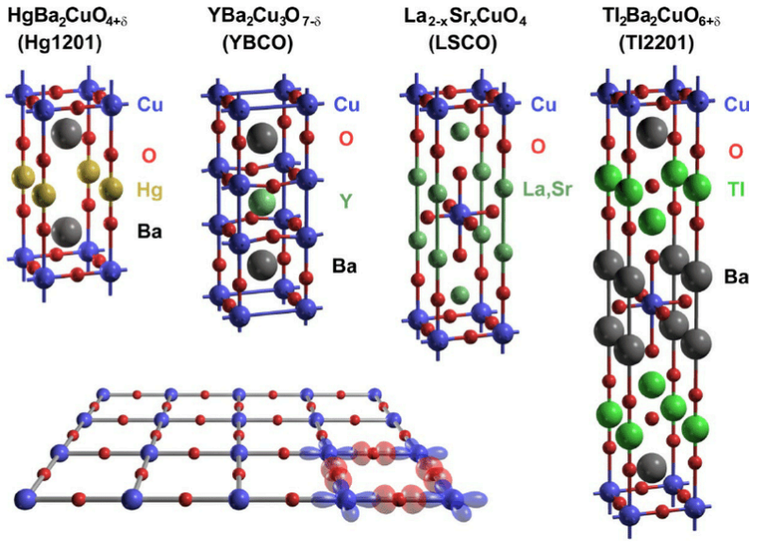


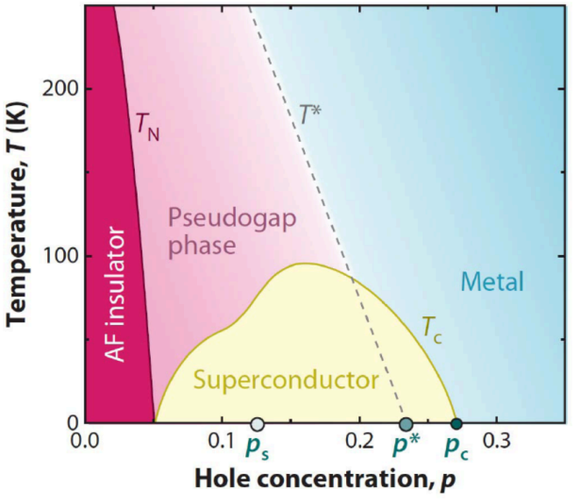
Dutch Physicist
Heike Kamerlingh Onnes in 1911



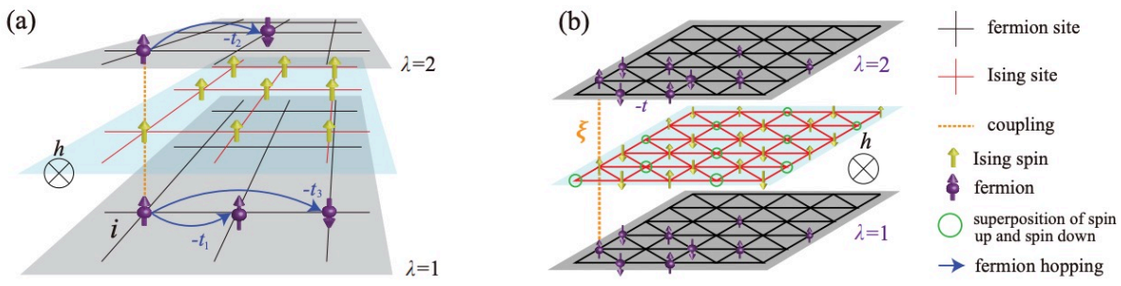


High-temperature superconductors at ~ -100°C

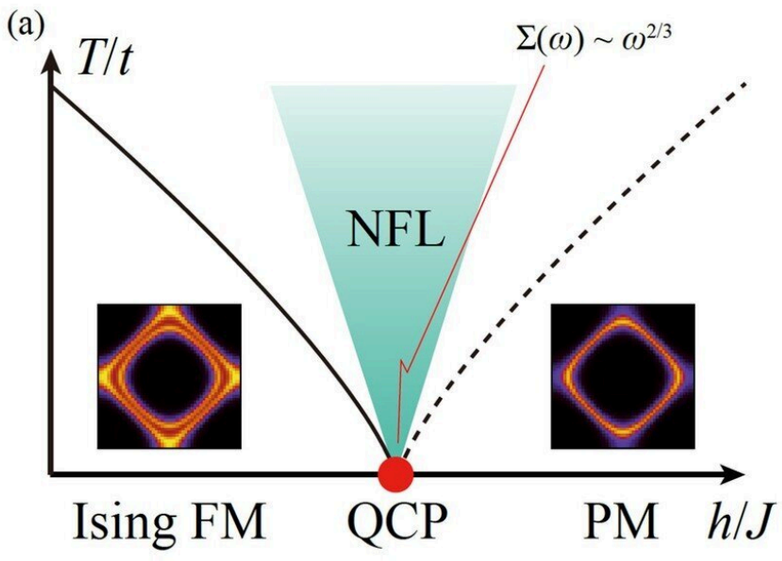




Understanding quantum critical Metals

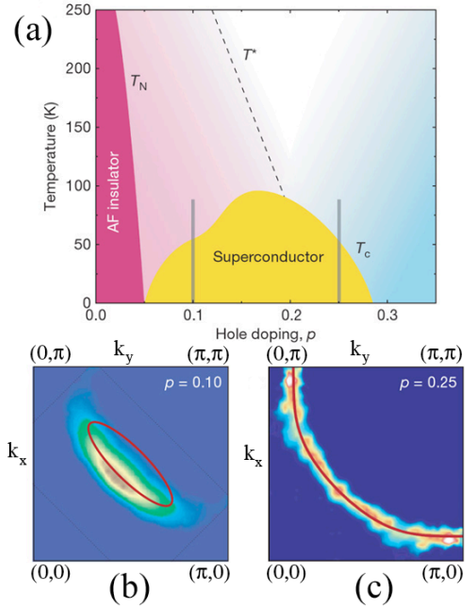


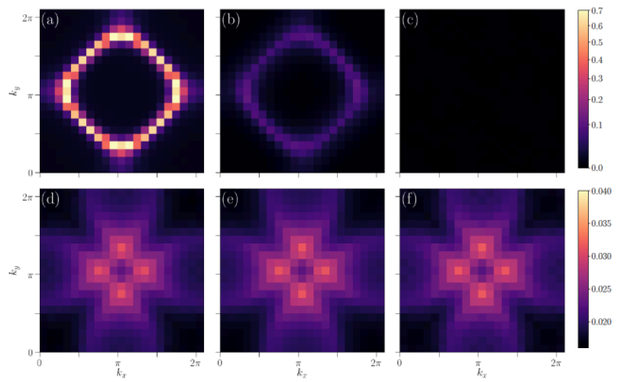
[PNAS 20, 116 (34) 16760-16767 (2019)]



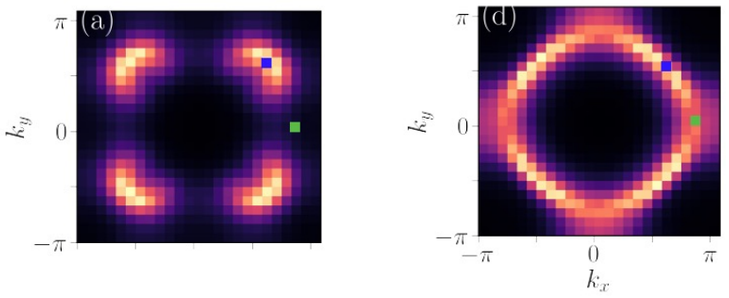
[npj Quantum Materials 5, 65 (2020)]

metals' awkward cousin is found



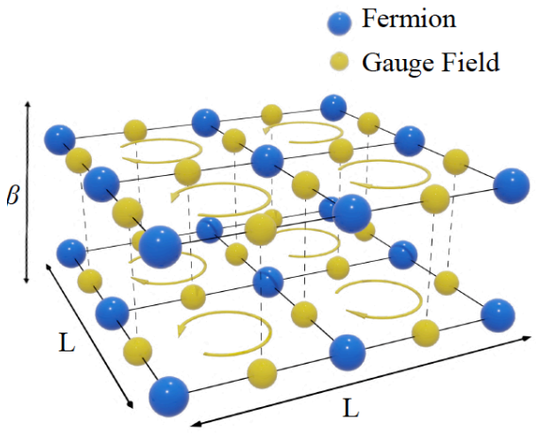


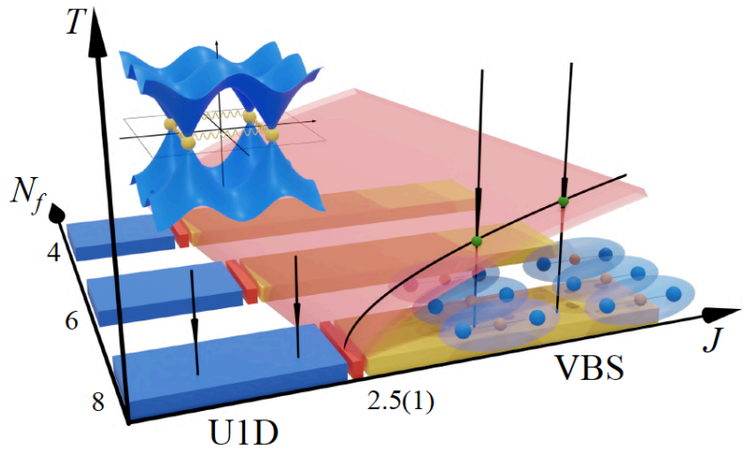
[Chin. Phys. Lett. 37 047103 (2020) Express Letters]



[Phys. Rev. B 103, 165131 (2021)]

Parent State of quantum phases

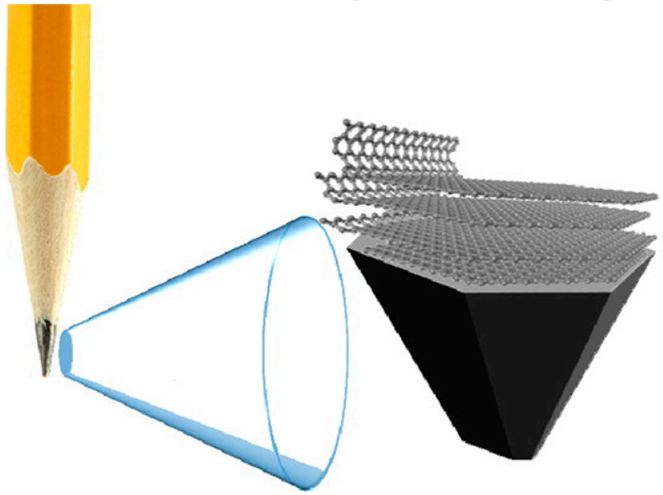


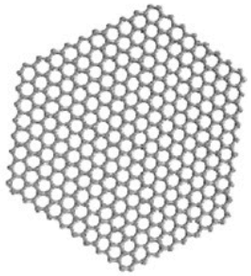


[Phys. Rev. X 9, 021022 (2019)]

Computation in graphene face masks

From graphite to graphene





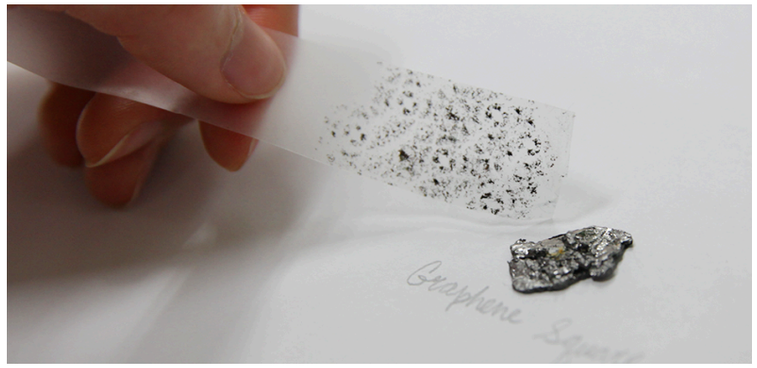
The Nobel Prize in Physics 2010



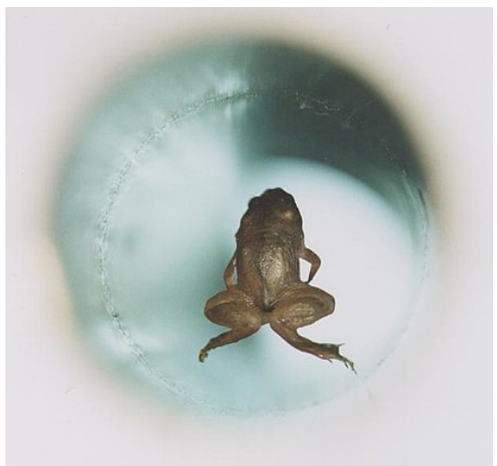
© The Nobel Foundation. Photo: U. Montan
Andre Geim
Prize share: 1/2



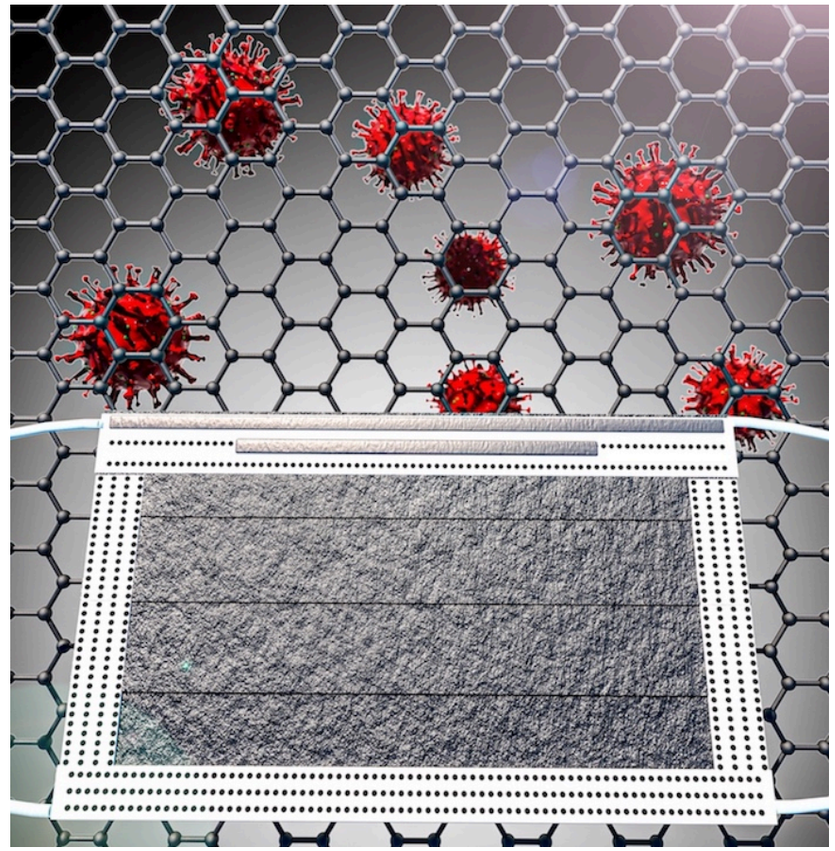
© The Nobel Foundation. Photo: U. Montan
Konstantin Novoselov
Prize share: 1/2



The 2000 Ig Nobel Prize in physics was awarded to Andre Geim, Radboud University Nijmegen, and Michael Berry, University of Bristol, UK, for the magnetic levitation of a live frog.



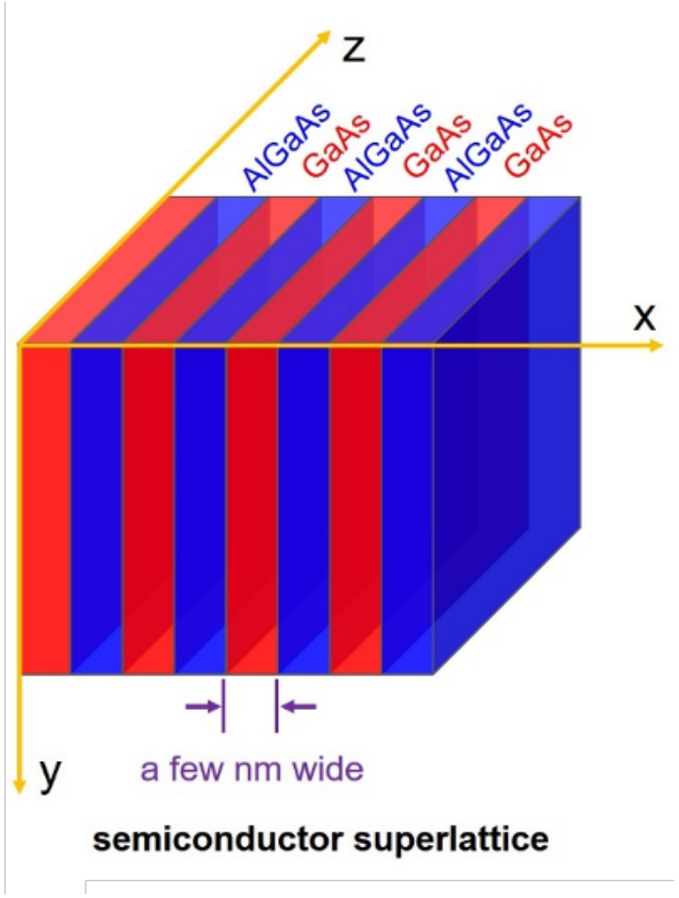
Graphene joins the fight against COVID-19





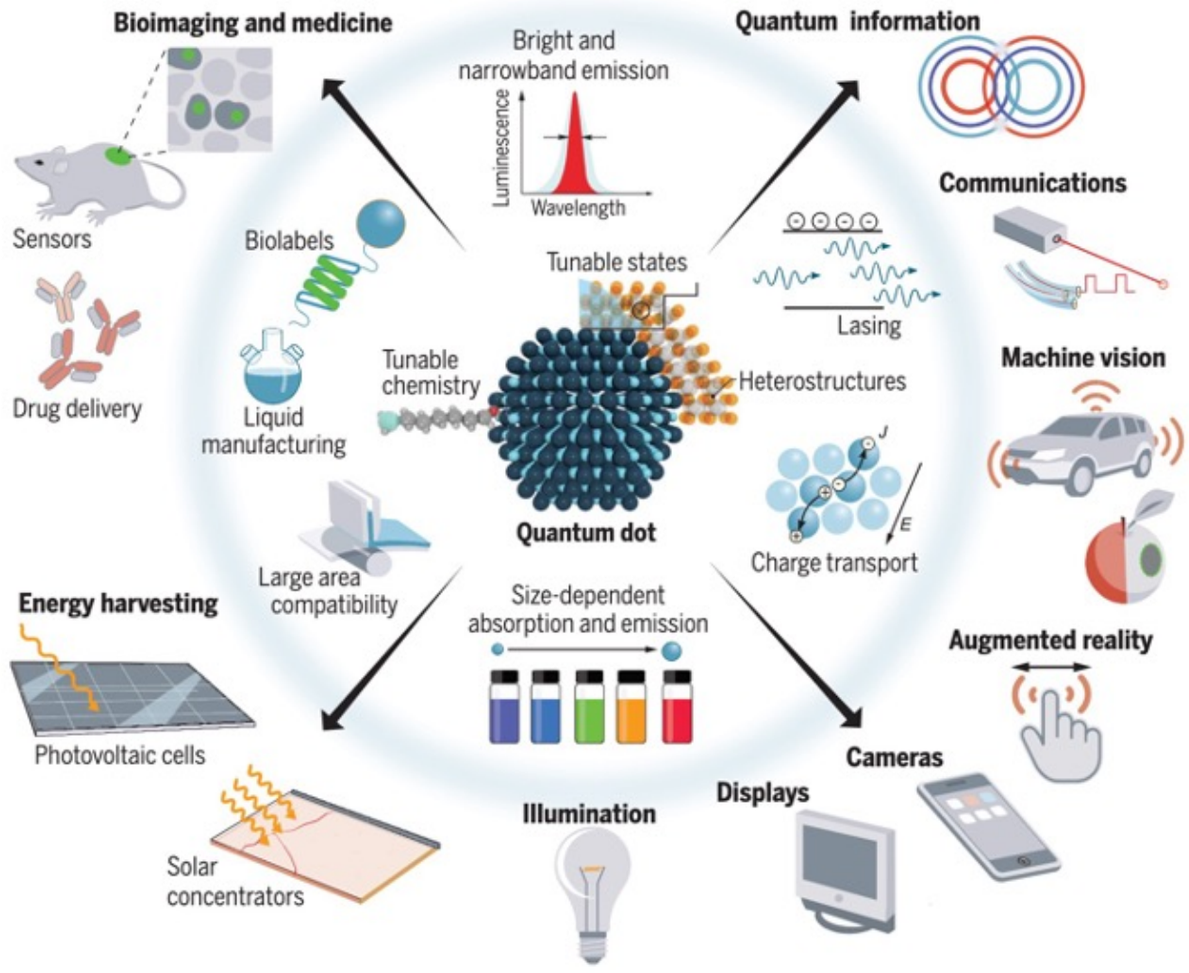
Superlattices are widely used as electric and optical devices

In semiconductor industry



Wikipedia

In semiconductor quantum dots / wires technologies



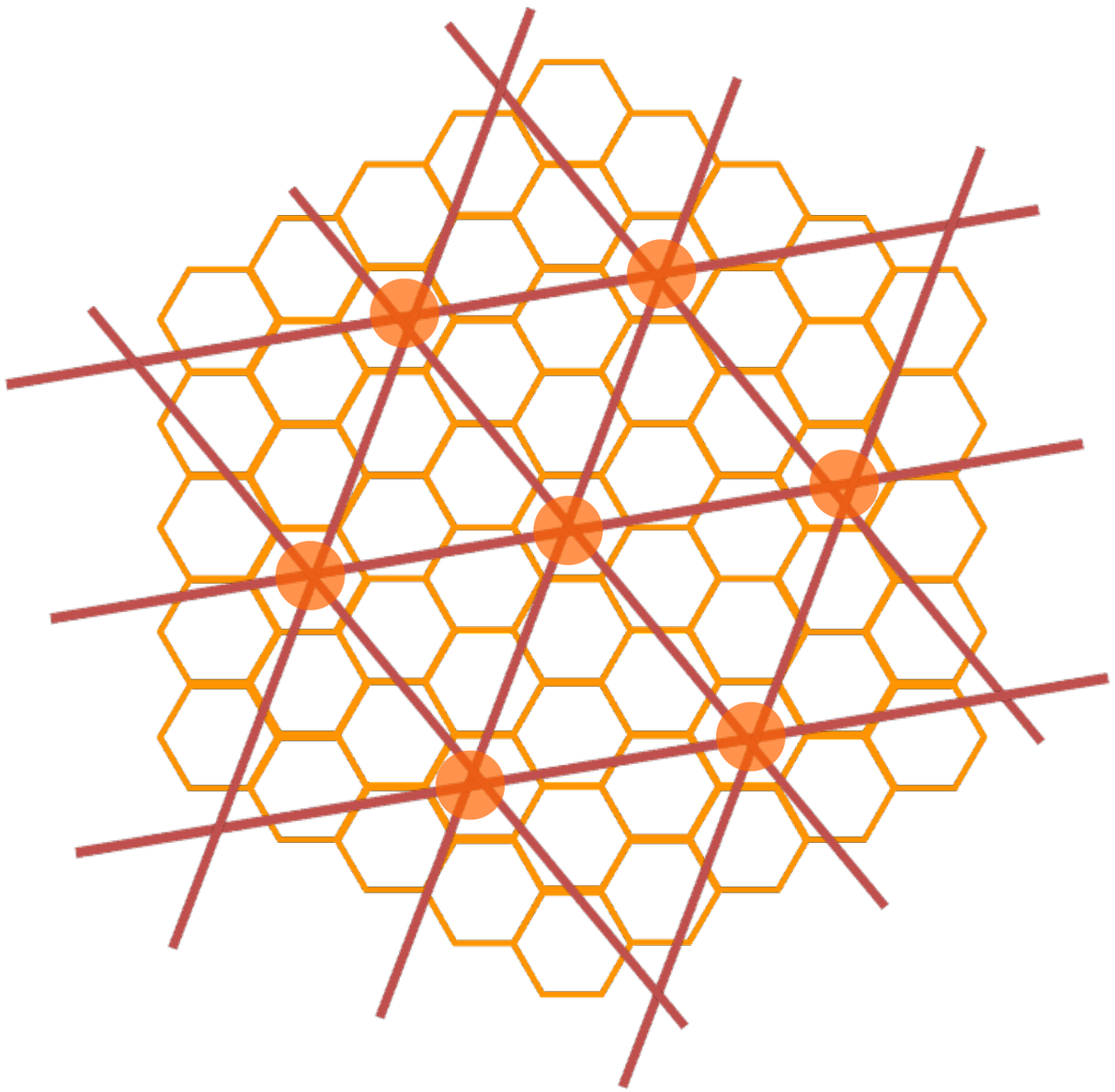
Garcia de Arquer et al., Science (2021)

- Periodic in growth direction (mainly 1D)
- Based on free electron band structure

- **Quantum moiré materials are new superlattices in 2D**
- **Based on many-body effects with novel properties (such as superconductivity)**

Quantum moiré materials are superlattice of 2D materials (e.g. graphene)

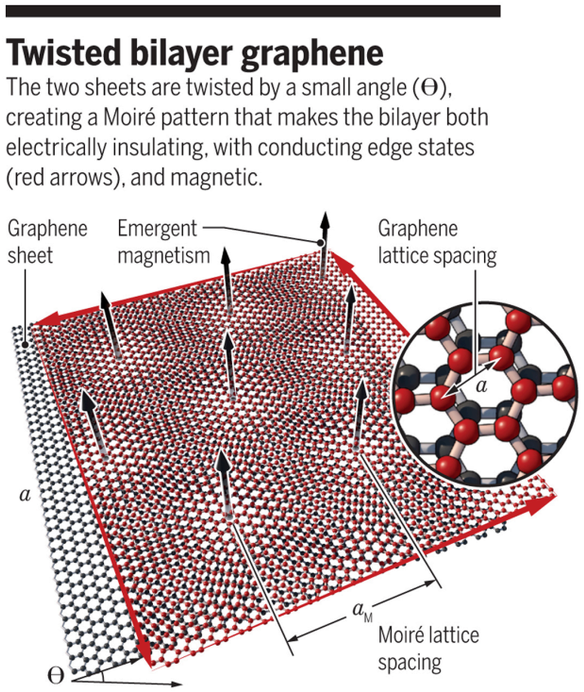
Moiré: stack, twist & new physics emerges
crystal from crystals
ideal playground & challenge for quantum many-body physics

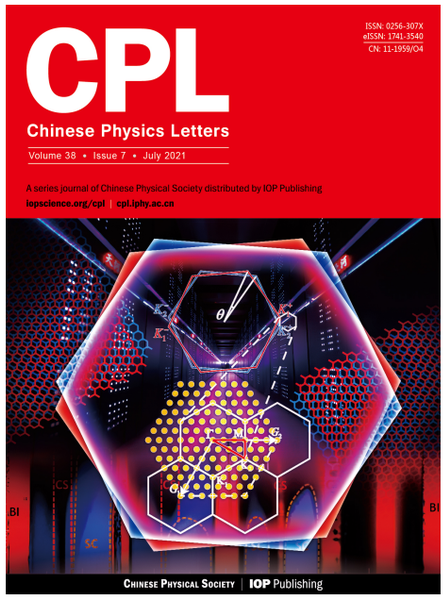


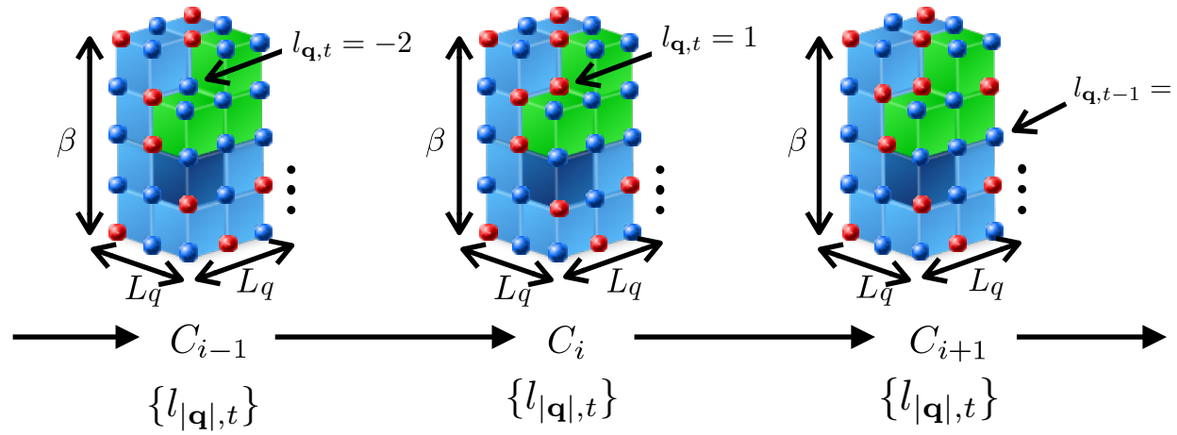
20° **rotation**

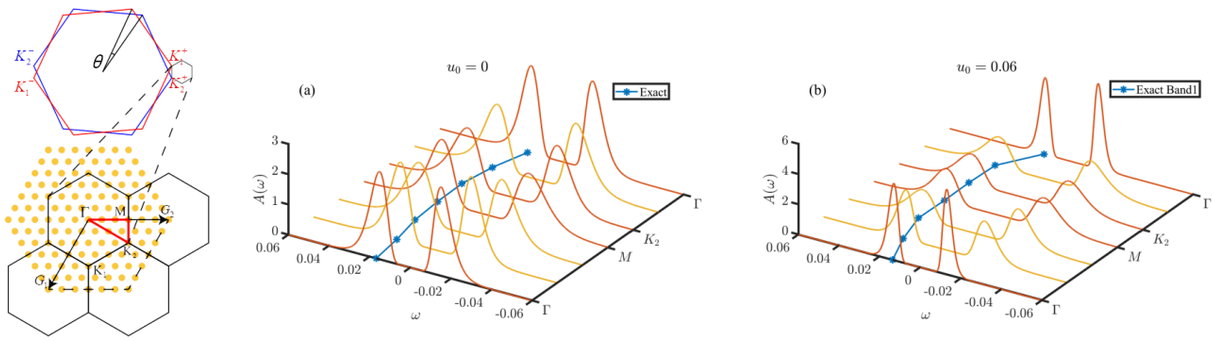
Computation in graphene face masks

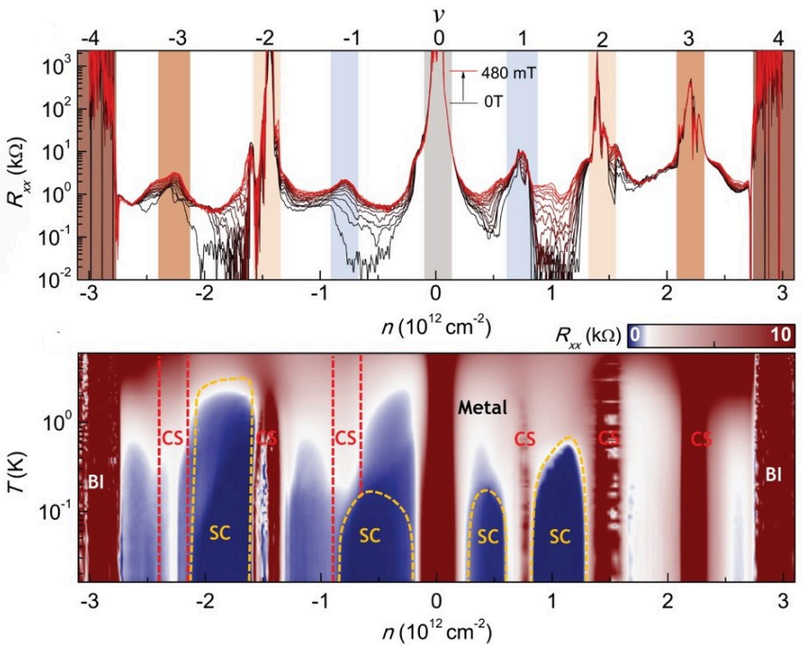
- The Samadhi of magic angle twisted bilayer graphene (转角石墨烯的三昧)



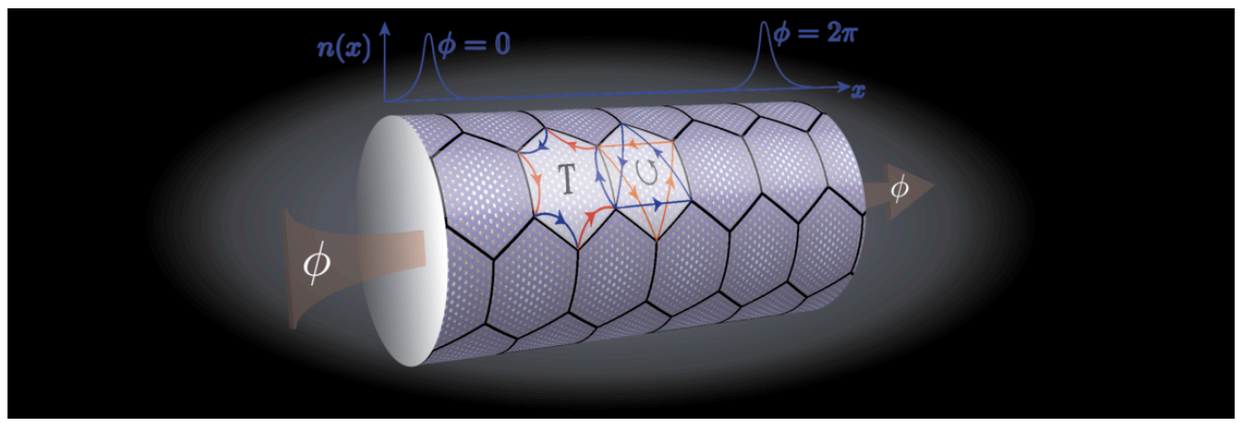








[Chin. Phys. Lett. 38, 077305 (2021) Cover story]



[Nature Communications 12, 5480 (2021)]

Momentum space quantum Monte Carlo algorithm



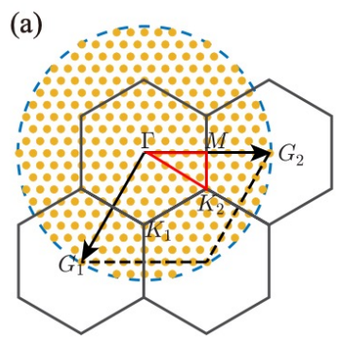
Long-range Coulomb + fragile topology

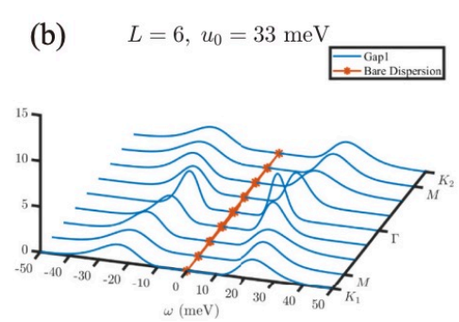
$$H = H_0 + H_{int} \qquad V(q) \sim \frac{1}{q}$$

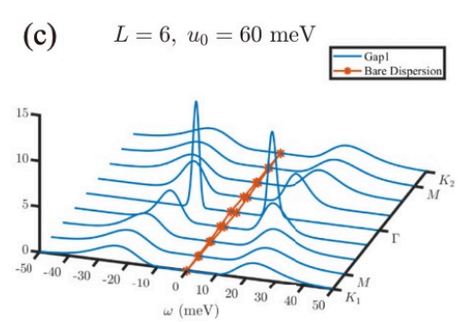
$$H_0 = \sum_m \sum_{\mathbf{k},\tau,s} \epsilon(\mathbf{k}) d^\dagger_{\mathbf{k},m,\tau,s} d_{\mathbf{k},m,\tau,s}$$

$$H_{int} = \frac{1}{2\Omega} \sum_{\mathbf{q},\mathbf{G}} V(\mathbf{q}+\mathbf{G})\, \delta\rho_{\mathbf{q}+\mathbf{G}}\, \delta_{-\mathbf{q}-\mathbf{G}}$$

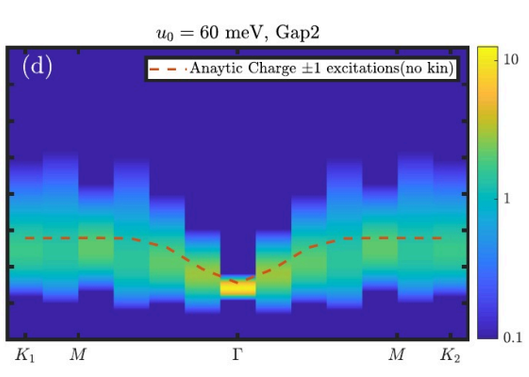
$$\delta\rho_{\mathbf{q}+\mathbf{G}} \sim \sum_{\mathbf{k}\in mBZ, m_1, m_2, \tau, s} \lambda_{m_1,m_2,\tau}(\mathbf{k}, \mathbf{k}+\mathbf{q}+\mathbf{G})\, d^\dagger_{\mathbf{k},m_1,\tau,s} d_{\mathbf{k}+\mathbf{q},m_2,\tau,s}$$

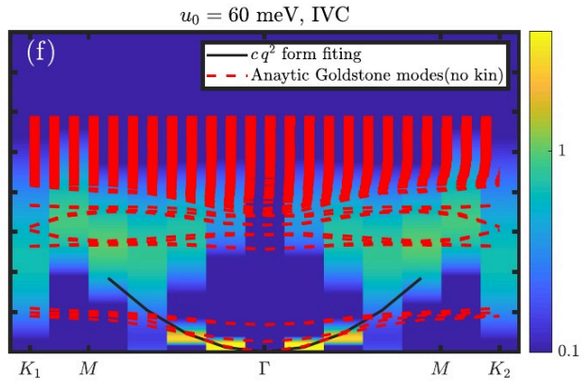




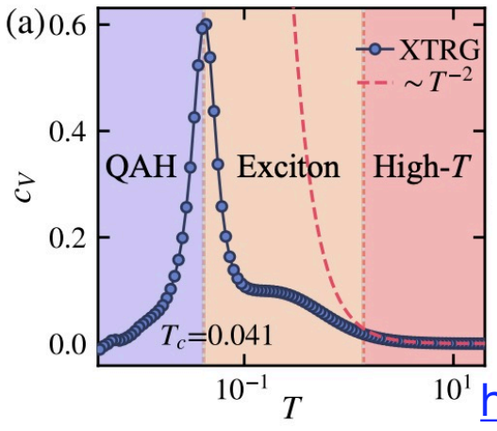


Collective excitations





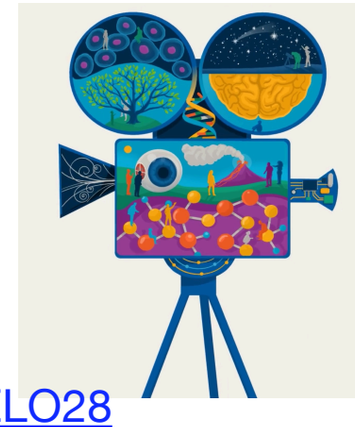
Tensor-network, thermodynamic computation



nature awards science in shorts

Science in Shorts playlist 2022

Watch and share the best Shorts from 2022. Which is your favourite?



https://youtu.be/c5-bFYELO28

[Phys. Rev. Lett. 131, 066301 (2023) Editors' Suggestion]
[Phys. Rev. Lett. 130, 016401 (2023)]
[Phys. Rev. Lett. 128, 157201 (2022)]
[Phys. Rev. B 105, L121110 (2022)]
[Nature Communications 12, 5480 (2021)]

The quantum teleportation pencil

Are you sitting comfortably? And concentrating hard? We're entering the realms of superfast computing based on quantum teleportation via twisted graphene lattices. But don't worry, you'll be fine as long as you have a pencil handy.

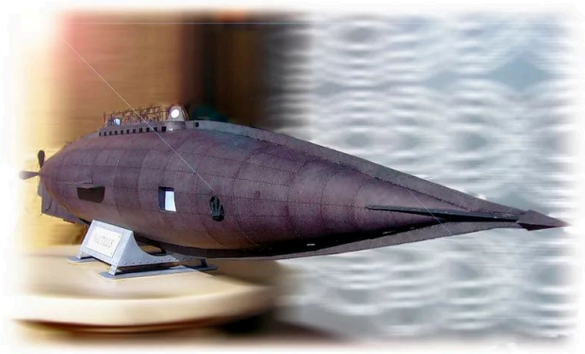
Bin Bin Chen & Zi Yang Meng
The University of Hong Kong

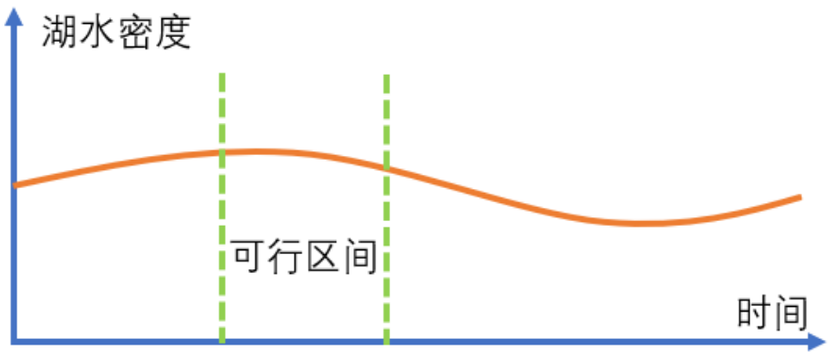


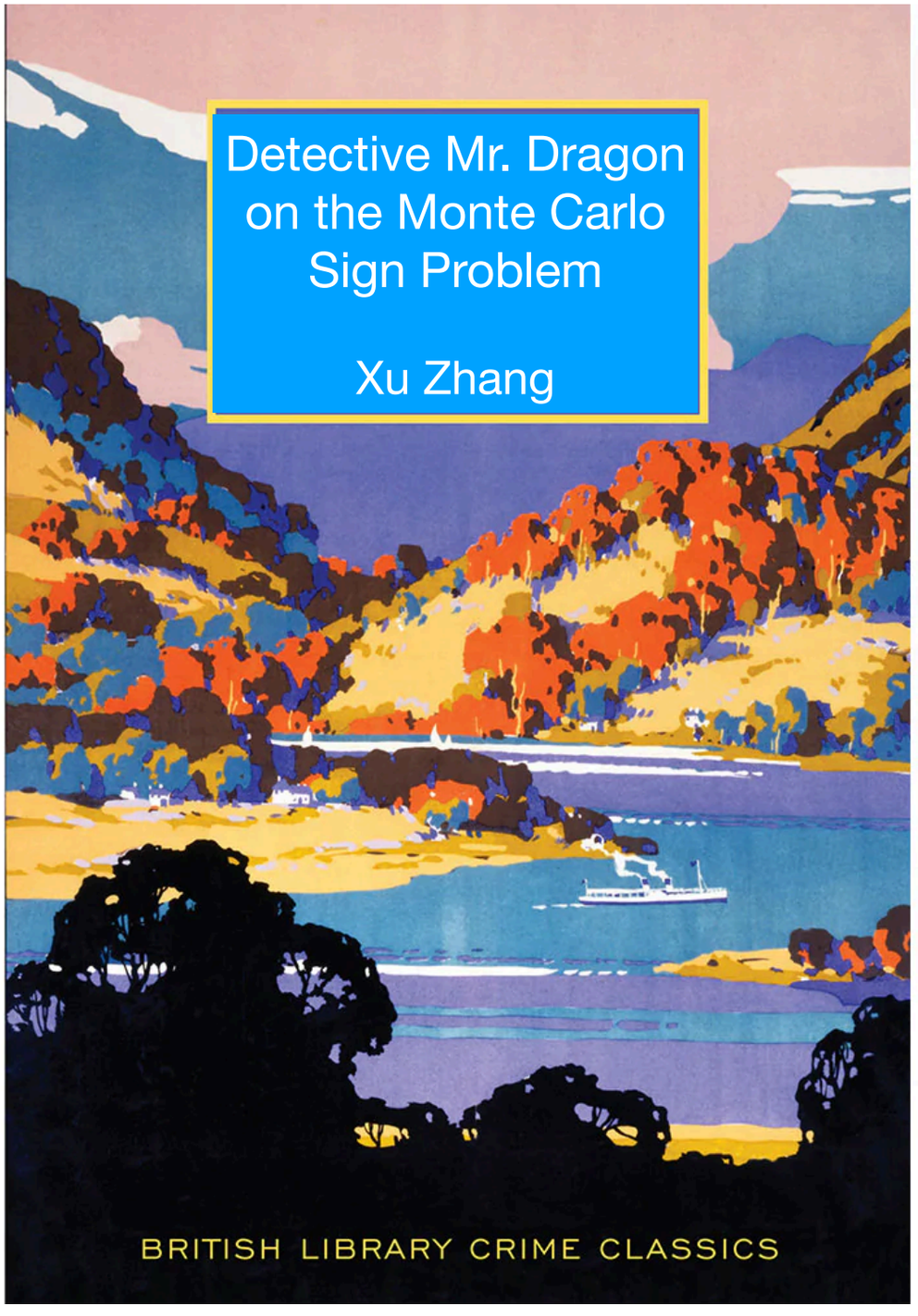
Xu Zhang



Caption Nemo and submarine Nautilus







$$\langle \rho \rangle_{V_i} = \frac{\sum_i V_i \rho_i}{\sum_i V_i} = \frac{\frac{\sum_i |V_i|(\pm\rho_i)}{\sum_i |V_i|}}{\frac{\sum_i |V_i|(\pm 1)}{\sum_i |V_i|}} = \frac{\langle \pm\rho_i \rangle_{|V_i|}}{\langle \pm 1 \rangle_{|V_i|}}$$

$\langle \pm 1 \rangle \sim e^{-N}$ **Sign problem and Sign bound**

- Twenty Thousand Leagues Under the Seas, Jules Verne
- Xu Zhang et al., Fermion sign bounds theory in quantum Monte Carlo simulation, PRB 106, 035121 (2022)
- Xu Zhang et al., Polynomial sign problem and topological Mott insulator in twisted bilayer graphene, PRB 107, L241105 (2023)

Entanglement entropy and conformal field theory
Calabrese & Cardy

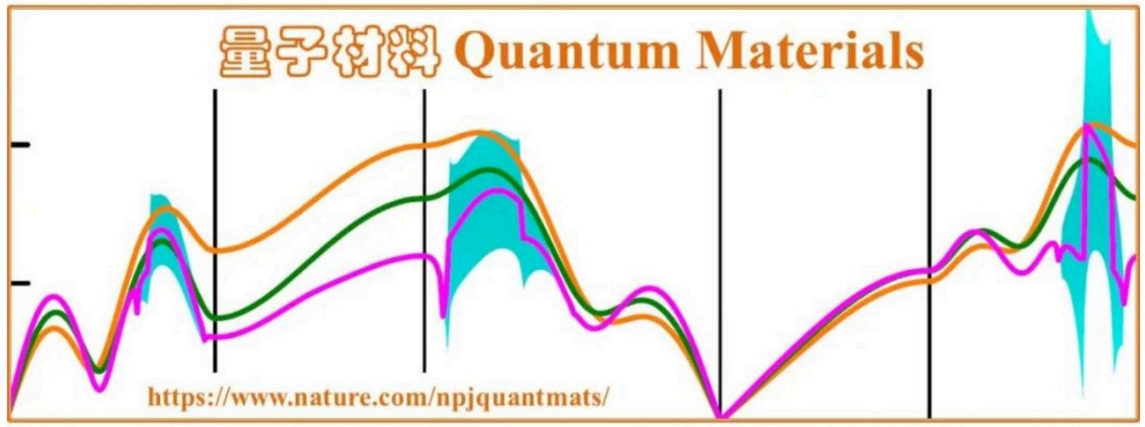
J. Stat. Mech. (2004) P06002

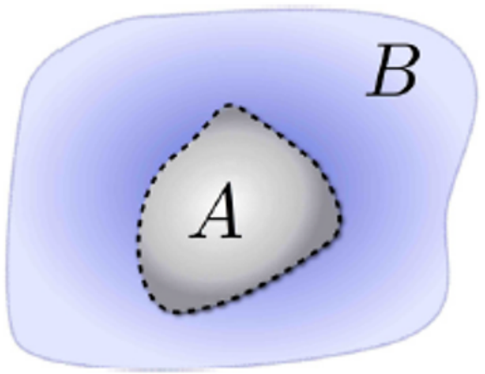


Jiarui Zhao

在纠缠中窥见自然的奥秘

Original 赵家瑞 量子材料QuantumMaterials 2022-06-30 08:25 Posted on 江苏





$$\rho = |\Psi\rangle\langle\Psi|$$

$$\rho_A = \mathbf{Tr}_B\, \rho$$

$$S_A = -\,\mathbf{Tr}_A\, \rho_A \ln(\rho_A)$$

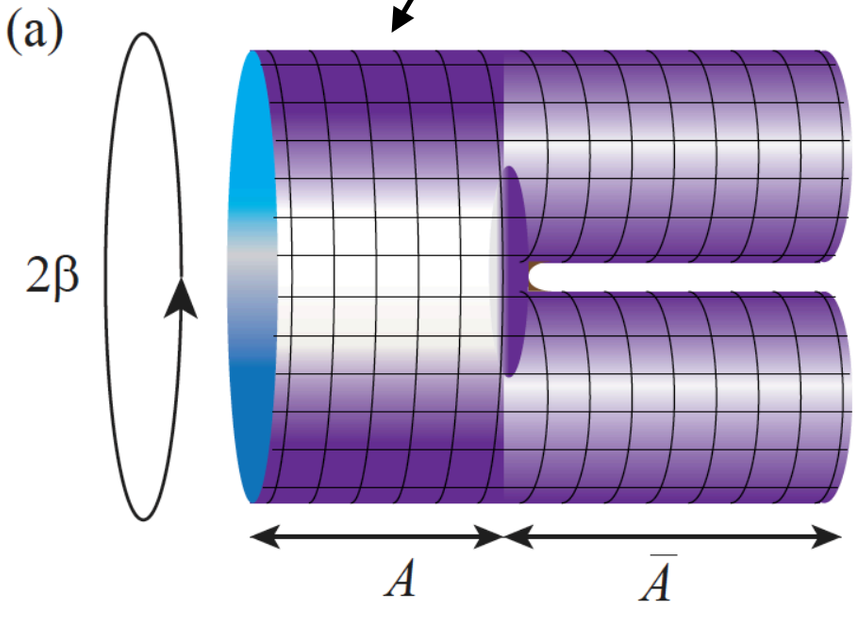
$$S_A^{(n)} = \frac{1}{1-n} \ln(\mathbf{Tr}_A(\rho_A^{(n)}))$$

“ discuss entropy in terms of the **Euclidean path integral** on an n-sheeted Riemann surface. ”

$$S_A^{(2)} = -\ln(\mathbf{Tr}_A(\rho_A^{(2)})) = -\ln(\frac{Z_A^{(2)}}{Z_\varnothing^2}) = \beta(F(Z_A^{(2)}) - F(Z_\varnothing^{(2)}))$$

“ Qiu Ku is the $Z_A^{(2)}$ ”

“ Renyi **EE** is **the difference in free energy** between partition functions with different trace topologies ” (in equilibrium)



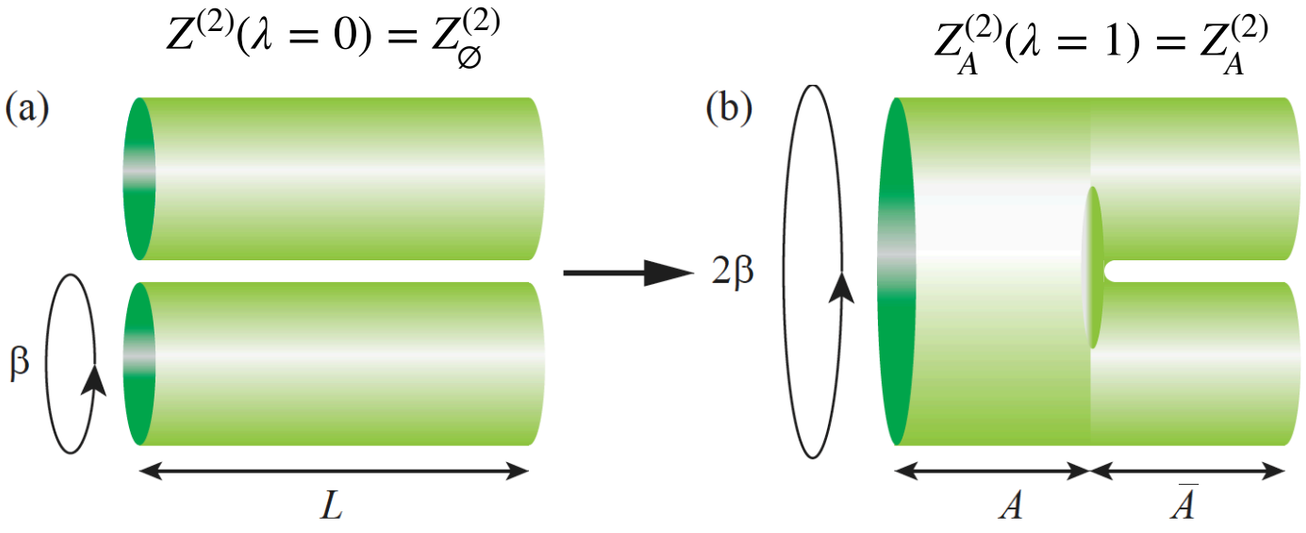
(b)



Incremental (Qiu Ku) method

- Jiarui Zhao, Yan-Cheng Wang, Zheng Yan, Meng Cheng, **ZYM**, PRL 128, 010601 (2022)
- Jiarui Zhao, Bin-Bin Chen, Yan-Cheng Wang, Zheng Yan, Meng Cheng, **ZYM**, npj Quantum Materials 7, 69 (2022)
- Gaopei Pan, Yuan Da Liao, Weilun Jiang, Jonathan D'Emidio, **ZYM**, PRB 108, L081123 (2023)

$$Z_A^{(2)}(\lambda) = \sum_{B\subseteq A} \lambda^{N_B}(1-\lambda)^{N_A-N_B} Z_B^{(2)} \qquad S_A^{(2)} = -\ln\left(\frac{Z_A^{(2)}}{Z_\varnothing^{(2)}}\right) = -\int_0^1 d\lambda \frac{\partial \ln Z_A^{(n)}(\lambda)}{\partial\lambda} = -\sum_{k=1,2,\cdots,N_\lambda} \int_{(k-1)\Delta}^{k\Delta} d\lambda \frac{\partial \ln Z_A^{(2)}(\lambda)}{\partial\lambda}$$



$$\frac{\partial \ln Z_A^{(2)}(\lambda)}{\partial\lambda} = \left\langle \frac{N_B}{\lambda} - \frac{N_A-N_B}{1-\lambda} \right\rangle_\lambda$$

$$= -\ln\left(\left\langle e^{-\beta W_A^{(2)}}\right\rangle\right) = -\sum_{k=1,2,\cdots,N_\lambda} \ln\left(\left\langle e^{-\beta W_{k,A}^{(2)}}\right\rangle\right)$$

$$\lambda(t_f) = k\Delta$$

$$W_{k,A}^{(2)} = -\frac{1}{\beta}\int_{t_i}^{t_f} dt\, \frac{d\lambda}{dt}\left\langle \frac{N_B}{\lambda(t)} - \frac{N_A-N_B}{1-\lambda(t)} \right\rangle_{\lambda(t)}$$

$$\lambda(t_i) = (k-1)\Delta$$

$$e^{-S_A^{(2)}} = \frac{Z(1)}{Z(0)} := \frac{Z(\lambda_1)}{Z(0)}\frac{Z(\lambda_2)}{Z(\lambda_1)}\cdots\frac{Z(\lambda_k)}{Z(\lambda_{k-1})}\cdots\frac{Z(1)}{Z(\lambda_{N_\lambda-1})}$$

Parallization does the job.
The Qiu Ku algorithm is
nostalgic, sentimental and useful

Computation in Physics



Tycho Brahe

Measure positions of plants for 20 years (big data)



Johannes Kepler

Deduce three empirical laws (unsupervised learning), without knowing the reason



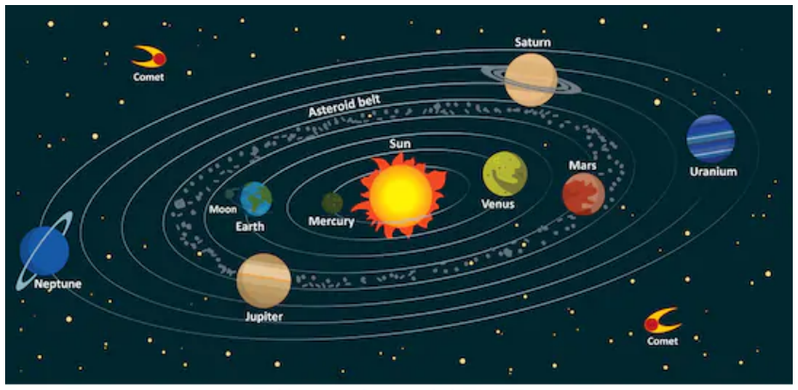
Issac Newton

Gravitation is the reason

$$F = GM_1M_2/r^2$$

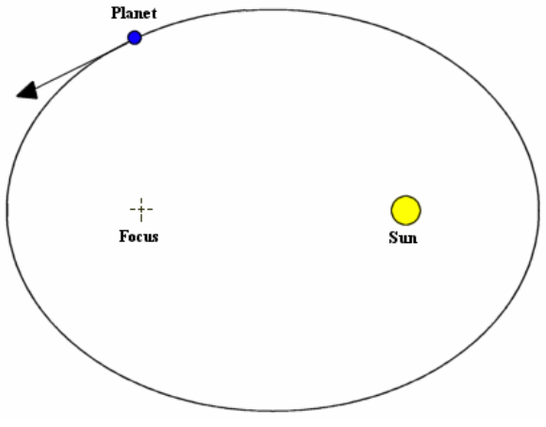
$$\dot{\vec{v}}(t) = \vec{a}(\vec{x}(t), \vec{v}(t), t)$$

$$\dot{\vec{x}}(t) = \vec{v}(t)$$

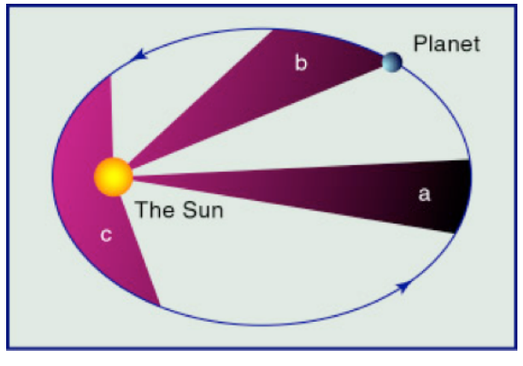


shutterstock.com • 319137437

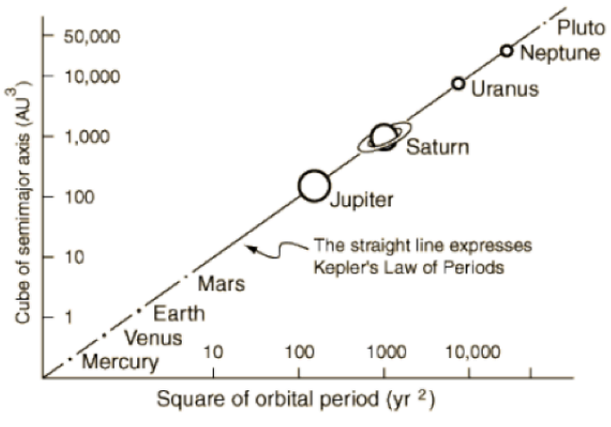
First law, ellipses



Second law, equal areas in equal time



Third law, T^2 ~ D^3



https://www.scifac.hku.hk/events/ai-computational-research

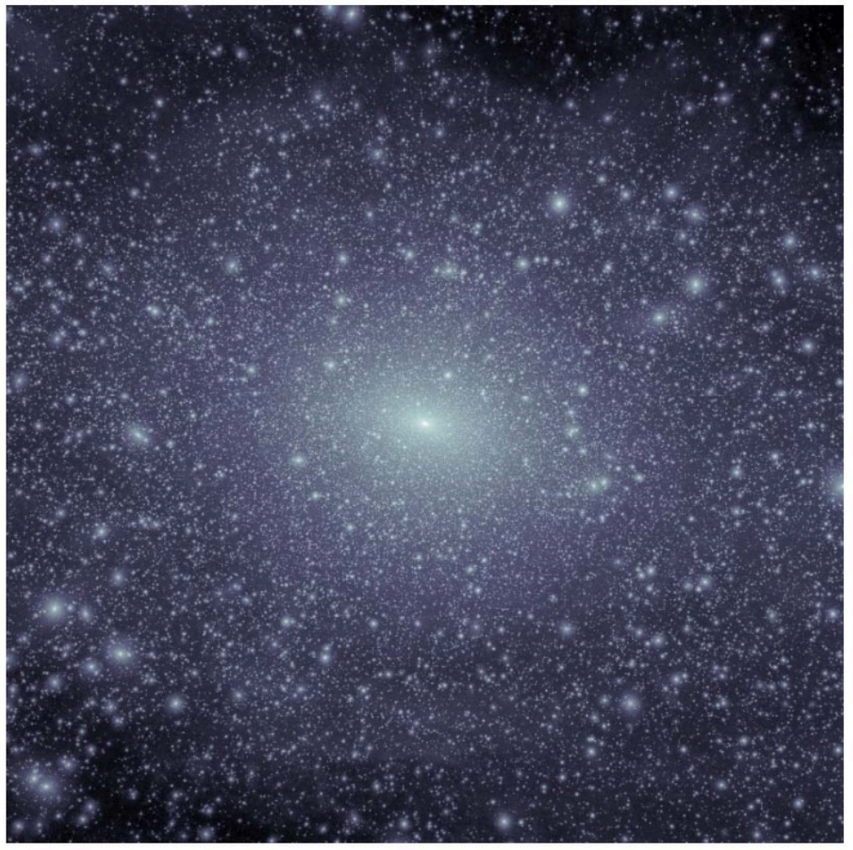
Some of the grand challenge problems

- Formation of starts and planetary systems
- Formation of galaxies and large scale structure
- Origin of cosmic magnetic fields
- Formation of supermassive black holes

Why grand challenge problems are difficult

- Complex: Dynamical, Multidimensional, Multiscale
- Inter-related
- Direct observations not possible (e.g. supernovae)

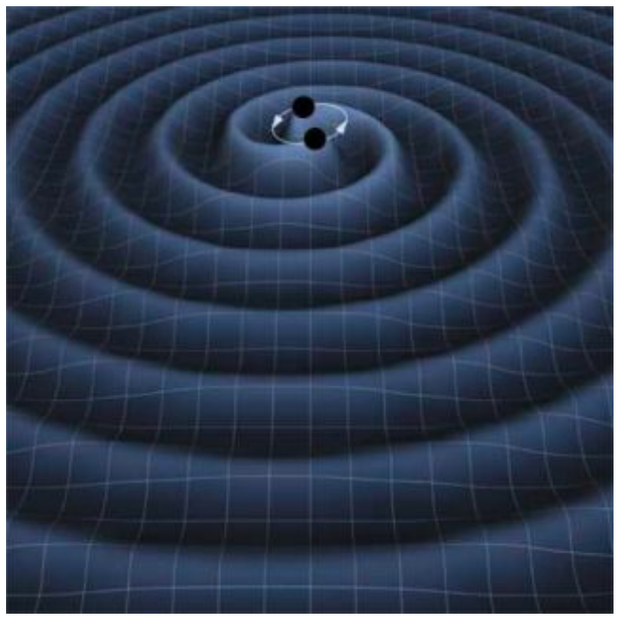
N-body/SPH tree codes



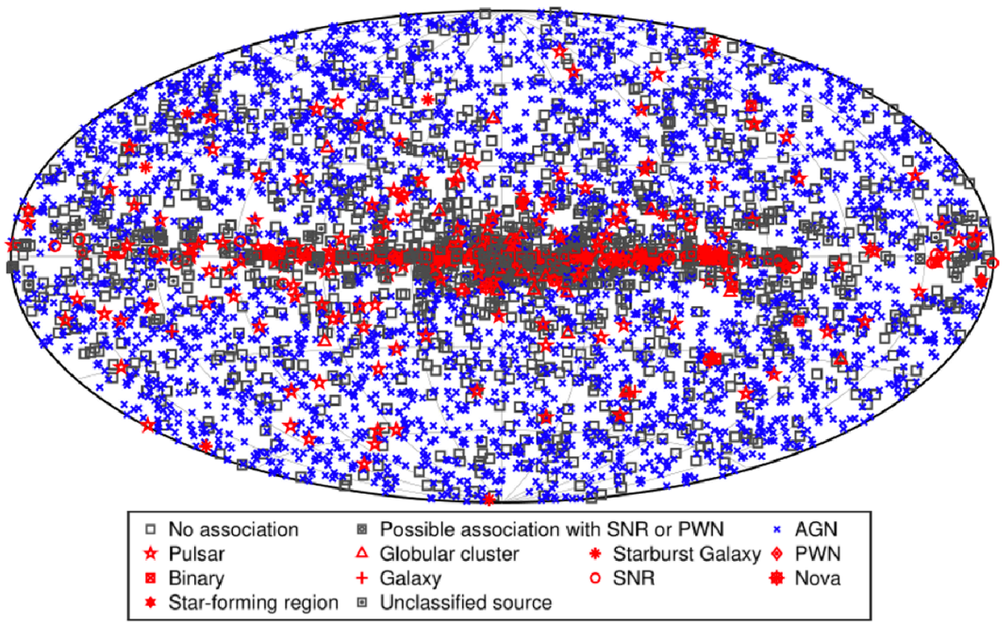
DM substructure in Milky Way
Diemand et al. (2008)

https://www.scifac.hku.hk/events/ai-computational-research

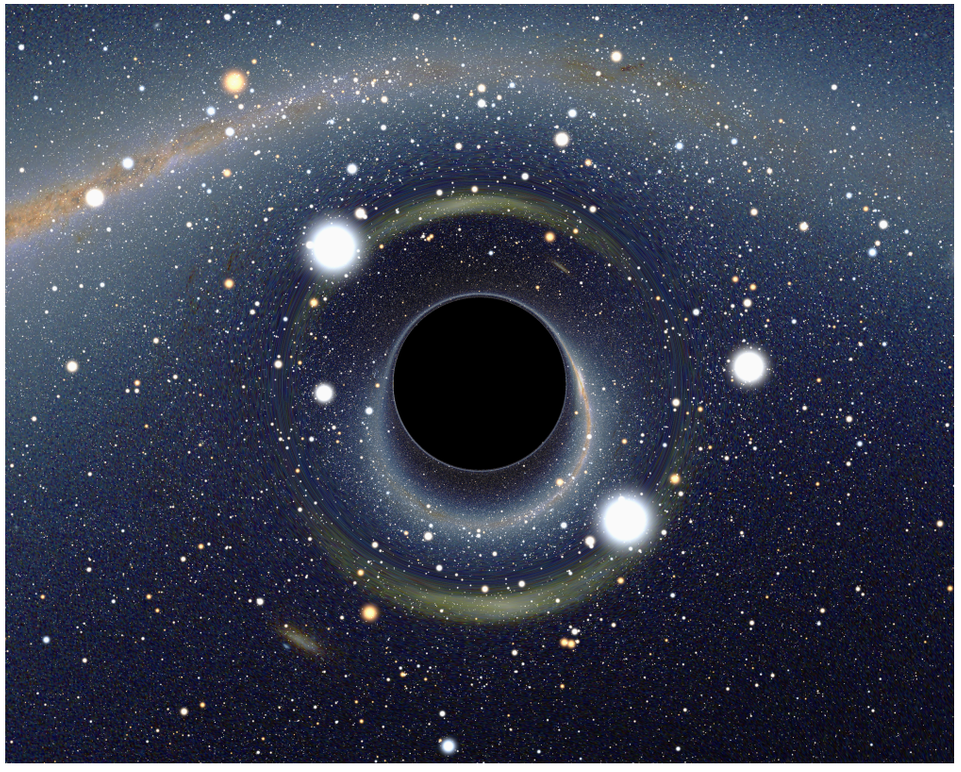
Computation in Physics







- Data volume (from different sky survey)
- Complexity (objects characterised by many parameters)
- Limitation of current knowledge (newly-emerged field e.g. gravitational wave)
- Search for “hidden” patterns



https://www.scifac.hku.hk/events/ai-computational-research