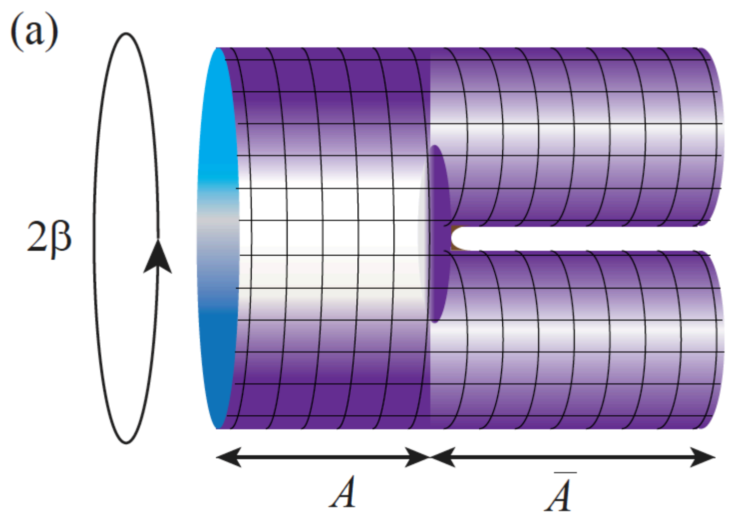
# Computational Physics

PHYS4150/8150 (6 credits)

Place: KKL 201

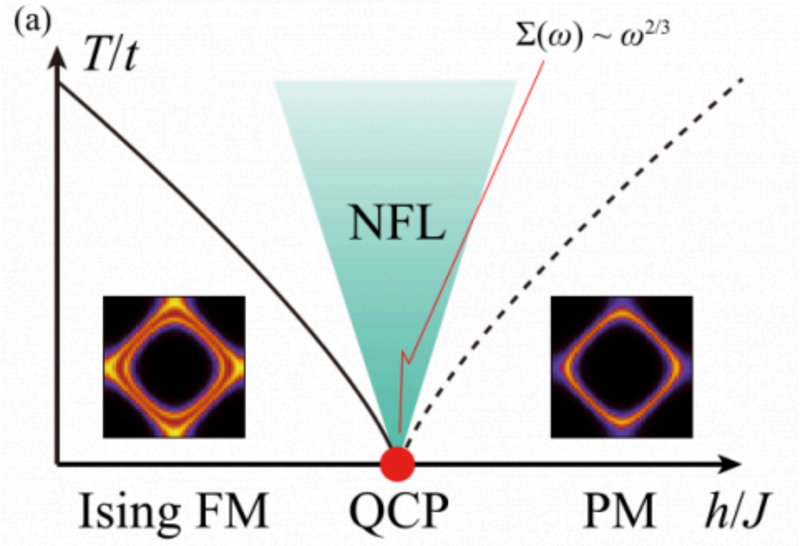
Time : Mon 17:30-18:20
Thu 16:30-17:20; 17:30-18:20

https://quantummc.xyz/teaching/hku-phys4150-8150-computational-physics-2024/

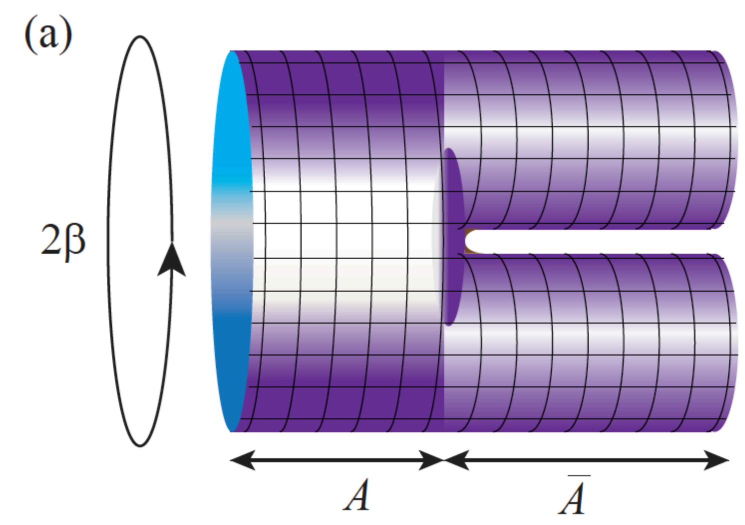



Teacher: Zi Yang Meng ( zymeng@hku.hk )

Tutor: Tim-Lok Chau (Justin) ( justintlchau@connect.hku.hk )
Min Long ( minlo@connect.hku.hk )



# Computational Physics




Teaching Materials:

https://quantummc.xyz/teaching/

Slides

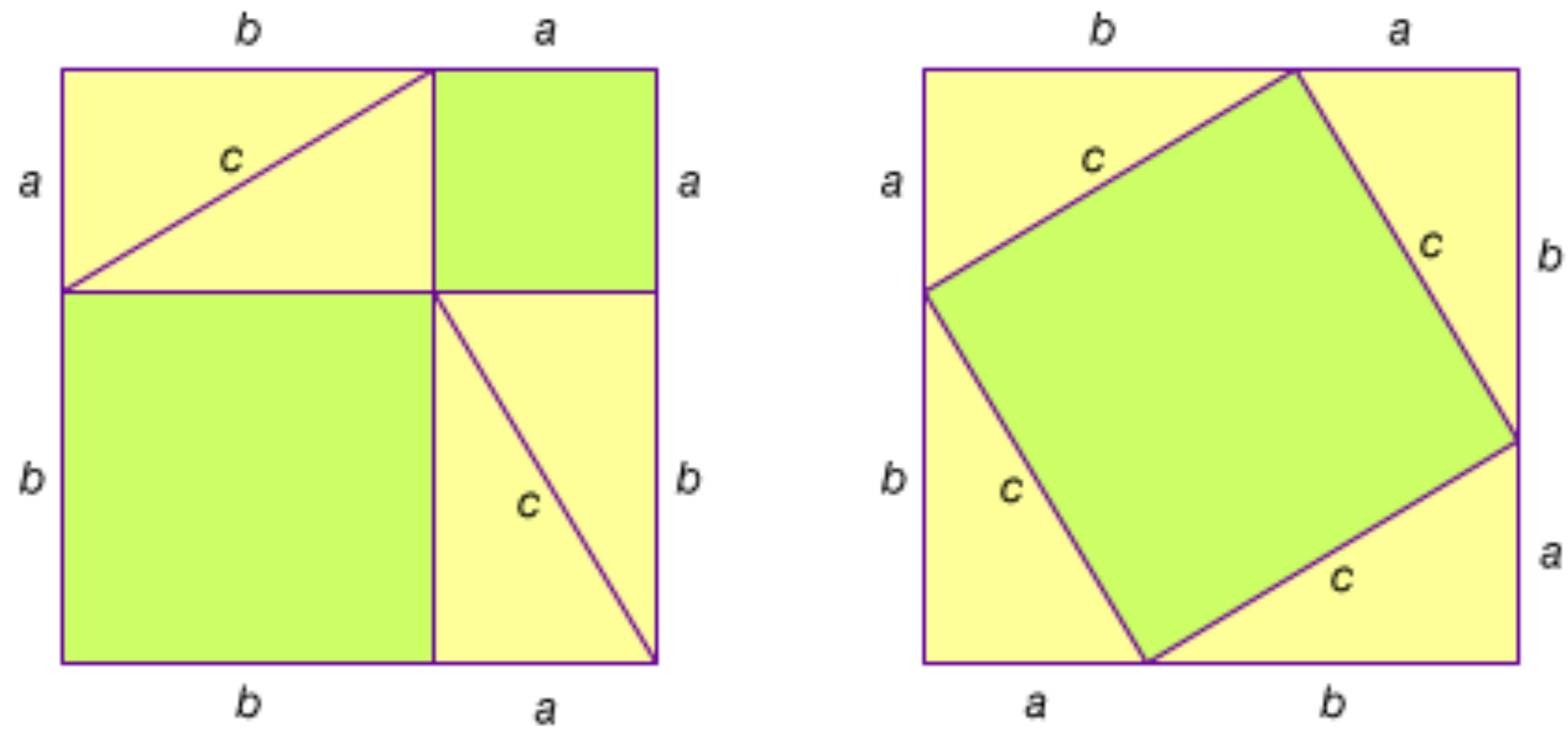
Reading materials

Python Notebooks

Assignments

Literature: Books, there are 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






**Proof of Pythagoras's theorem**

# How Archimedes compute the area under a parabola

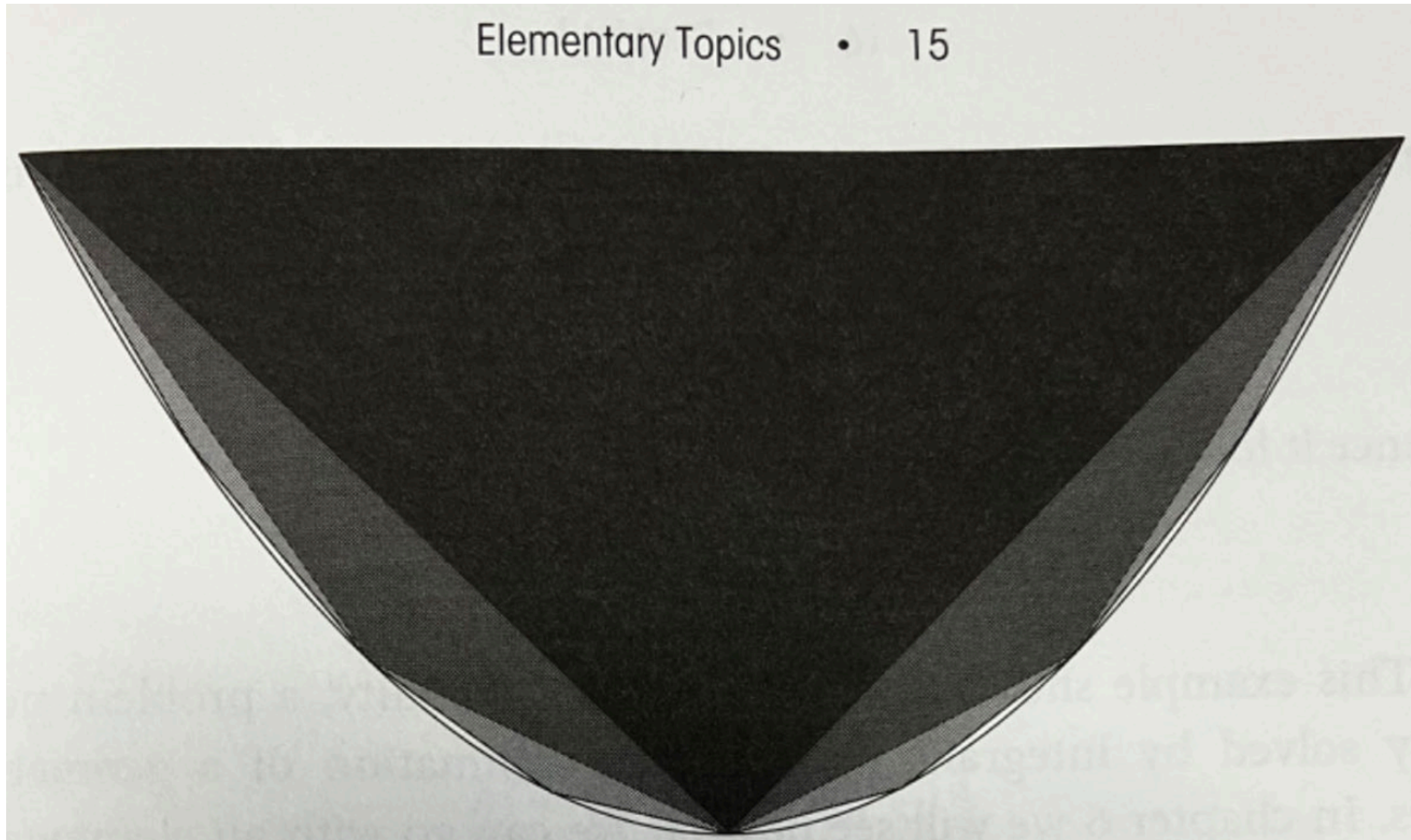



Figure 1.5: Filling the parabolic segment with triangles.

**Newton**

$$a + ar + ar^2 + ar^3 + \cdots = \frac{a}{1-r} \qquad |r| < 1$$

$$\ln 2 = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots$$

**Power series for the logarithm**

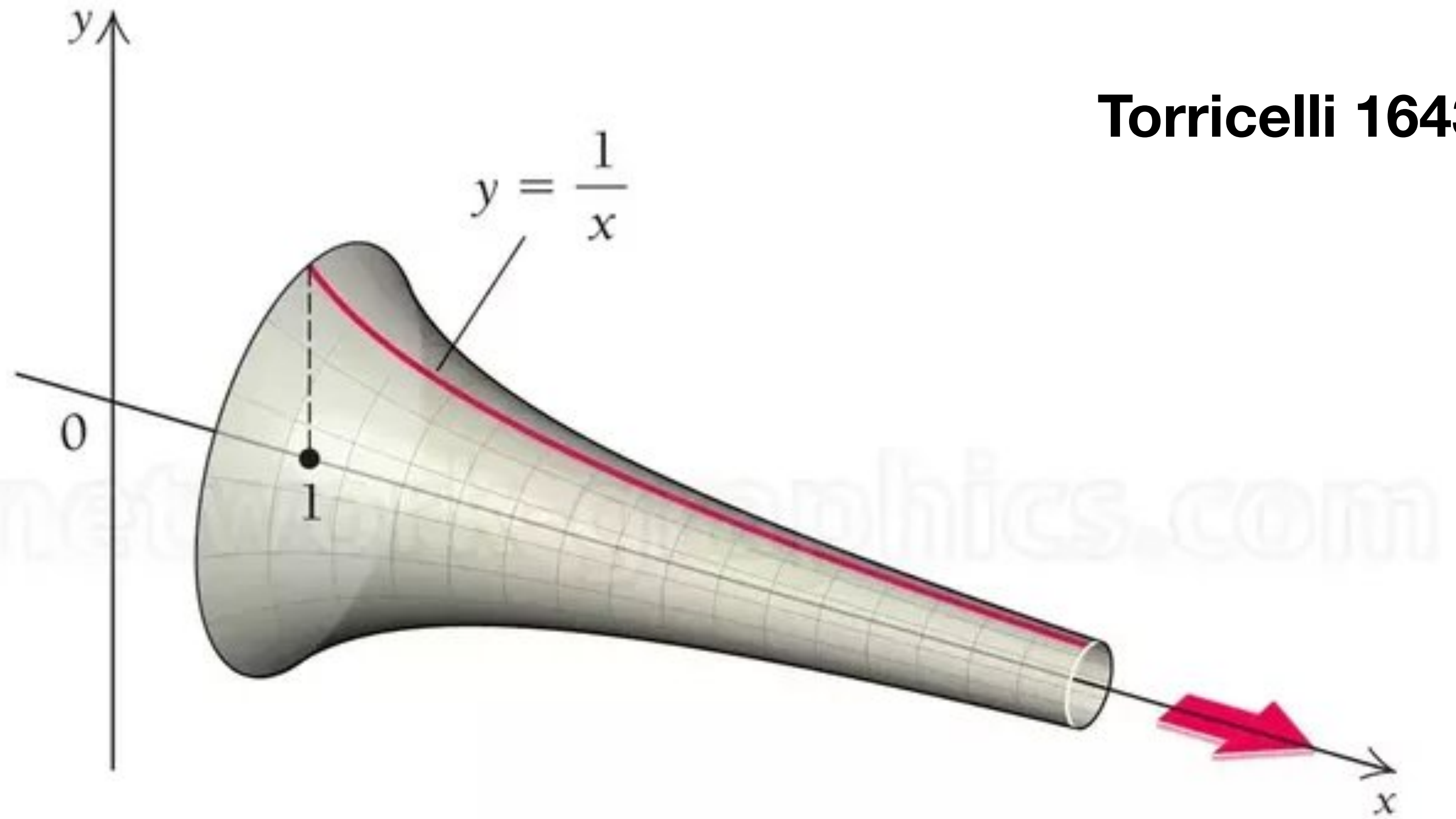
$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \cdots$$

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots$$

**Inverse Tangent function and pi**

$$\frac{1}{1+x^2} = 1 - x^2 + x^4 - x^6 + \cdots$$

**How can Gabriel's horn have a finite volume but infinite surface area?**




**volume =** $$\int_1^\infty \pi(\frac{1}{x})^2 dx = \pi[-\frac{1}{x}]_0^\infty = \pi$$

**area =** $$\int_1^\infty 2\pi \frac{1}{x}\sqrt{(dx)^2 + (\frac{dy}{dx})^2} = \int_1^\infty 2\pi \frac{1}{x}\sqrt{1 + \frac{1}{x^4}}dx > \int_1^\infty 2\pi \frac{1}{x}dx = 2\pi \ln(\infty) \rightarrow \infty$$

Philosopher Hobbes (1672) wrote of Torricelli's results that "to understand this for sense, it is not required that a man should be a geometrician or logican, but that he should be mad."

# 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

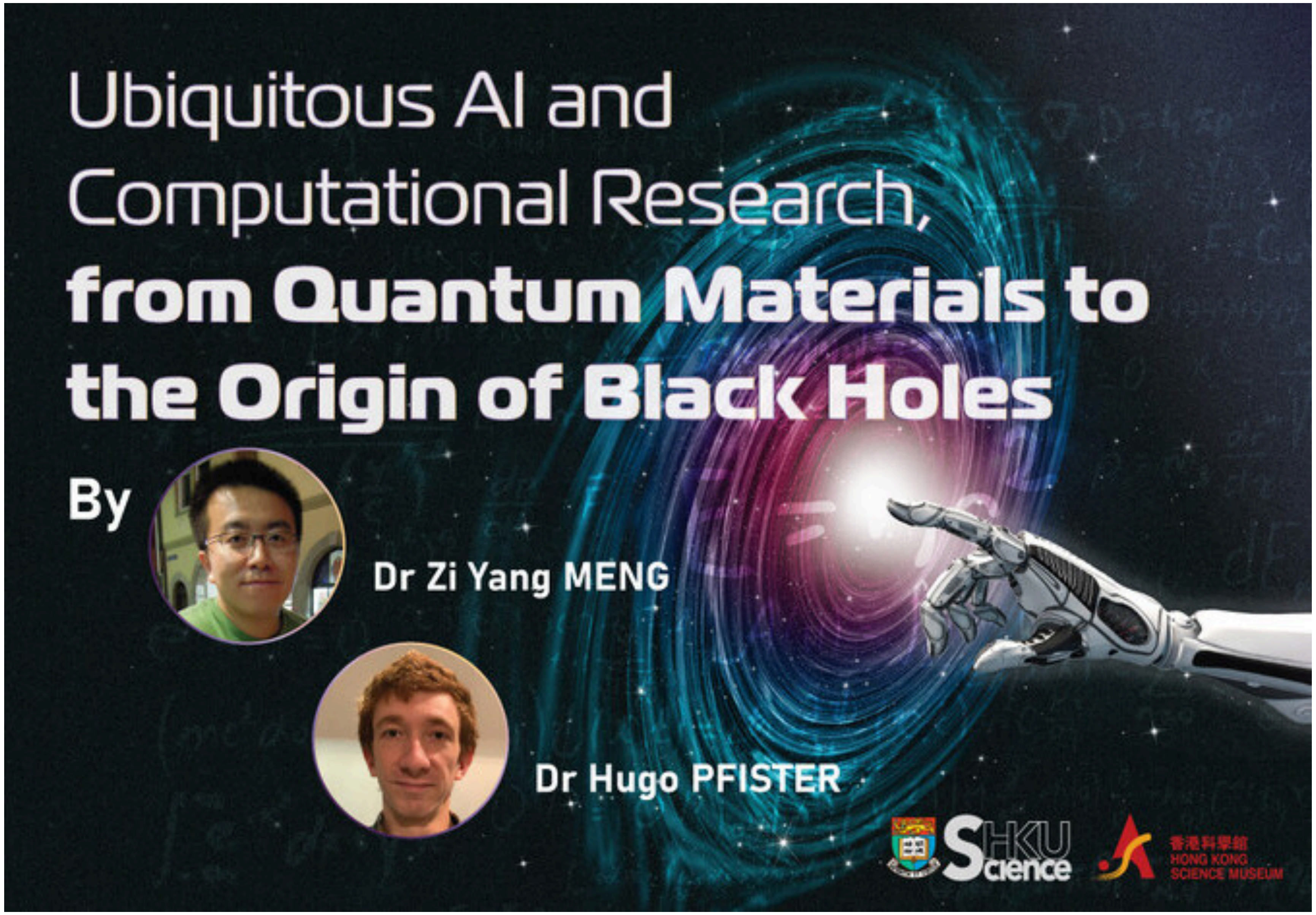
# Content


**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**

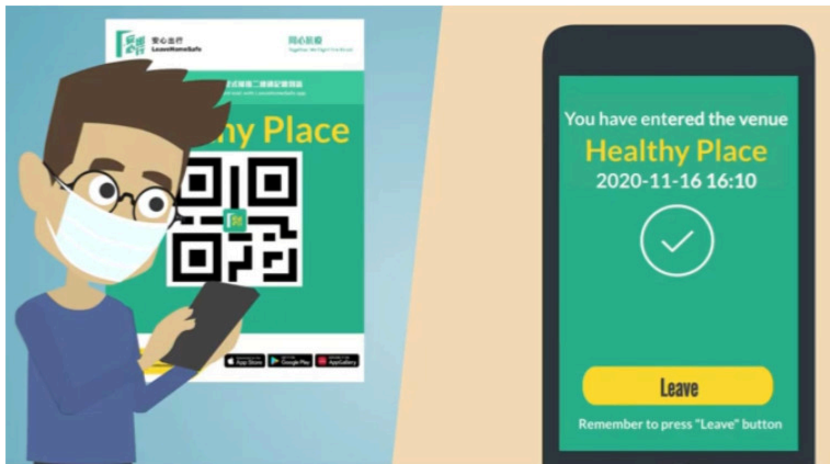
- **4.1 AI in quantum physics**
- **4.2 HPC and parallelism**
- **4.3 …**




**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

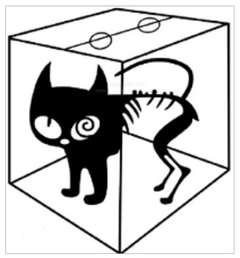

- The machine played perfect…
- I am so behind, unbelievable…
- AlphaGo is not the God, but it is a superior species than human being…

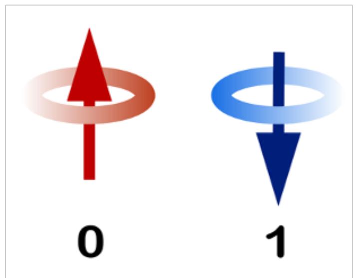
**AlphaGo**

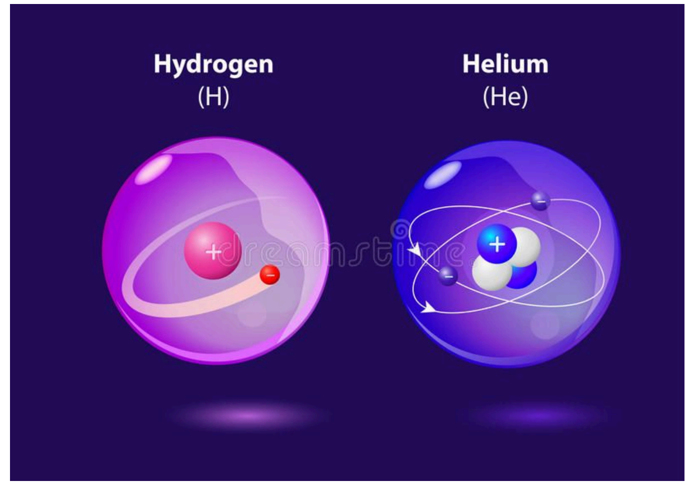

**Smart Robots** https://www.bostondynamics.com/

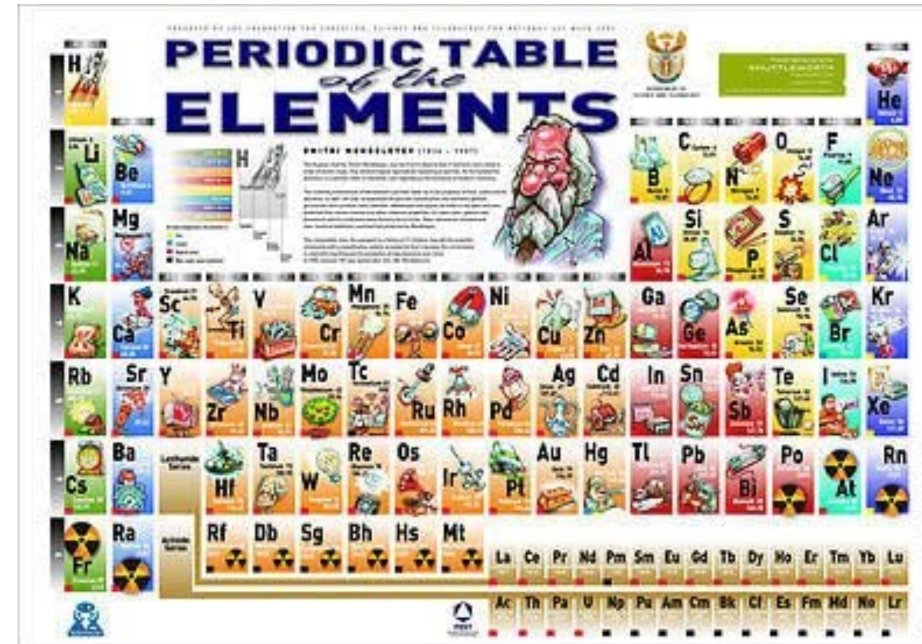
**Self-driving Car**

# Computation on quantum bit and quantum entanglement





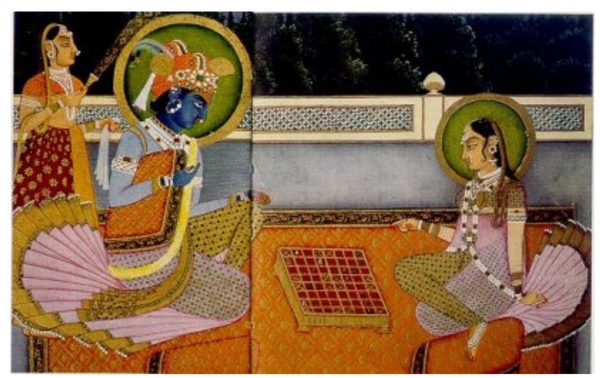




**Lead to the famous "exponential wall"**

Krishna and Radha playing chaturanga

Multi-electron atoms, cannot be solved exactly



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.

$2^N$

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

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

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

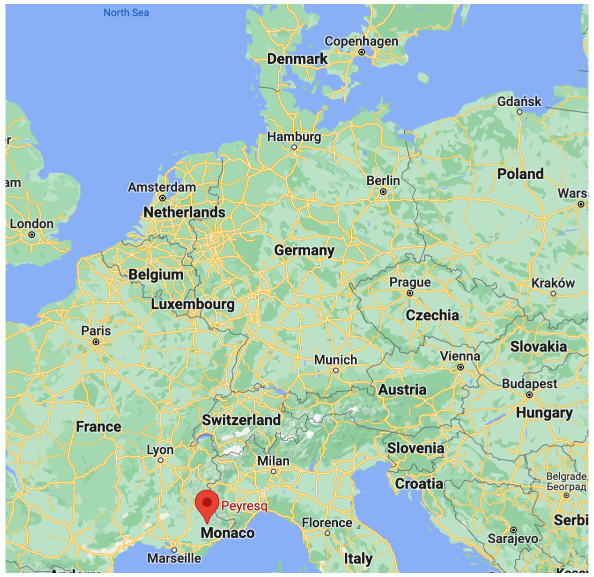
$N = 40 \quad 2^{40} = 1{,}099{,}511{,}627{,}776 \sim 10^{12}$

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

**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

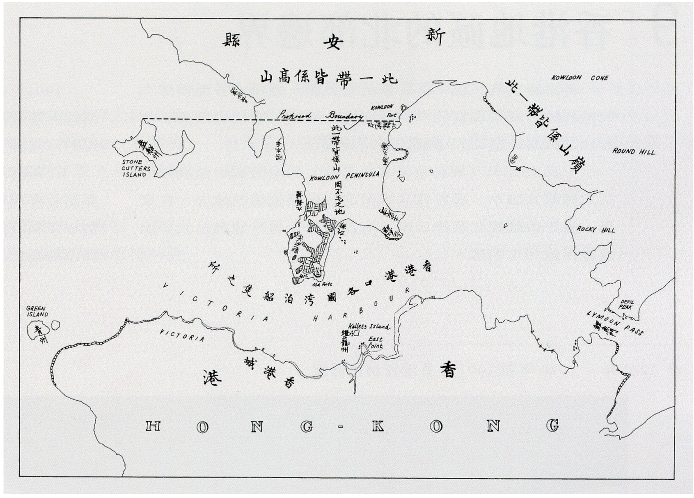
Edward Teller,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

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



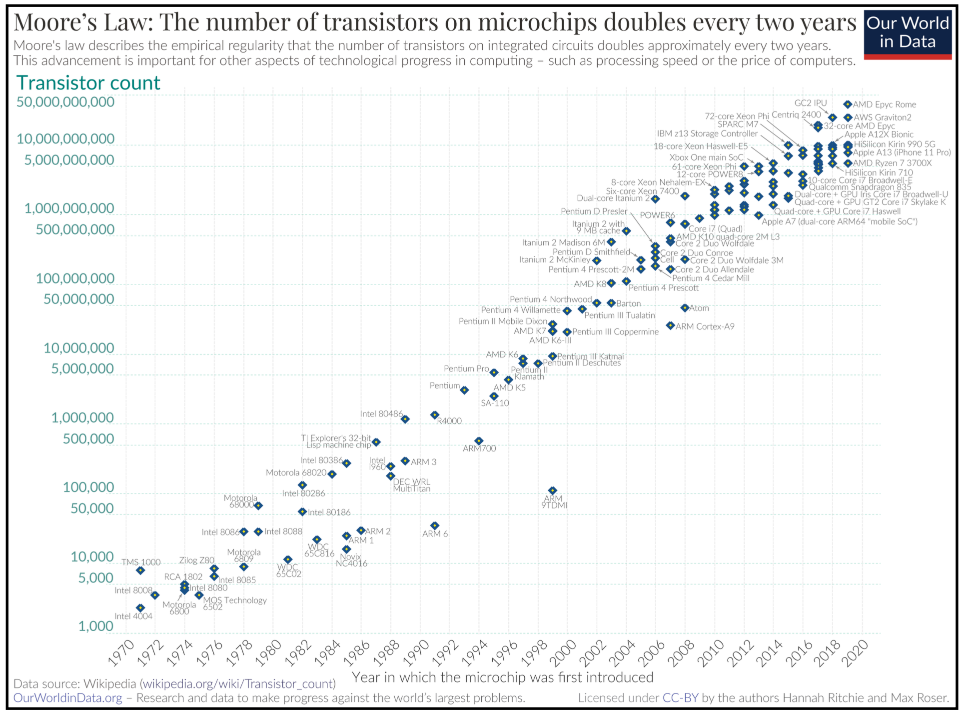

8 million taels of silver apiece

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

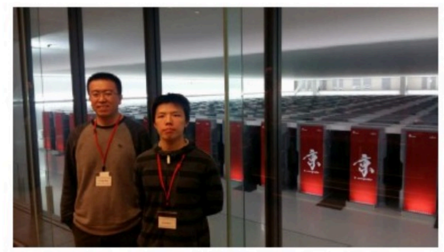
TeraFLOPS: 10^12

PetaFLOPS: 10^15

ExaFLOPS: 10^18

NSCC 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

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

Tianhe-2 (天河2号): 100 PetaFLOPS

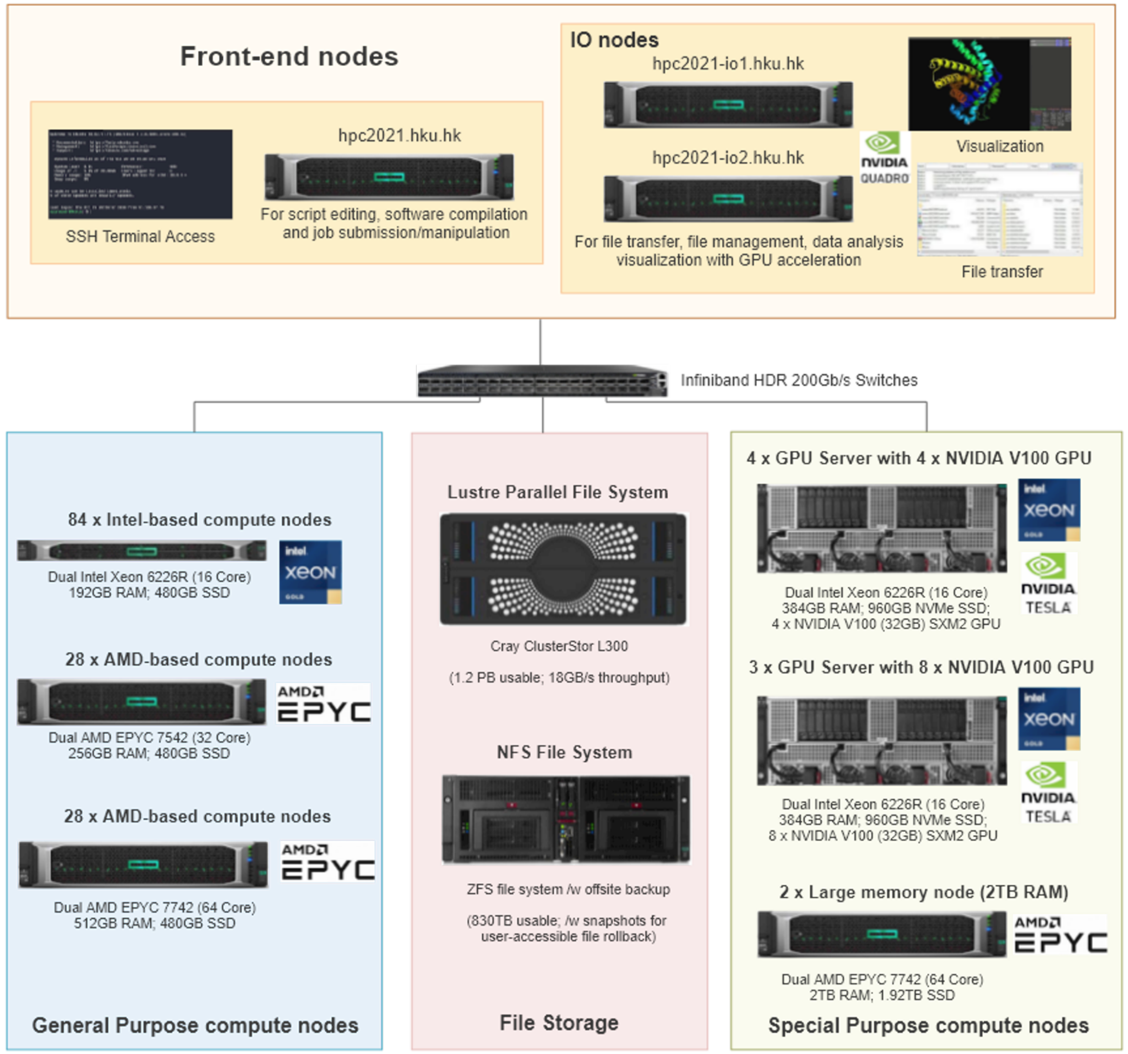
| | Supercomputer | Personal Computer | Human Brain |
|---|---|---|---|
| Computational Units | 32,000 Xeon CPUs<br>10^12 transistors | 4 CPUs, 10^9 transistors | 10^11 neurons |
| Cycle time | 10^-9 sec | 10^-9 sec | 10^-3 sec |
| Operations/sec | 10^15 | 10^10 | 10^17 |
| Memory updates/sec | 10^14 | 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

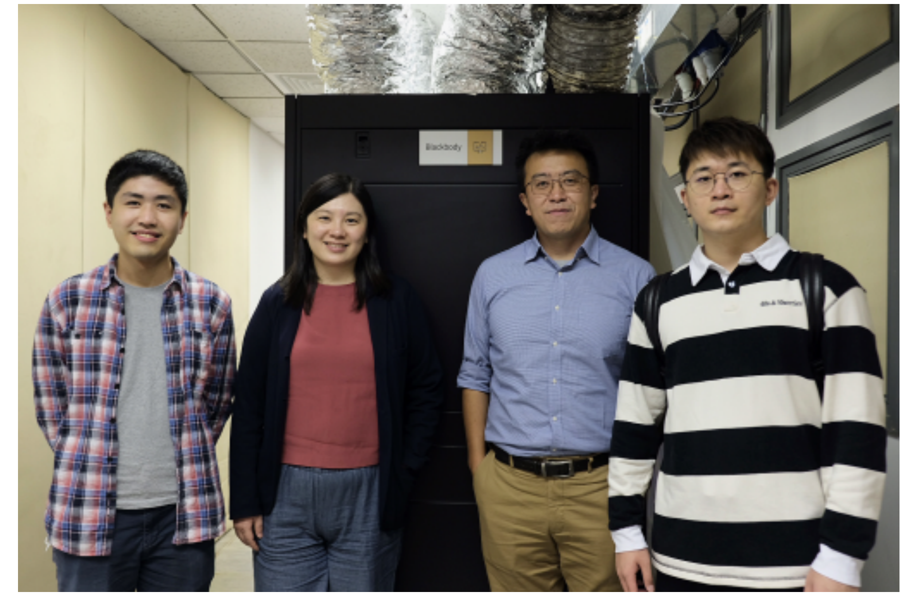



Tianhe-II: 16,000 node, 24 Intel Xeon E5 core CPU, 384,000 in total

# Our own Blackbody

1024 cpu cores

2022/09



2023/11

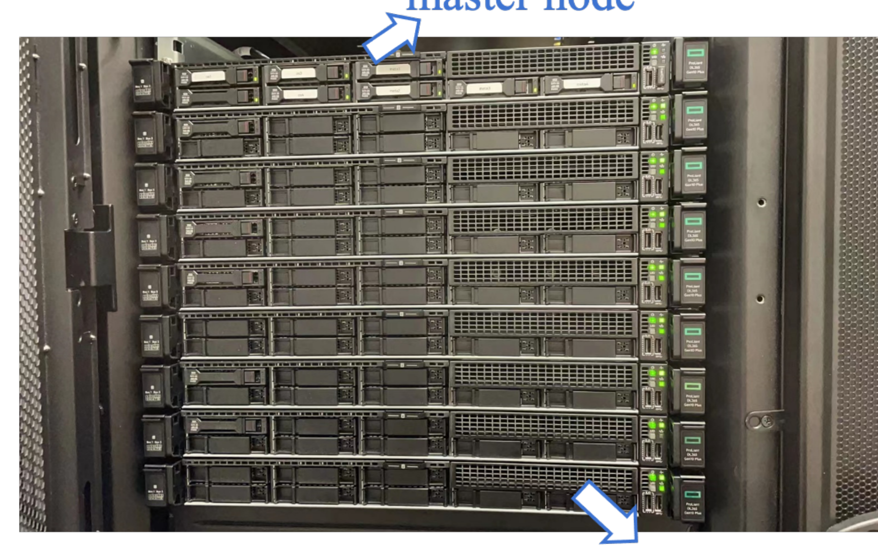
AMD 7702P (64 core) x 2 x 10 = 1280 cores
AMD 7573X (32 core) x 2 x 1 = 64 cores
AMD 7763 (64 core) x 2 x 7 = 896 cores
AMD 9654 (96 core) x 2 x 2 = 384 cores

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

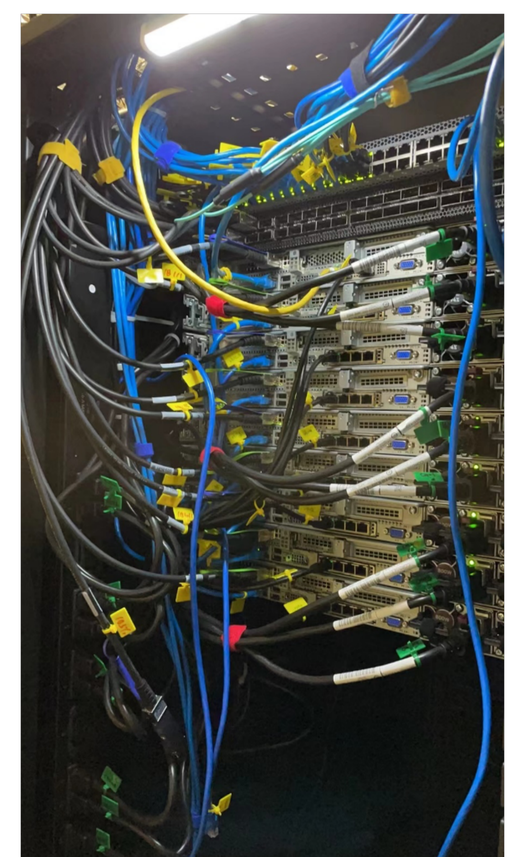
# Our Blackbody Cluster in Room 311 of CYM Building

master node



compute node

Cable Management & Labeling



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

1024 cpu cores

## Exhaust Pipes and Inrow Cooling



## Electricity

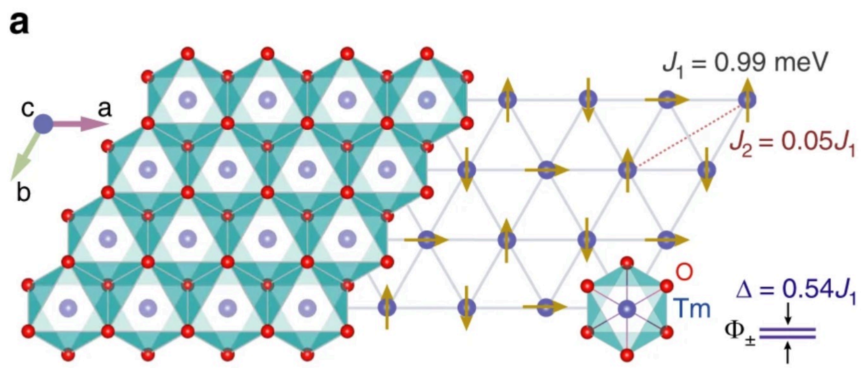
Total Electricity: 24 kW
Current Usage:
cluster ~ 5.4 kW (computing nodes 0.55 kW × 8, head node, storage)
cooling ~ 8 kW (each ~ 2.4 kW)

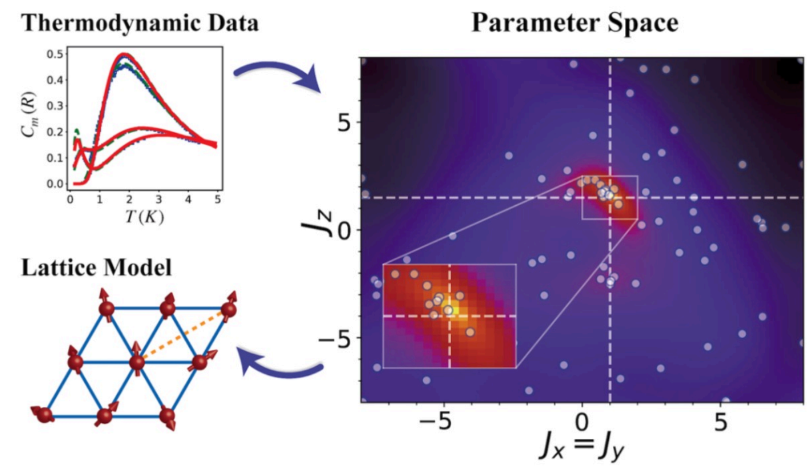
Around 10 kW electricity for future use.

# Computation in Quantum Physics

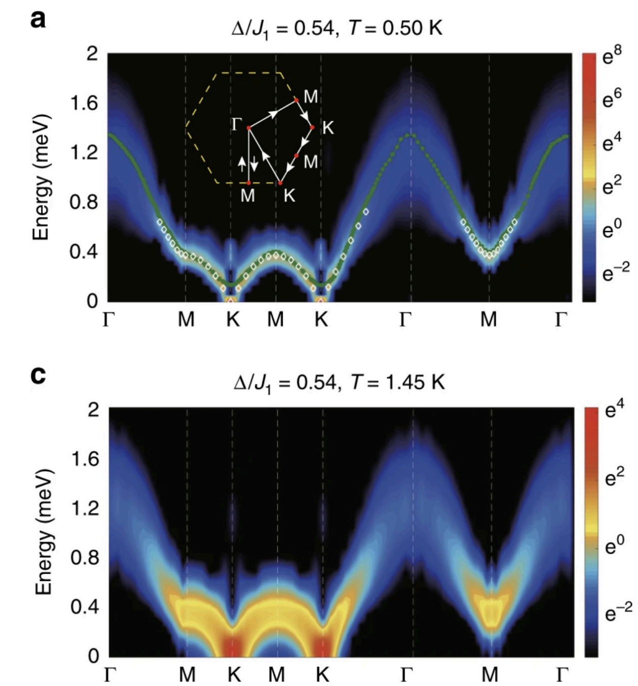
- Quantum material research connecting physicists in Hong Kong, Beijing and Shanghai

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



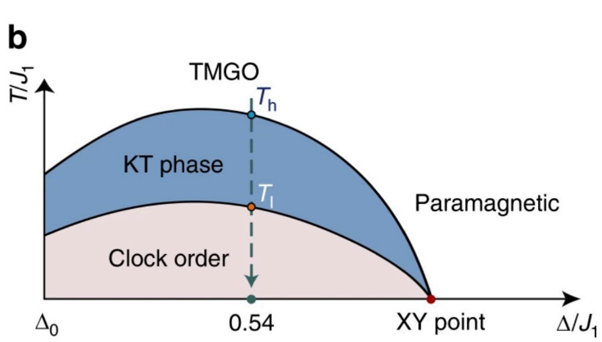

auto-gradient, Bayesian optimization

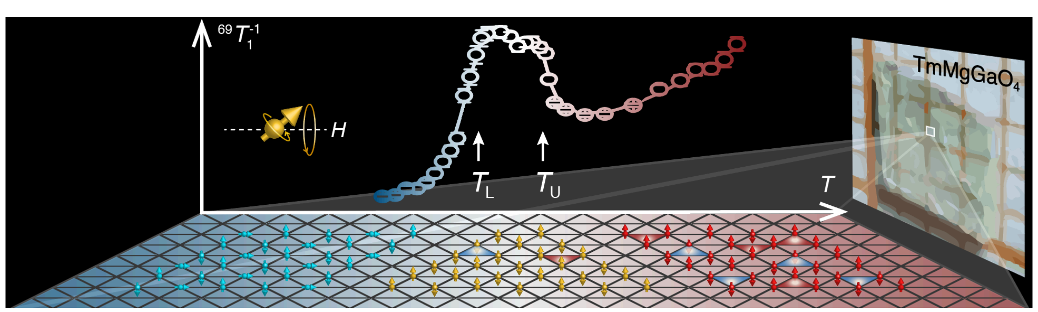



[Nature Communications 11, 1111 (2020)]

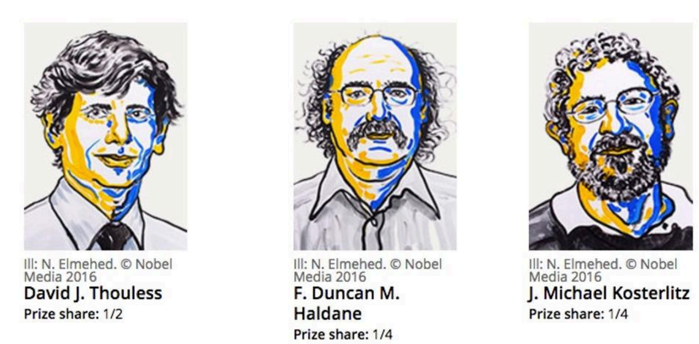
- Confirming simulated calculations, quantum material research reveals topological KT phase

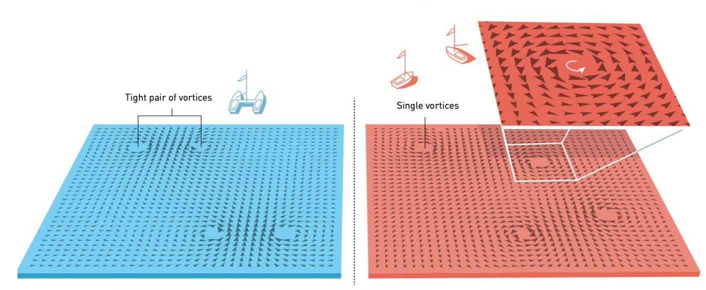
Nuclear magnetic resonance — MRI / CT scans




The Nobel Prize in Physics 2016




[Nature Communications 11,5631 (2020)]

# Computation in Quantum Physics

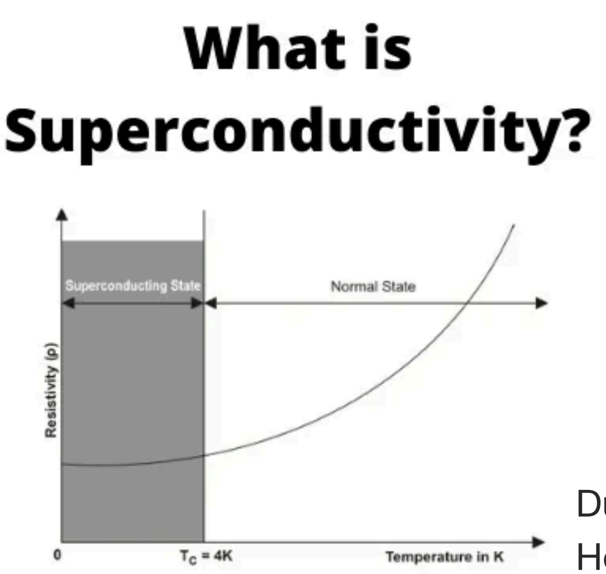
CLP 中電 electric power transmission at high voltage

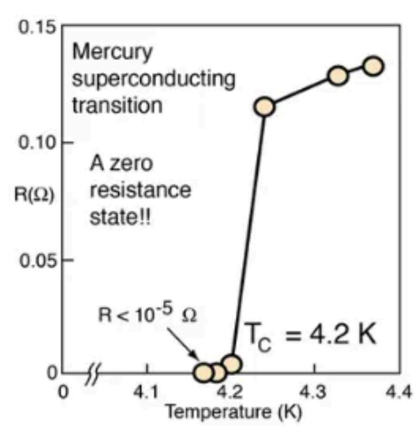
Maglev (magnetic levitation) bullet train with 600 k/h

High speed rail

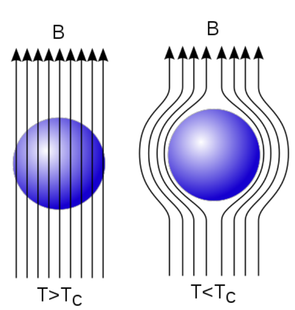

superconductors at ~ -270°C

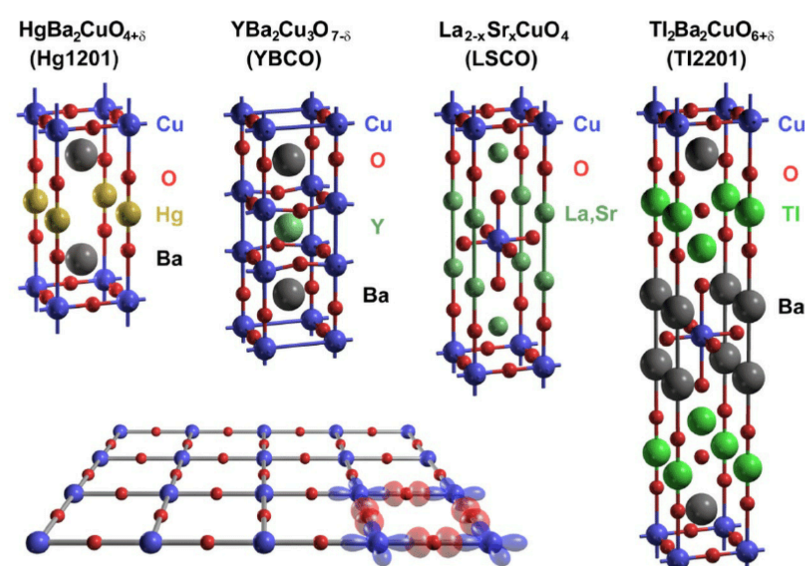
High-temperature superconductors at ~ -100°C

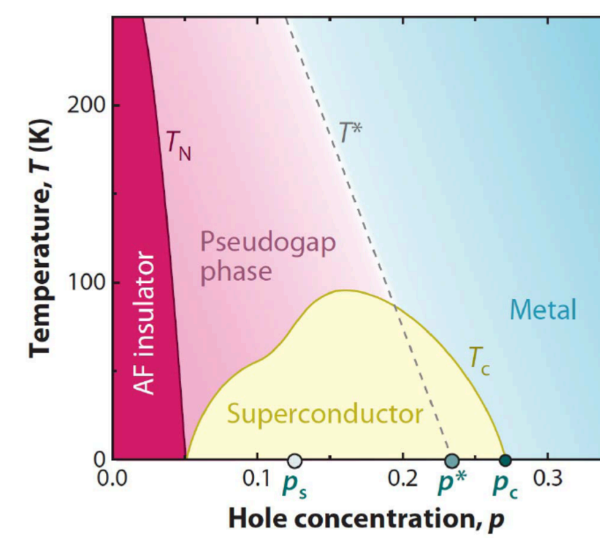


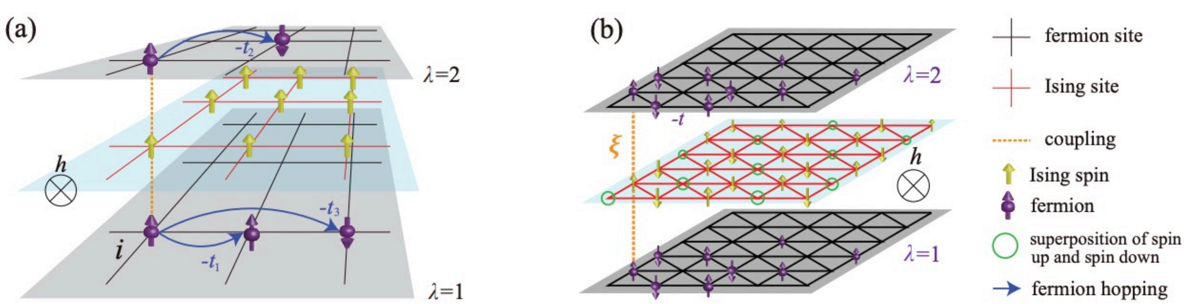

Dutch Physicist
Heike Kamerlingh Onnes in 1911



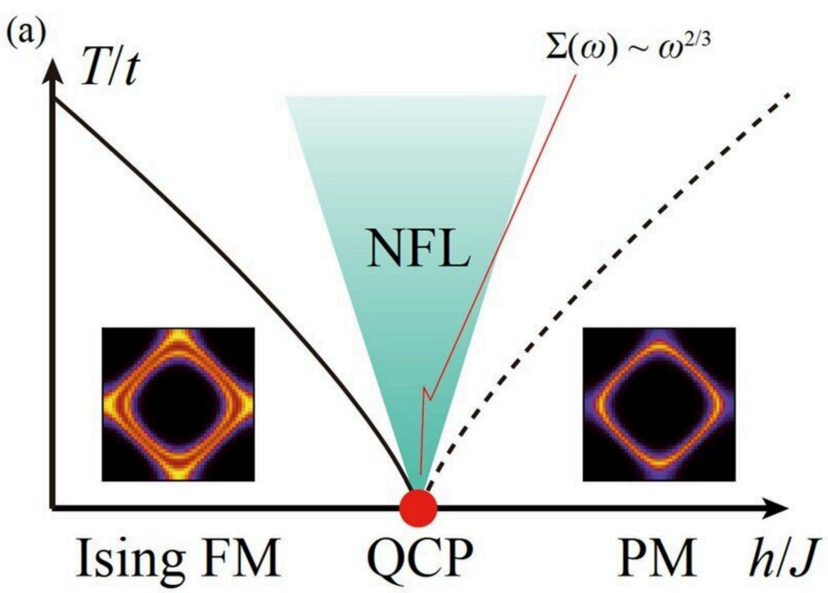



## Understanding quantum critical Metals

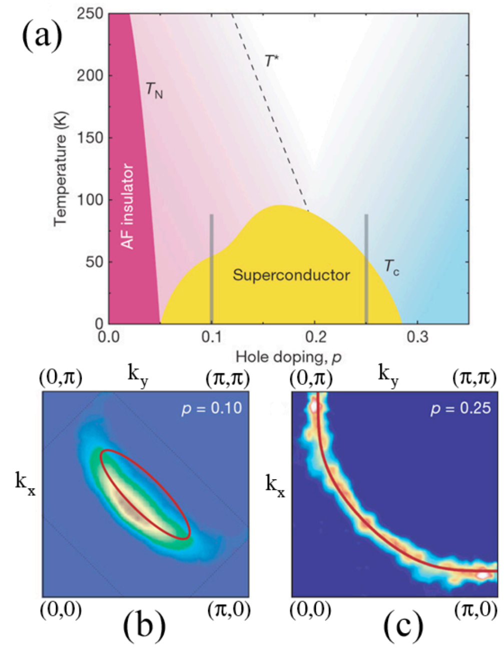



PNAS 20, 116 (34) 16760-16767 (2019)

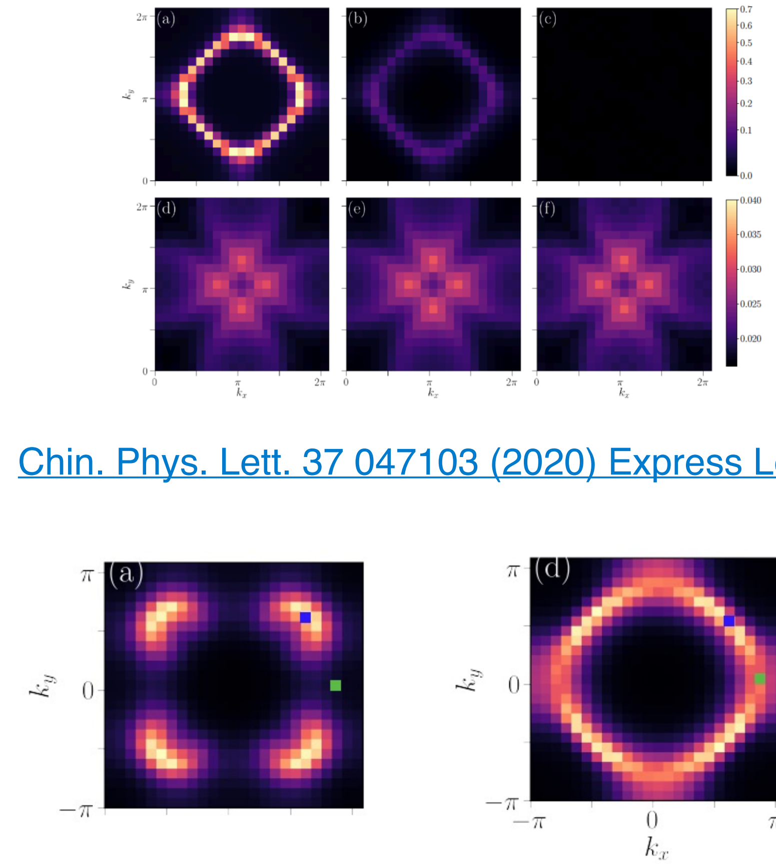



npj Quantum Materials 5, 65 (2020)

## metals' awkward cousin is found

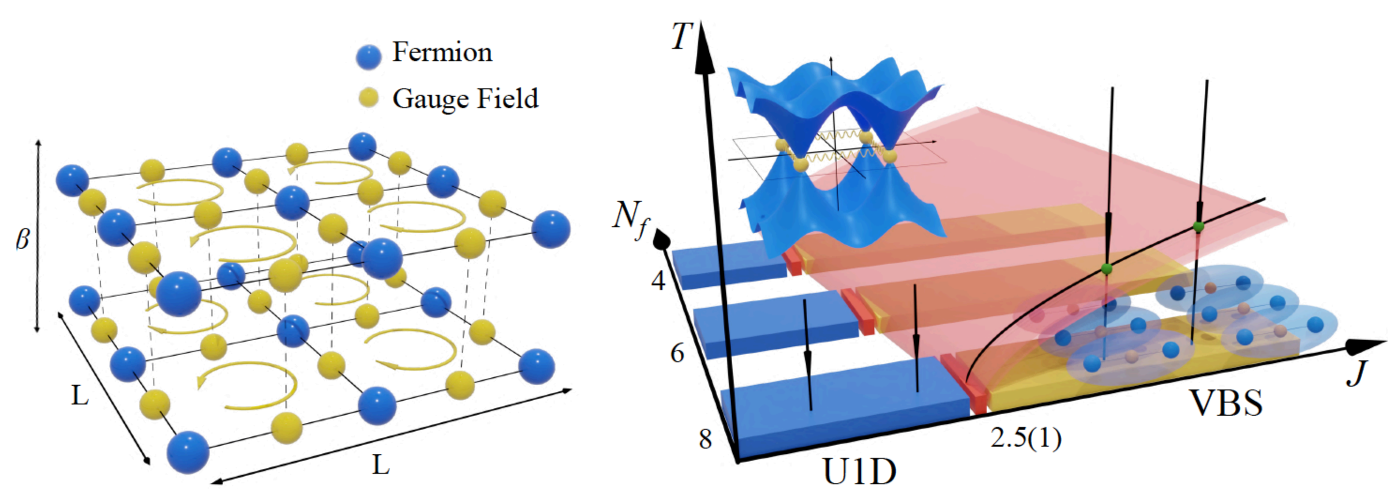



Chin. Phys. Lett. 37 047103 (2020) Express Letters




Phys. Rev. B 103, 165131 (2021)

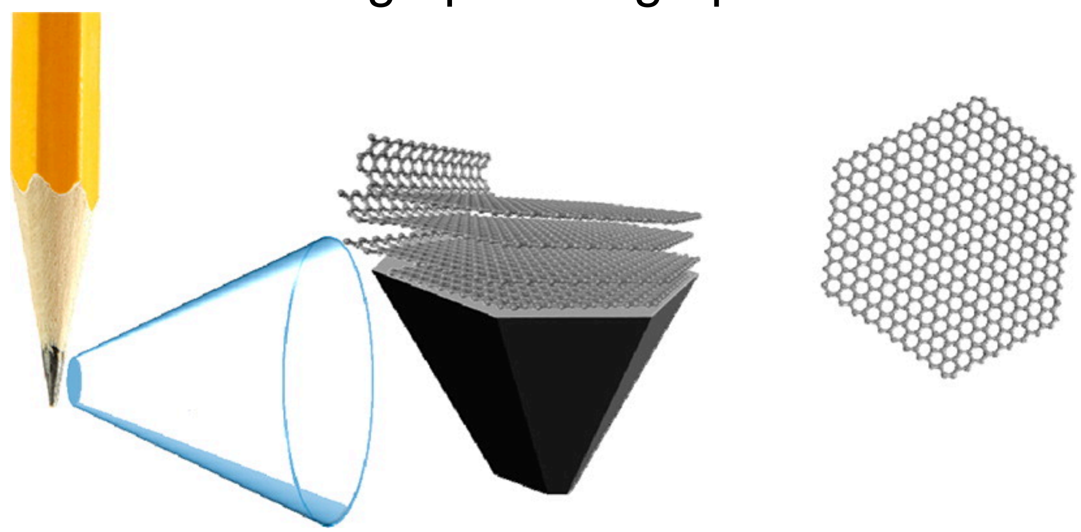
## Parent State of quantum phases



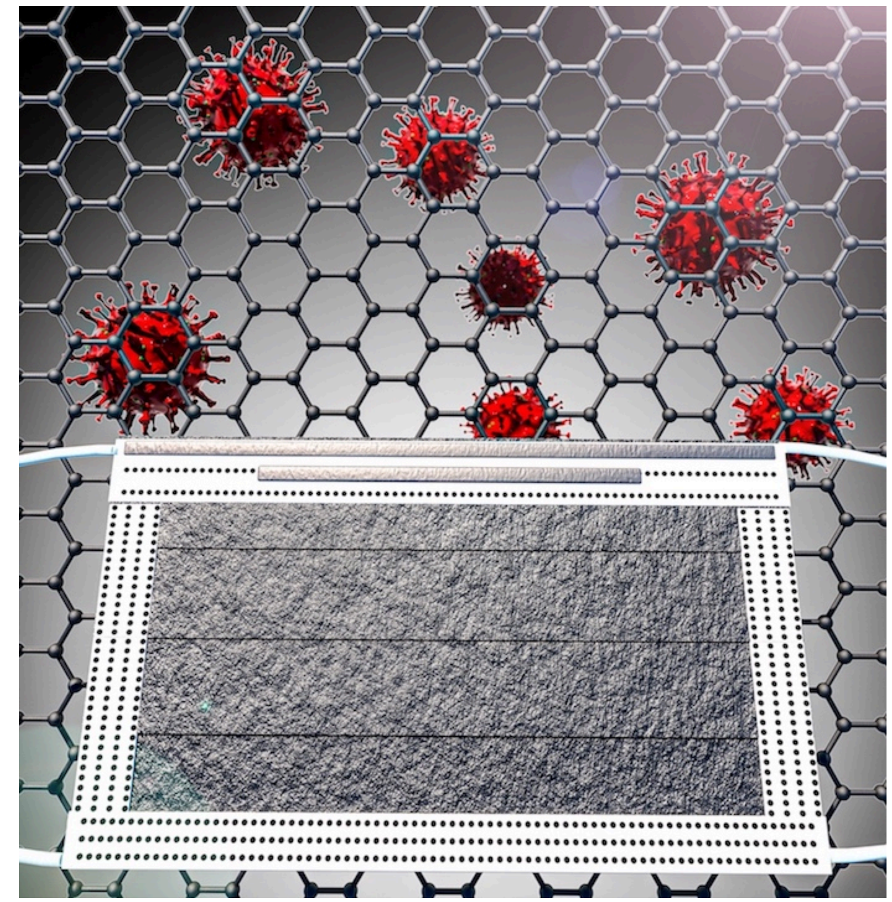

Phys. Rev. X 9, 021022 (2019)

# Computation in graphene face masks

## From graphite to graphene



## Graphene joins the fight against COVID-19



The Nobel Prize in Physics 2010

© The Nobel Foundation. Photo: U. Montan

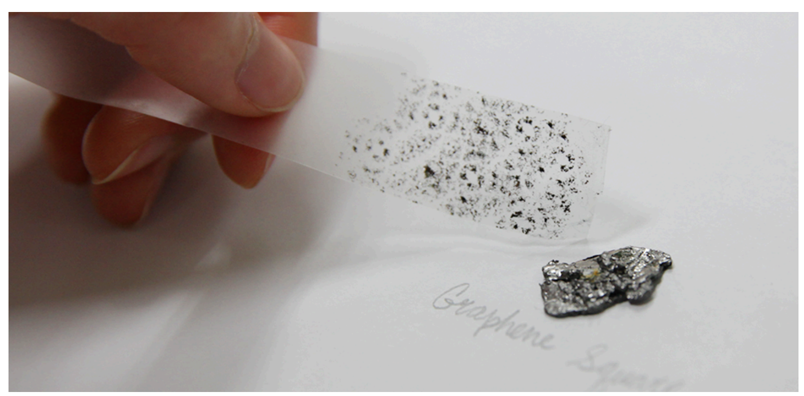
Andre Geim

Prize share: 1/2

© The Nobel Foundation. Photo: U. Montan

Konstantin Novoselov

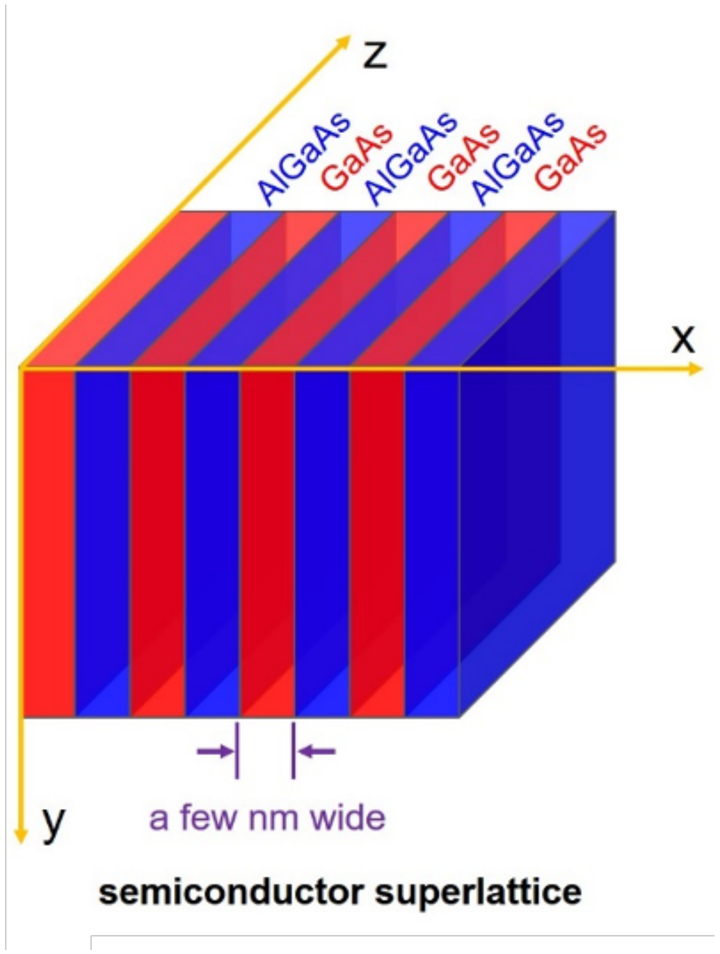
Prize share: 1/2



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.

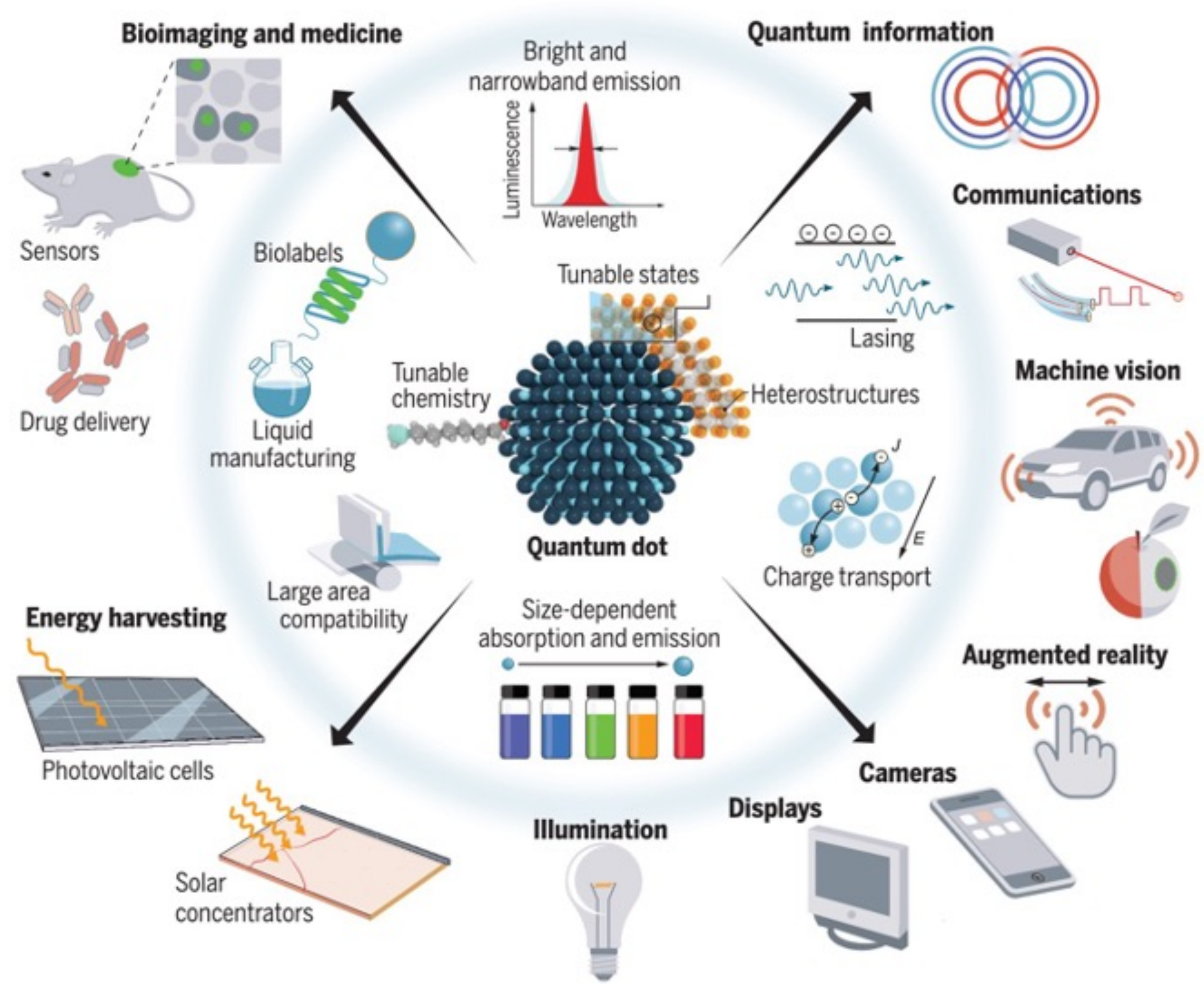
# Superlattices are widely used as electric and optical devices

In semiconductor industry




Wikipedia

In semiconductor quantum dots / wires technologies



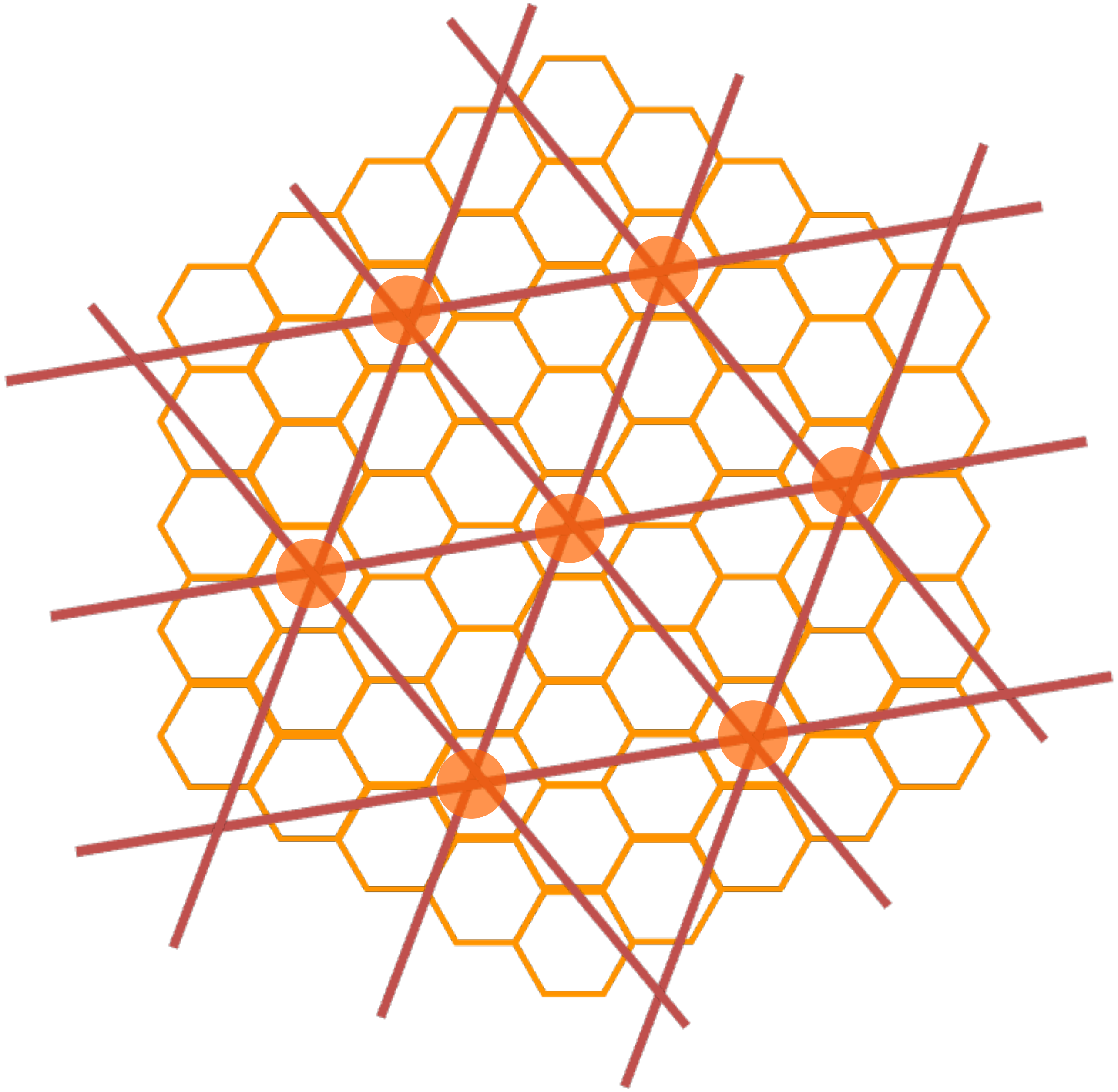

Garcia de Arquer et al., Science (2021)

- 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



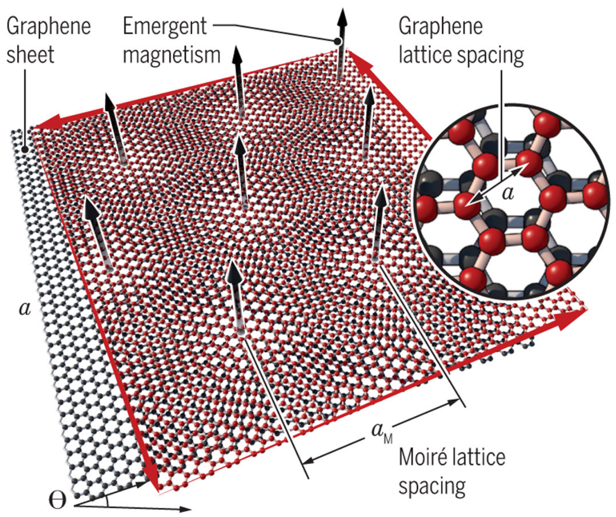
$20^{\circ}$ **rotation**

# Computation in graphene face masks

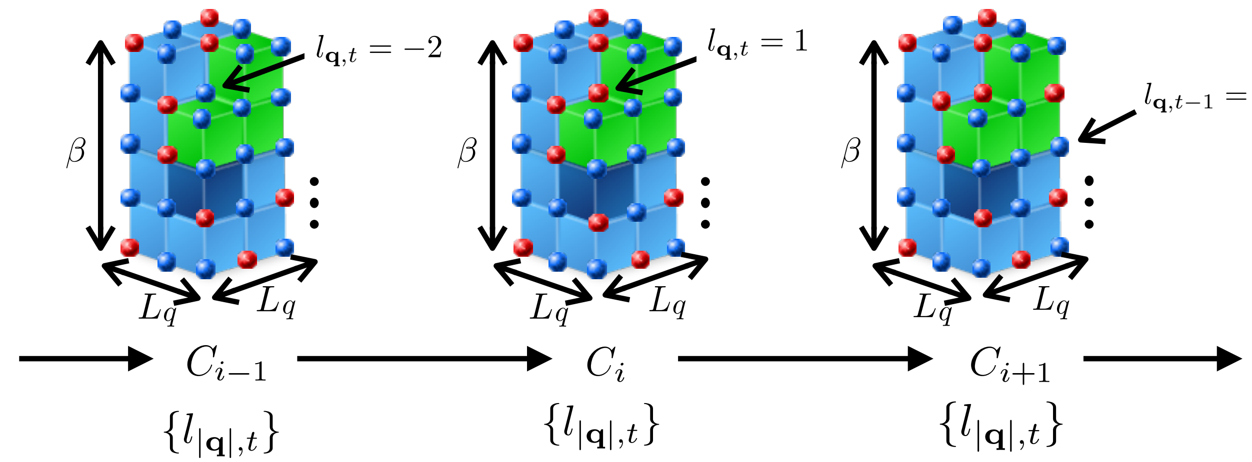
The Samadhi of magic angle twisted bilayer graphene (转角石墨烯的三昧)

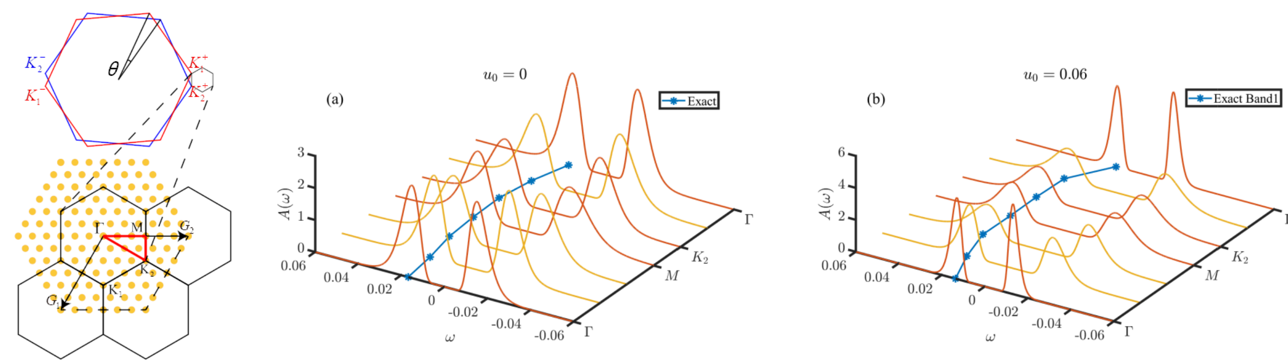
**Twisted bilayer graphene**

The two sheets are twisted by a small angle (Θ), creating a Moiré pattern that makes the bilayer both electrically insulating, with conducting edge states (red arrows), and magnetic.

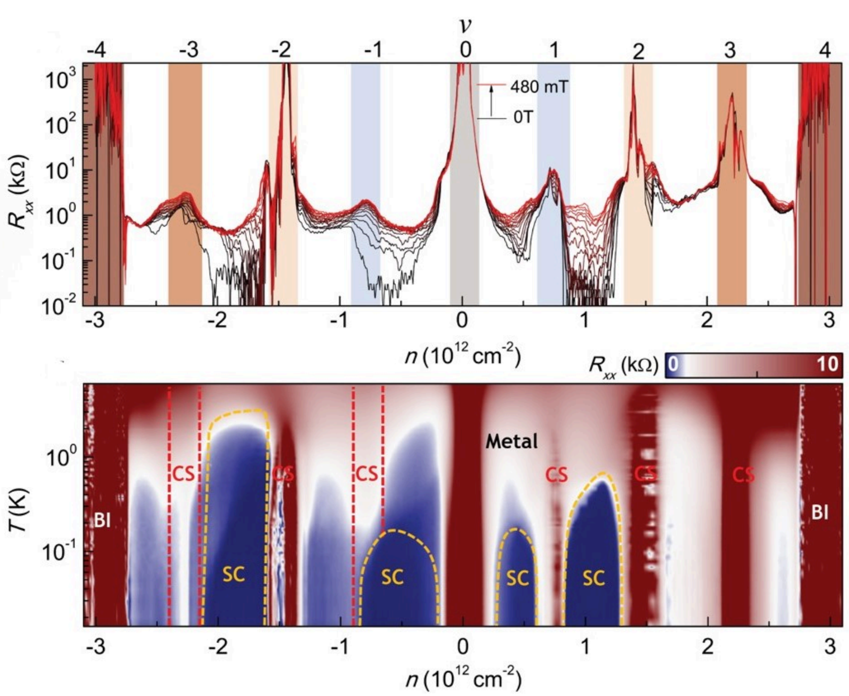


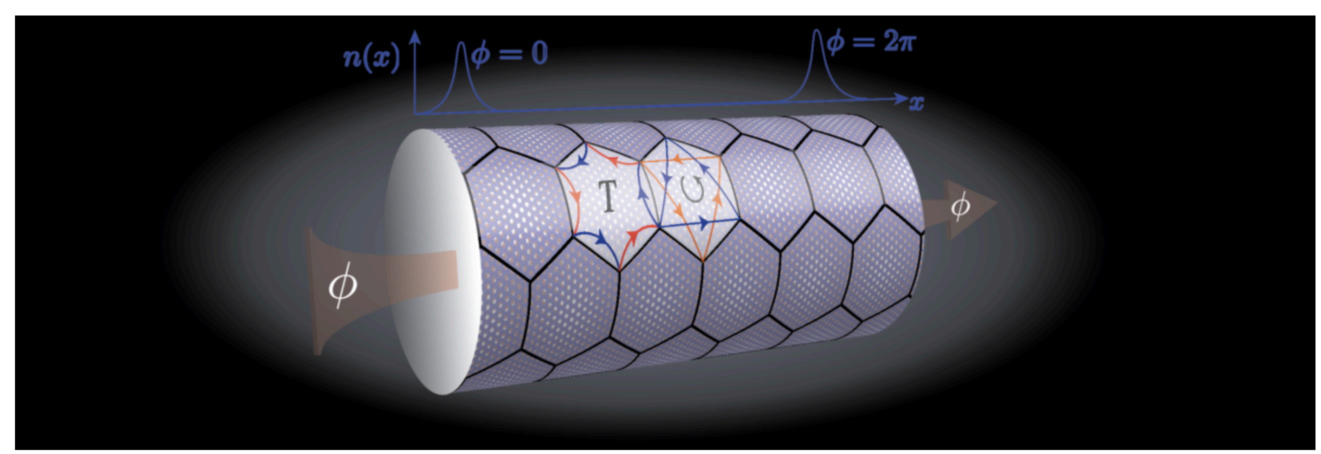





Chin. Phys. Lett. 38, 077305 (2021) Cover story




Nature Communications 12, 5480 (2021)

# Momentum space quantum Monte Carlo algorithm


## Long-range Coulomb + fragile topology

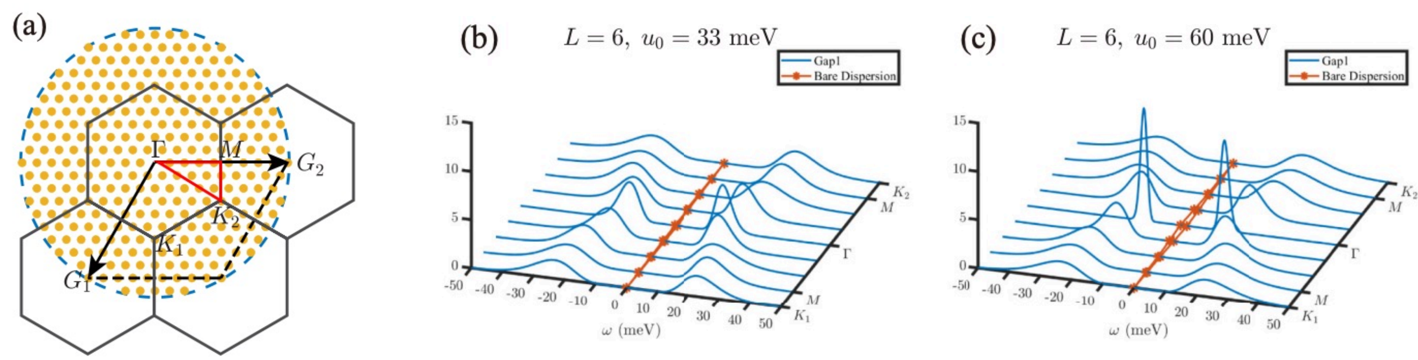
$$H = H_0 + H_{int}$$

$$V(q) \sim \frac{1}{q}$$

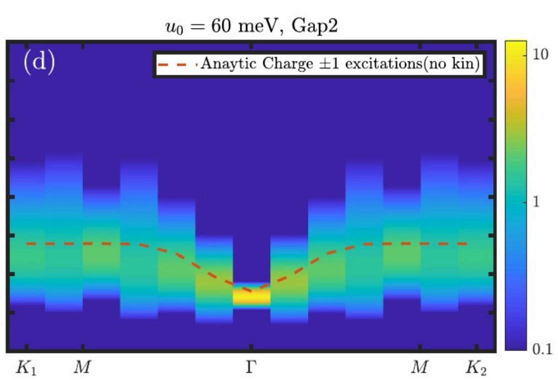
$$\delta\rho_{\mathbf{q}+\mathbf{G}} \sim \sum_{\mathbf{k}\in mBZ, m_1, m_2, \tau, s} \lambda_{m_1,m_2,\tau}(\mathbf{k}, \mathbf{k}+\mathbf{q}+\mathbf{G})\, d^\dagger_{\mathbf{k},m_1,\tau,s} d_{\mathbf{k}+\mathbf{q},m_2,\tau,s}$$

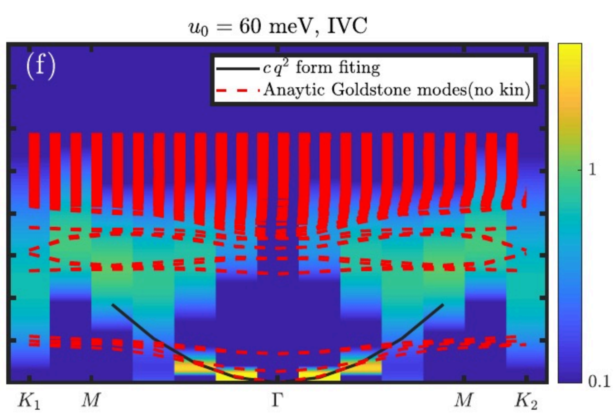
$$H_0 = \sum_m \sum_{\mathbf{k},\tau,s} \epsilon(\mathbf{k}) d^\dagger_{\mathbf{k},m,\tau,s} d_{\mathbf{k},m,\tau,s}$$

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

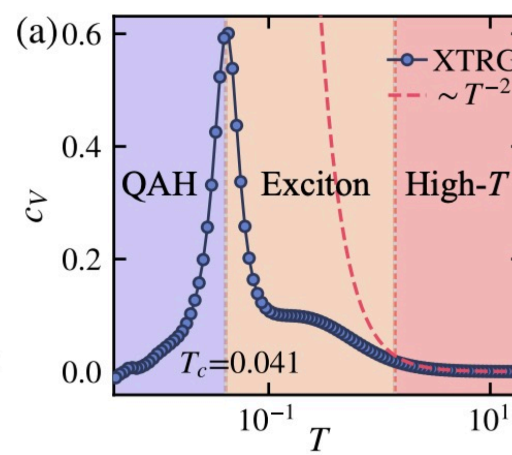



## Collective excitations




## 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)](#)

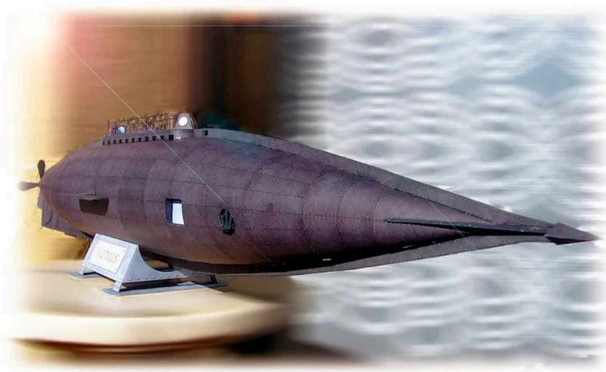
**The quantum teleportation pencil**

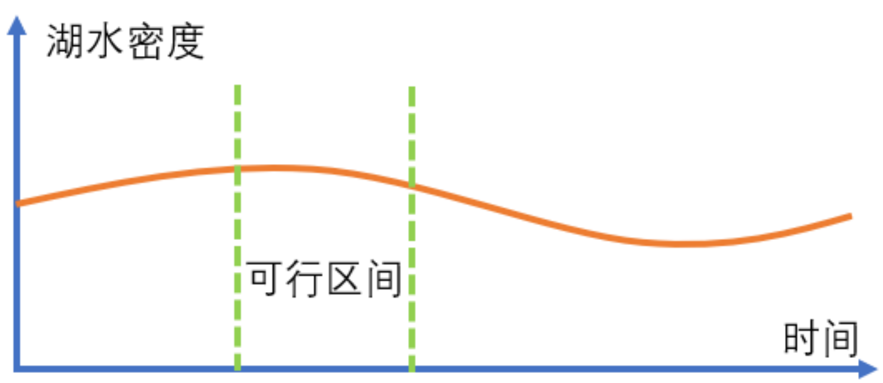
Are you sitting comfortably? And concentrating hard? We're entering the realms of superfast computing based on quantum teleportation via twisted graphene lattices. But don't worry, you'll be fine as long as you have a pencil handy.

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

Xu Zhang

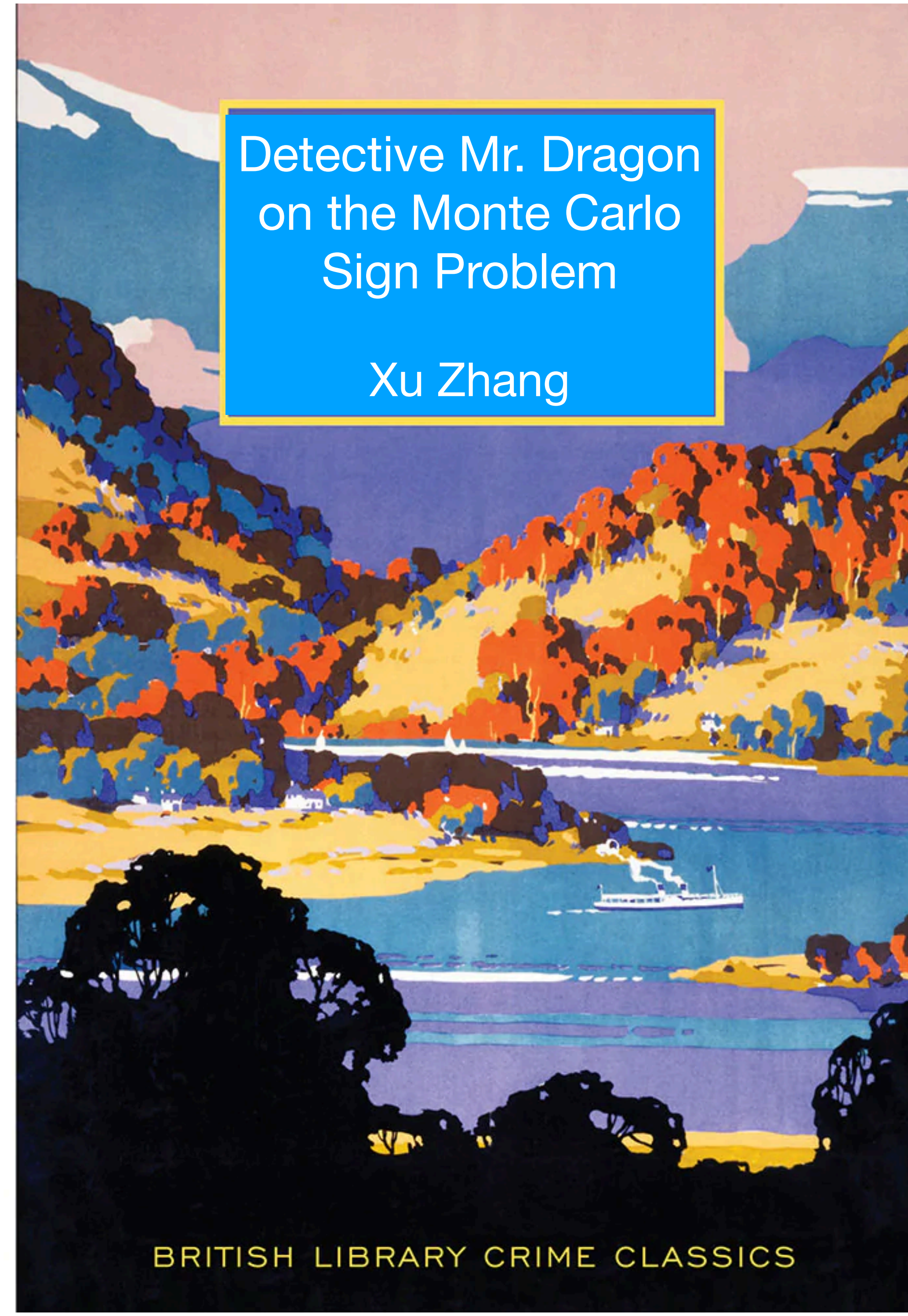

Caption Nemo and submarine Nautilus






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

$\langle \pm 1 \rangle \sim e^{-N}$ **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)

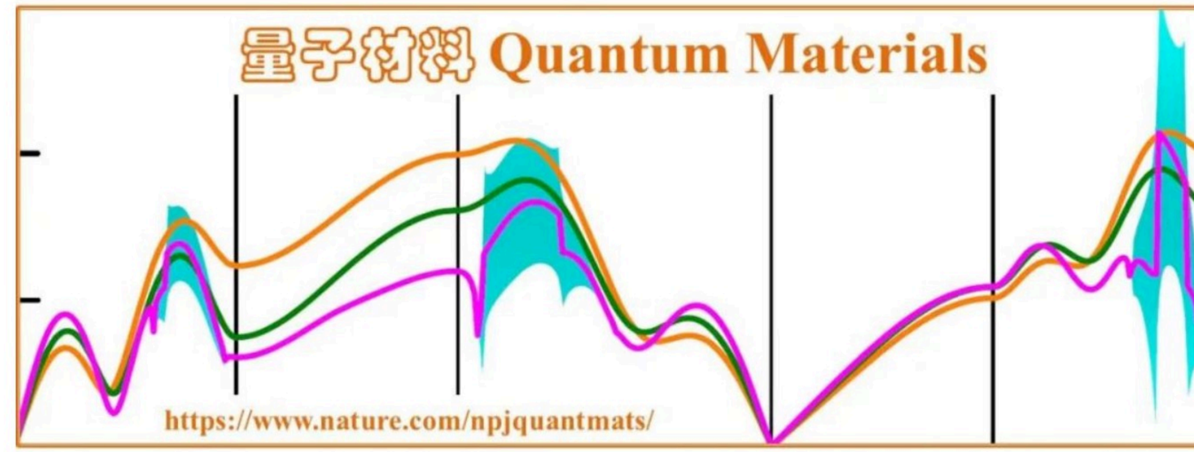
Entanglement entropy and conformal field theory
Calabrese & Cardy

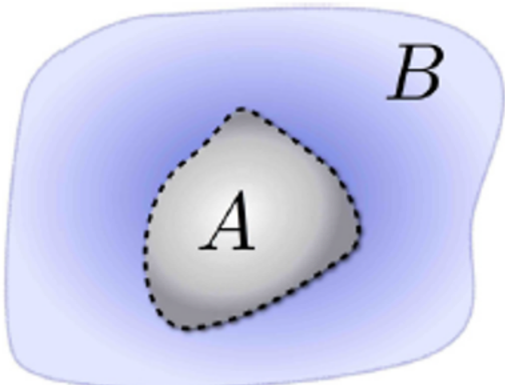
J. Stat. Mech. (2004) P06002

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




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

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

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

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

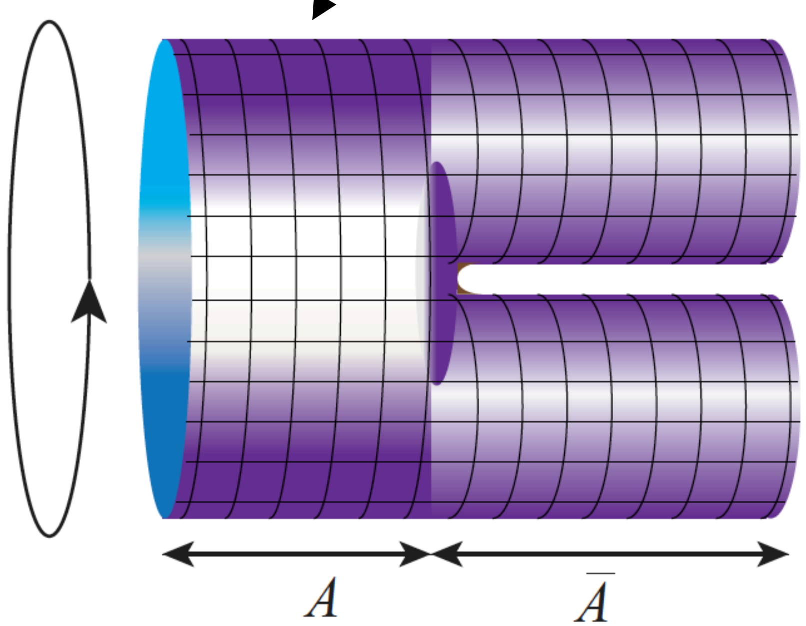
" discuss entropy in terms of the **Euclidean path integral** on an n-sheeted Riemann surface. "

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

**" Qiu Ku is the $Z_A^{(2)}$ "**

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

(a)




(b)

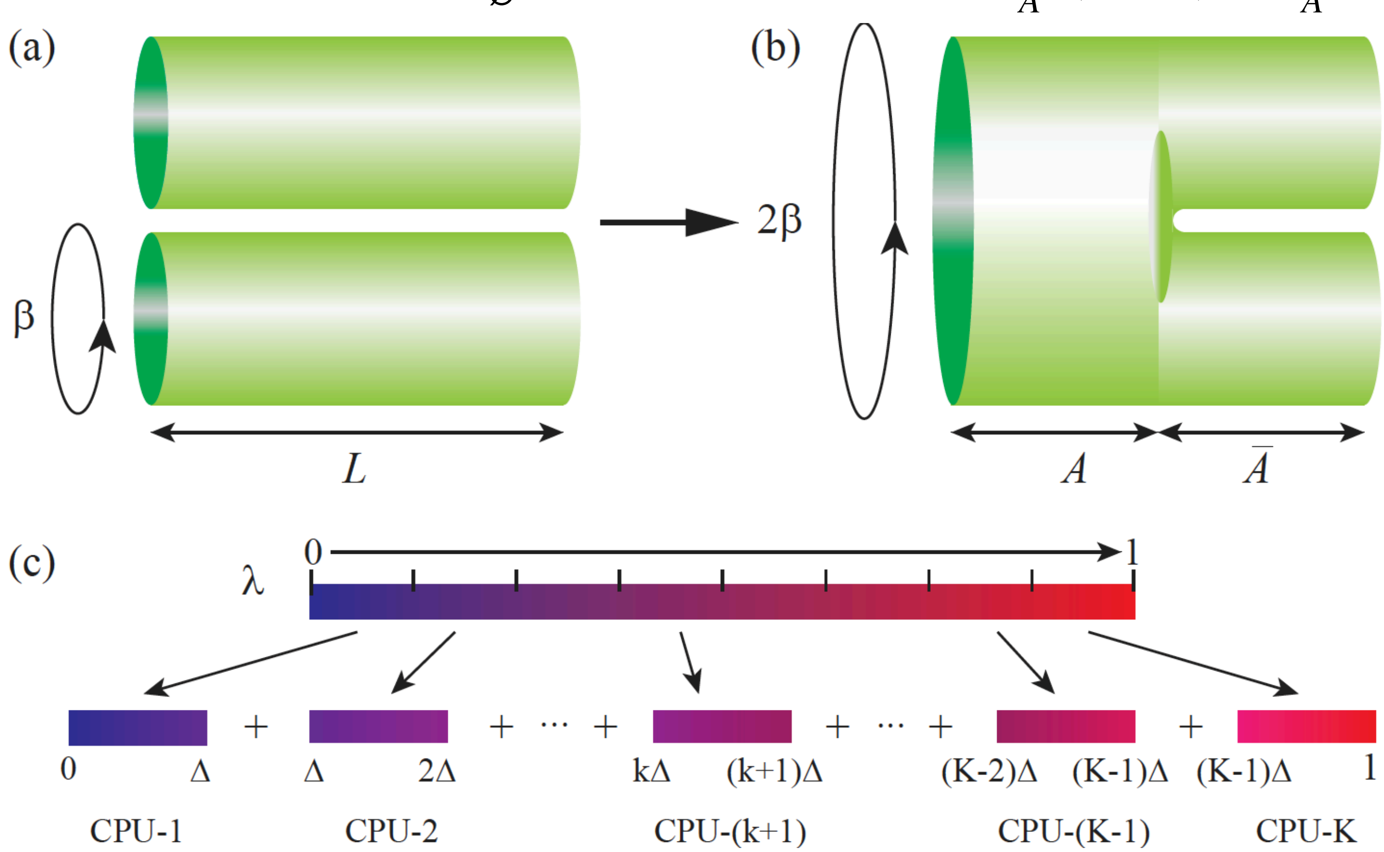
# Incremental (Qiu Ku) method

- 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)

$$Z_A^{(2)}(\lambda) = \sum_{B\subseteq A} \lambda^{N_B}(1-\lambda)^{N_A-N_B} Z_B^{(2)}$$

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

$$Z^{(2)}(\lambda=0) = Z_\varnothing^{(2)} \qquad Z_A^{(2)}(\lambda=1) = Z_A^{(2)}$$




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

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

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

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

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

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

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

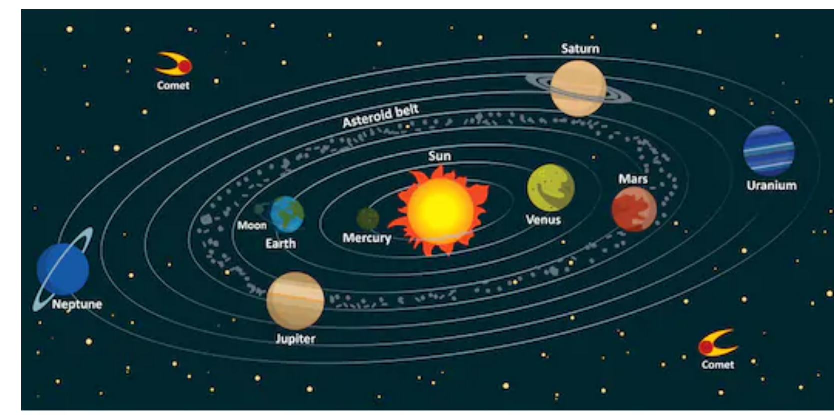
Issac Newton

Gravitation is the reason

$$F = GM_1M_2/r^2$$

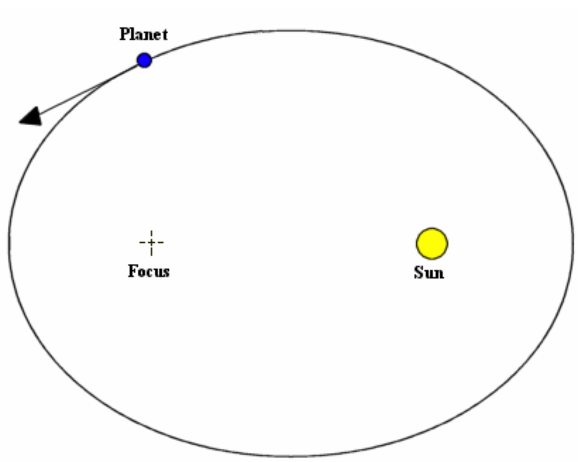
$$\dot{\vec{v}}(t) = \vec{a}(\vec{x}(t), \vec{v}(t), t)$$

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

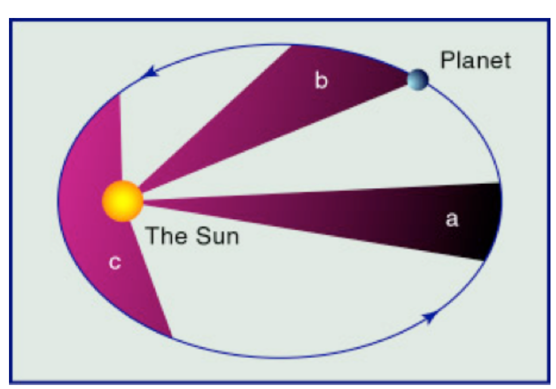



shutterstock.com • 319137437

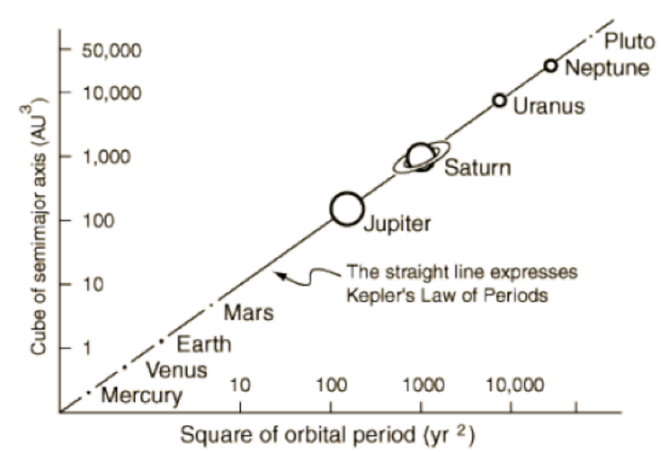
First law, ellipses




Second law, equal areas in equal time

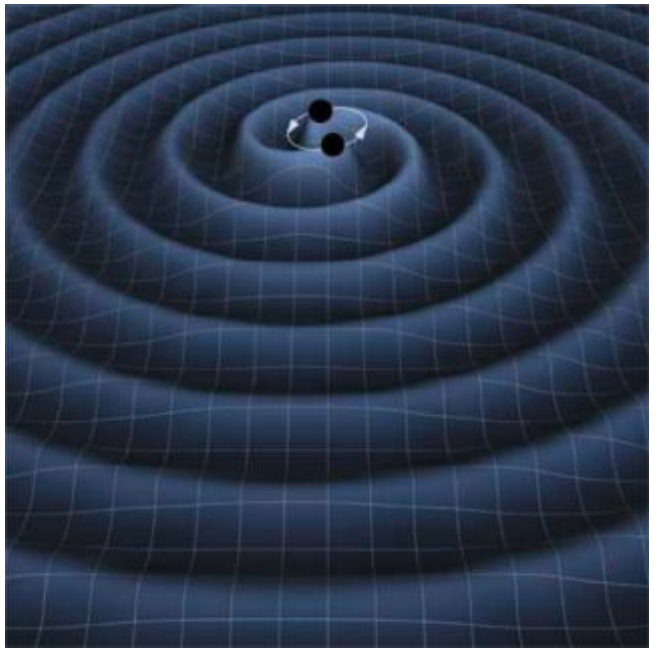


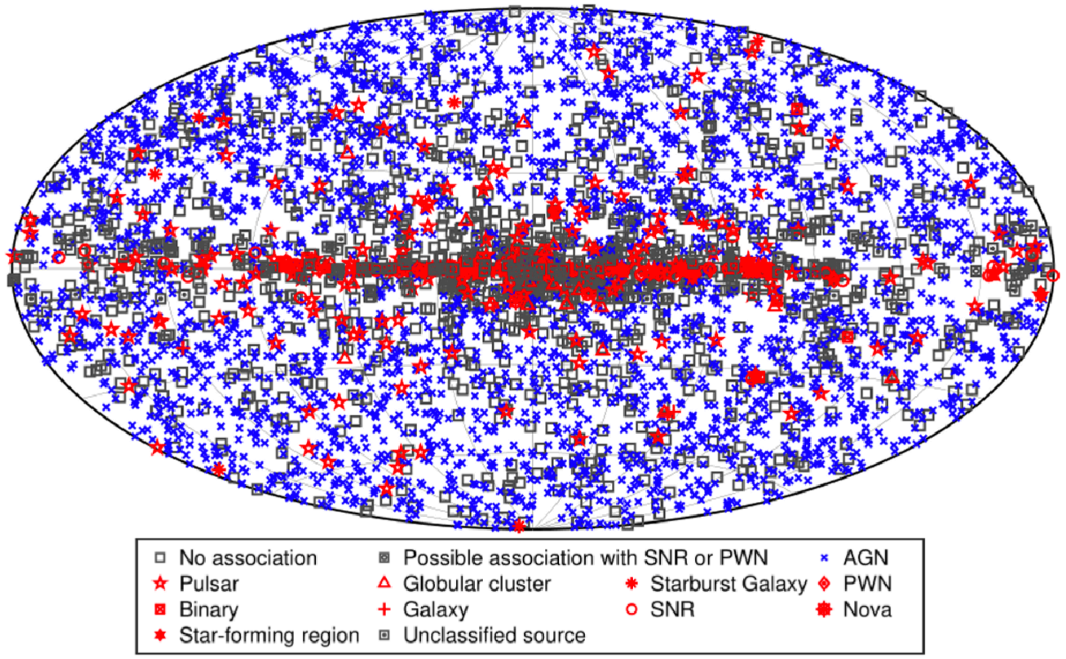

Third law, T^2 ~ D^3



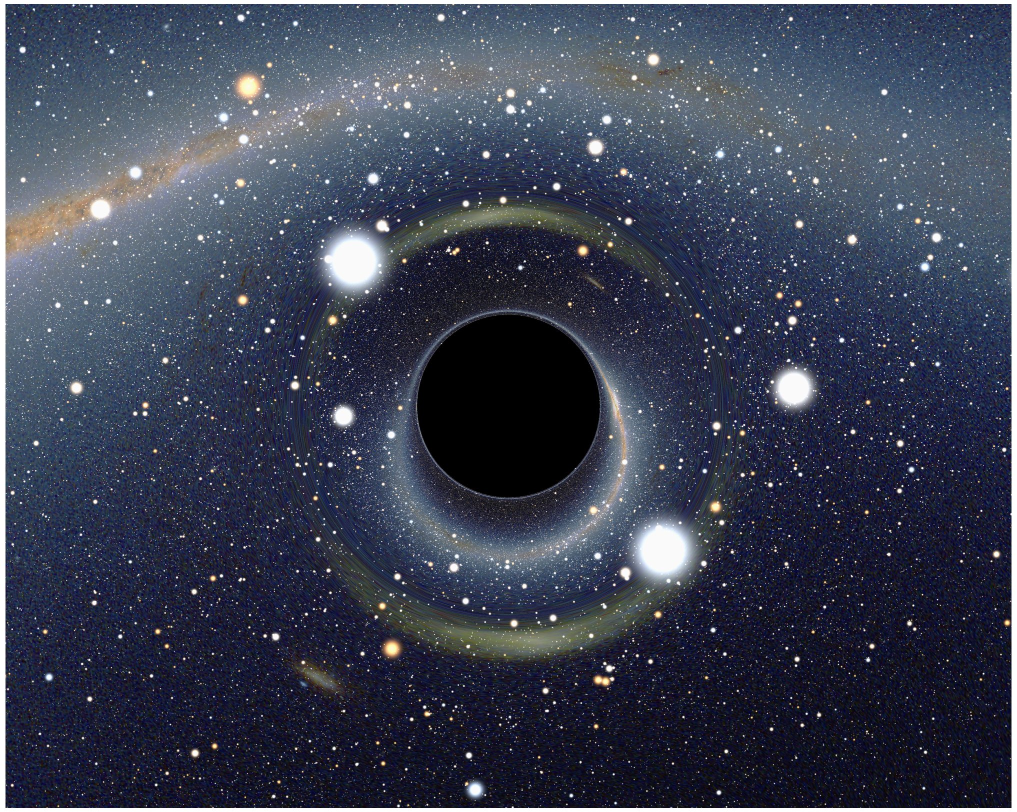

https://www.scifac.hku.hk/events/ai-computational-research

# 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