

Computational Physics

Teaching Materials:

<https://quantummc.xyz/teaching/>

Slides

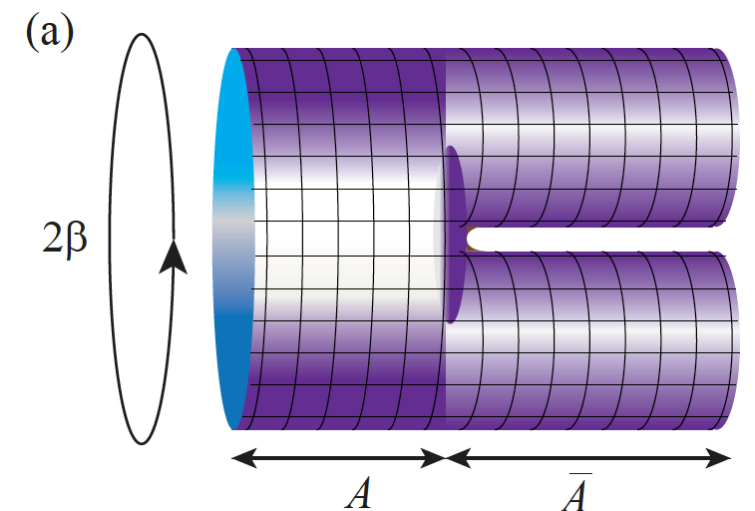
Reading materials

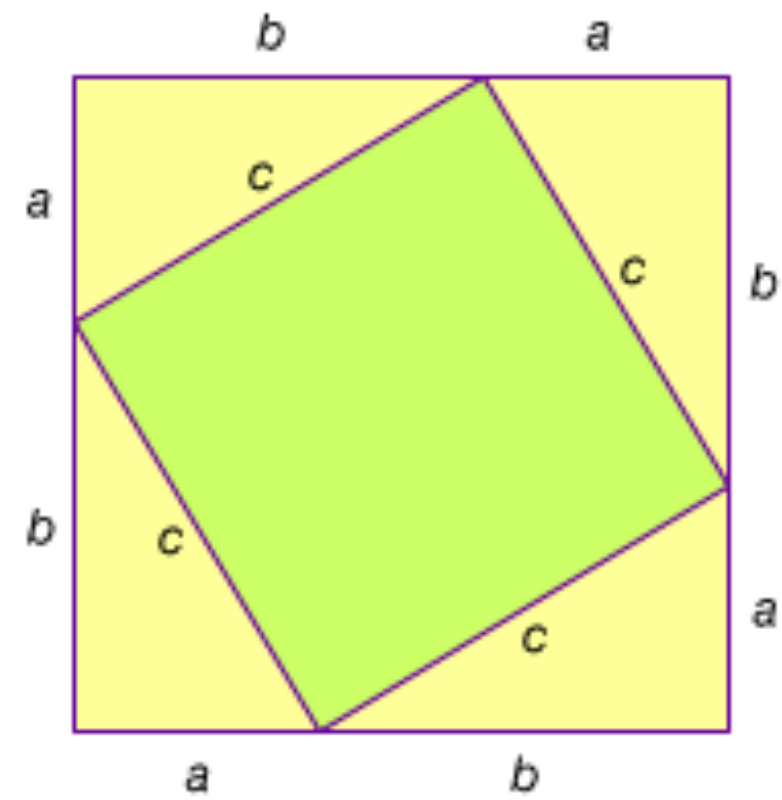
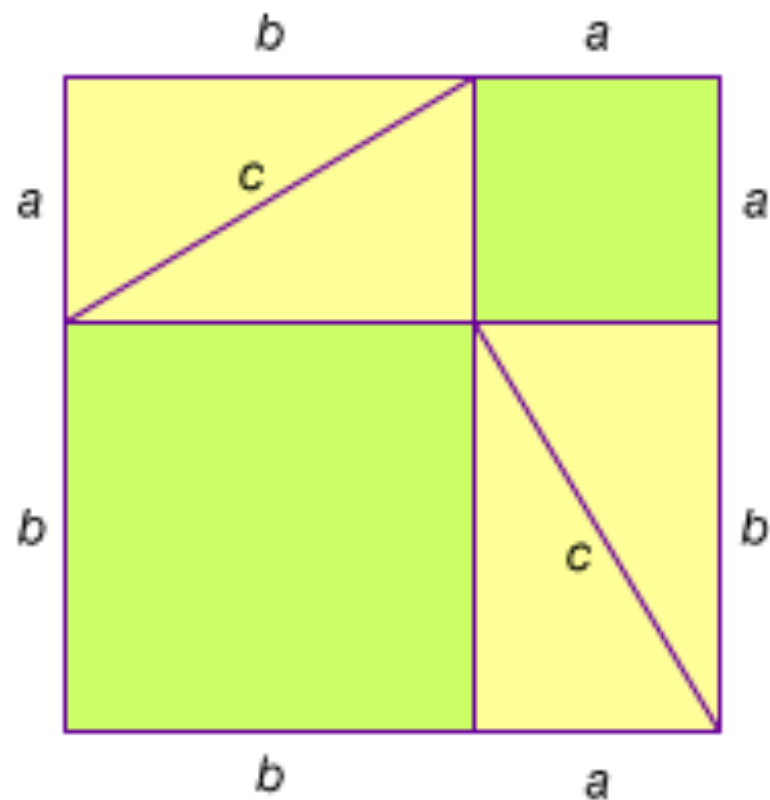
Python Notebooks

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

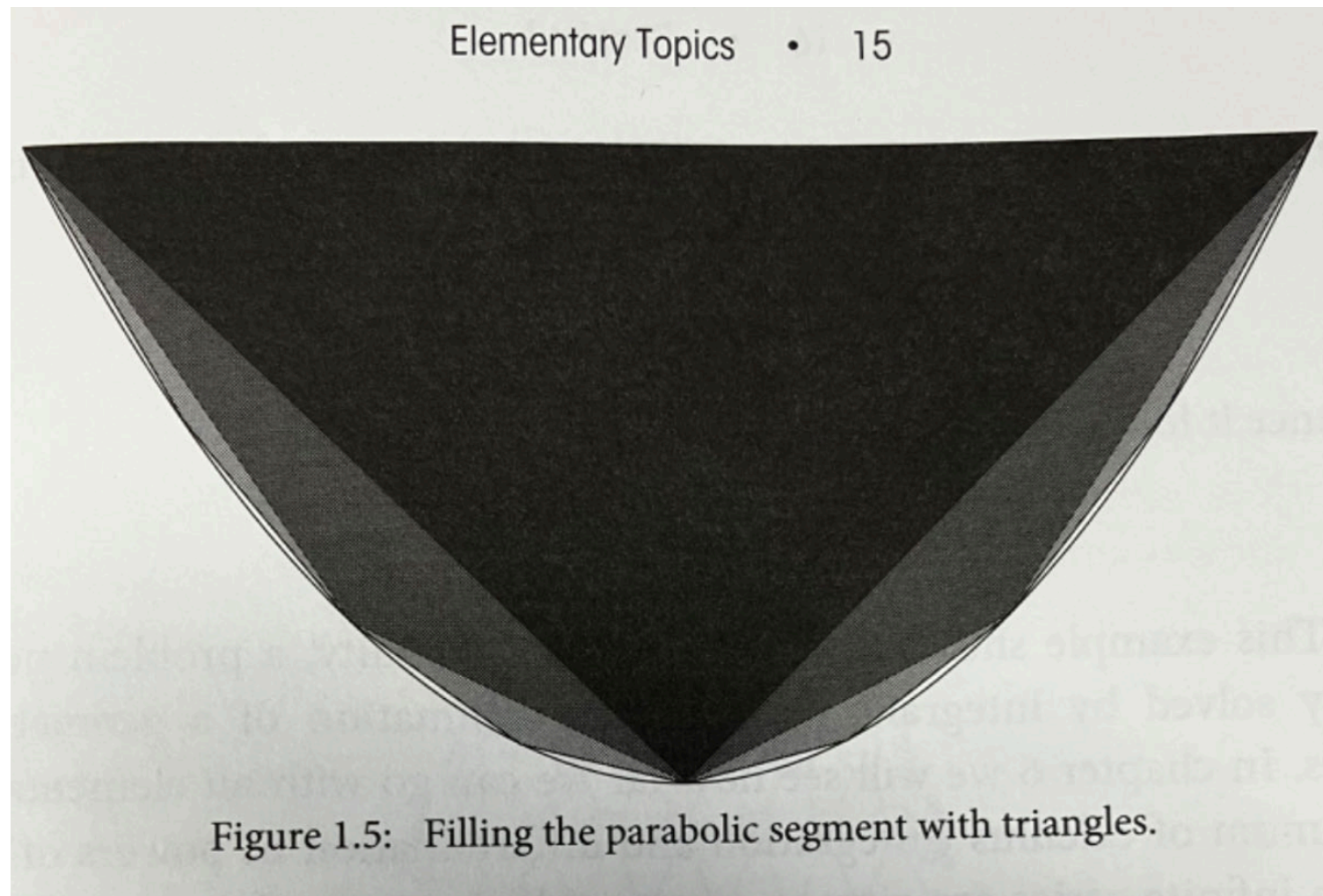




© 2002 Encyclopædia Britannica, Inc.

Proof of Pythagoras's theorem

How Archimedes compute the area under a parabola



Newton

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

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

Power series for the logarithm

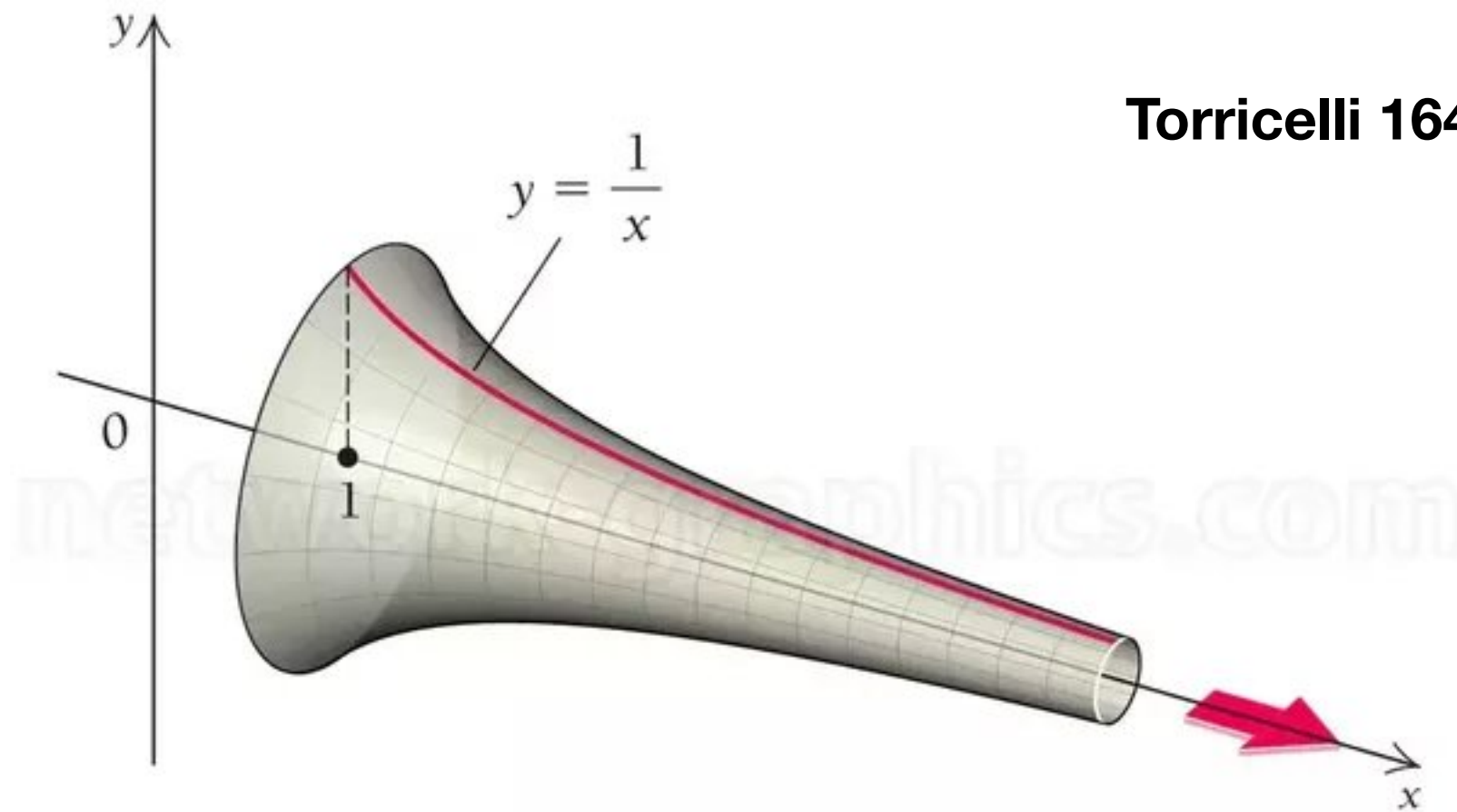
$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \dots$$

Inverse Tangent function and pi

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

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

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



$$\text{volume} = \int_1^{\infty} \pi \left(\frac{1}{x} \right)^2 dx = \pi \left[-\frac{1}{x} \right]_1^{\infty} = \pi$$

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

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 logician, 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



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 Hilbert 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 ...

Ubiquitous AI and Computational Research, **from Quantum Materials to the Origin of Black Holes**

By



Dr Zi Yang MENG



Dr Hugo PFISTER



SHKU
science

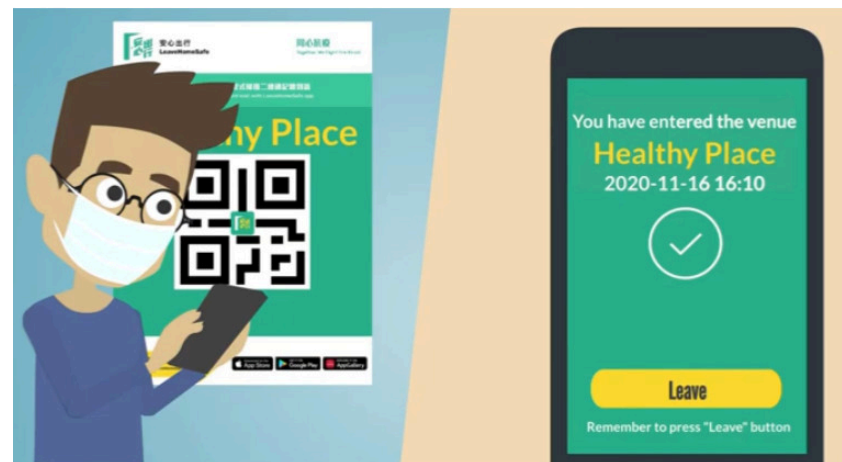


香港科學館
HONG KONG
SCIENCE MUSEUM

Hong Kong Science Museum 01/15/2022

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

Computation is everywhere



QR / Face Recognition



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

In April 2017, AlphaGo vs. Jie Ke



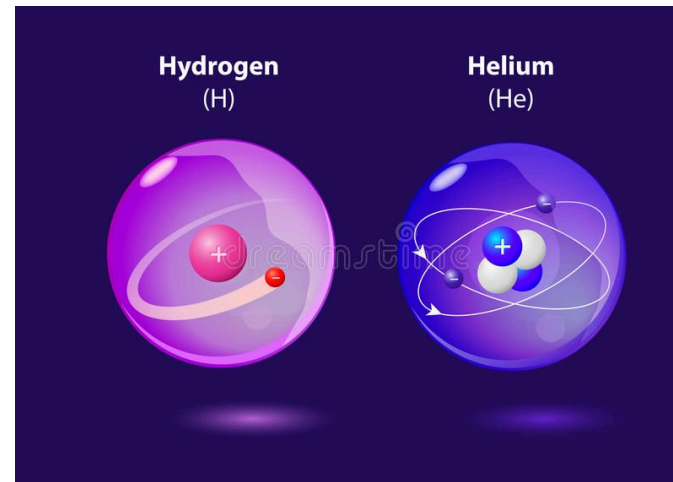
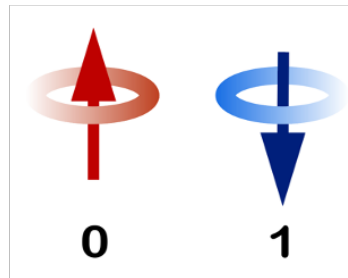
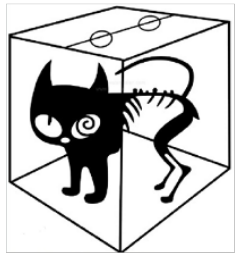
- The machine played perfect...
- I am so behind, unbelievable...
- AlphaGo is not the God, but it is a superior species than human being...

AlphaGo



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



$$2^N$$

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

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

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

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

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



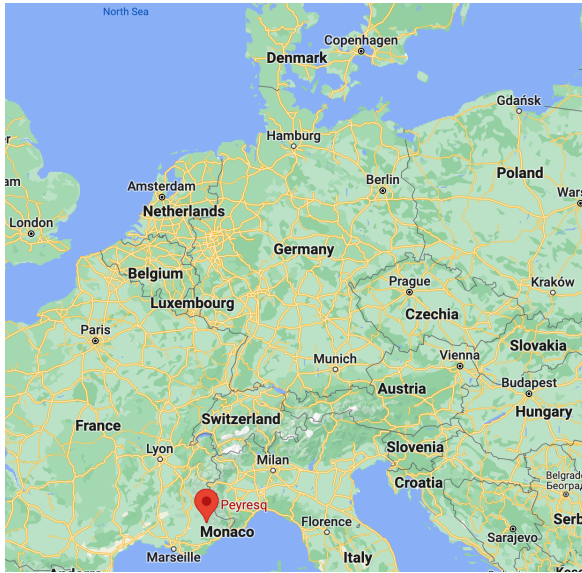
Wheat grains on chessboard — Sissa ibn Dahir, inventor of Chaturanga

$2^{64} - 1 = 18,446,744,073,709,551,615$ 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

Burning of the summer palaces

Convention of Peking

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

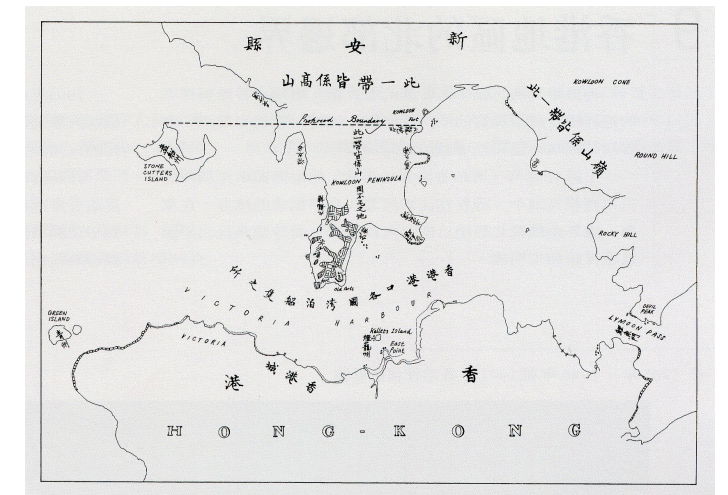
AND

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.



Late Qing Dynasty
1856-1860 2nd Opium war



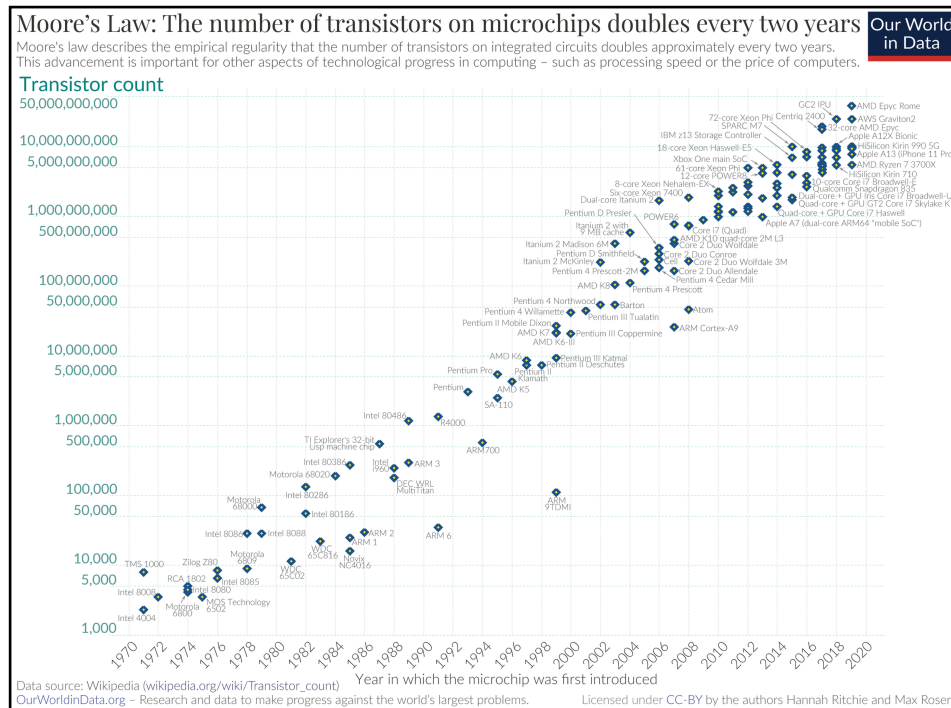
8 million taels of silver apiece

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

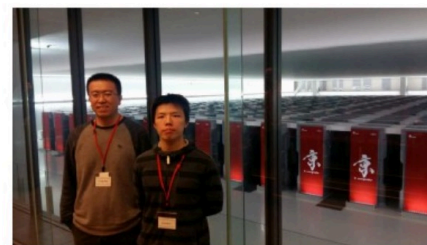
TeraFLOPS: 10^{12}

PetaFLOPS: 10^{15}

ExaFLOPS: 10^{18}



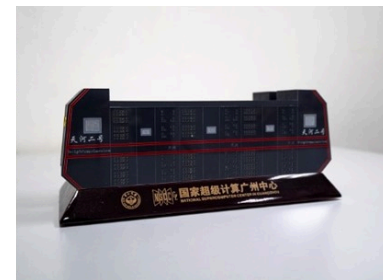
Tianhe-1 (天河1号): 5 PetaFLOPS



K-computer (京): 10 PetaFLOPS



Tianhe-2 (天河2号): 100 PetaFLOPS

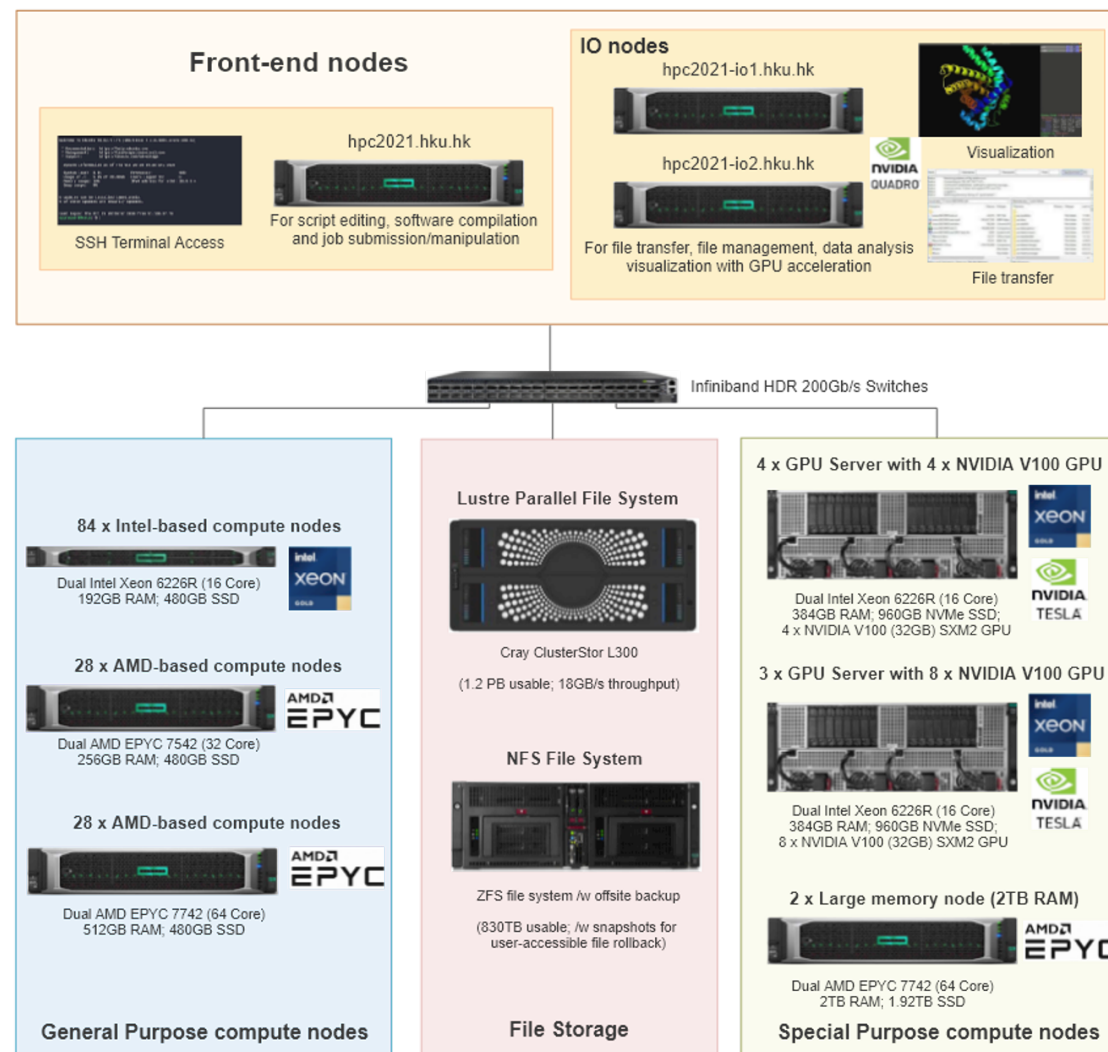


	Supercomputer	Personal Computer	Human Brain
Computational Units	32,000 Xeon CPUs 10 ¹² transistors	4 CPUs, 10 ⁹ transistors	10 ¹¹ neurons
Cycle time	10 ⁻⁹ sec	10 ⁻⁹ sec	10 ⁻³ sec
Operations/sec	10 ¹⁵	10 ¹⁰	10 ¹⁷
Memory updates/sec	10 ¹⁴	10 ¹⁰	10 ¹⁴
Weight / Space	150 tons / Basketball court	1 Kg / A4 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)

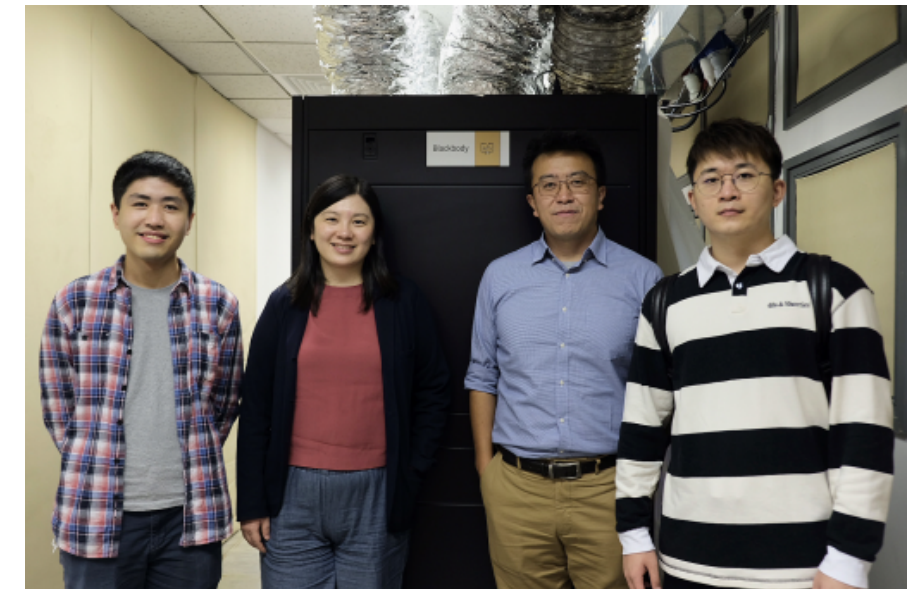
Intel(R) Xeon(R) Platinum 9242 (48 cores) 2 x 4 = 384 cores (computation node)

3056 CPU cores

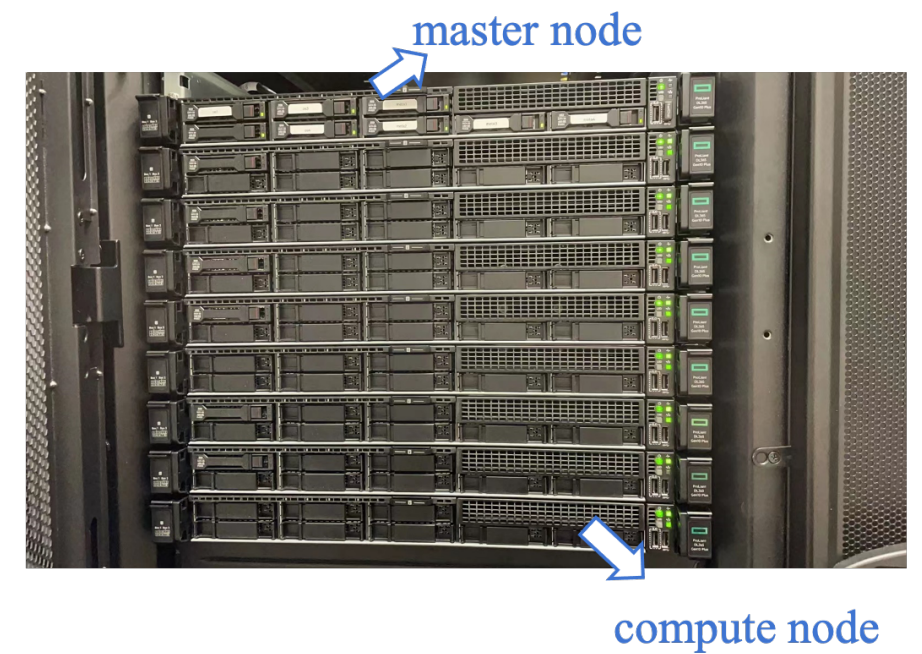
Our own Blackbody

1024 cpu cores

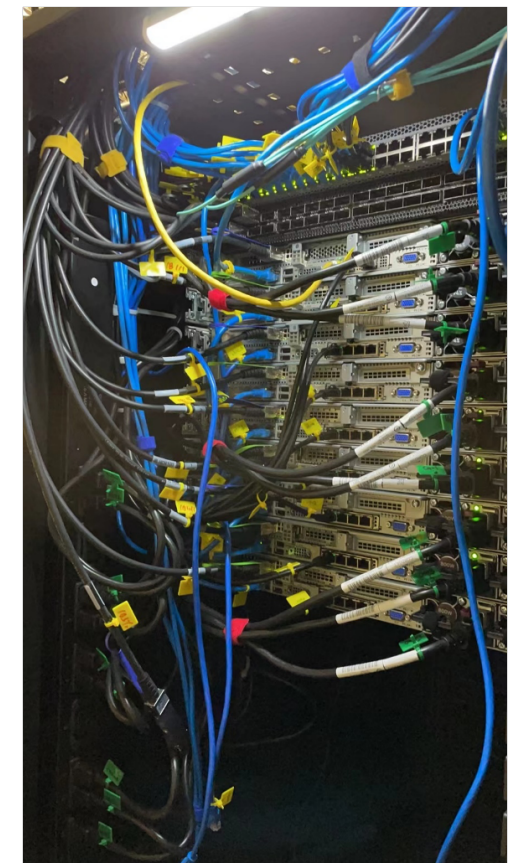
2022/09



Our Blackbody Cluster in Room 311 of CYM Building



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 $0.55 \text{ kW} \times 8$, head node, storage)

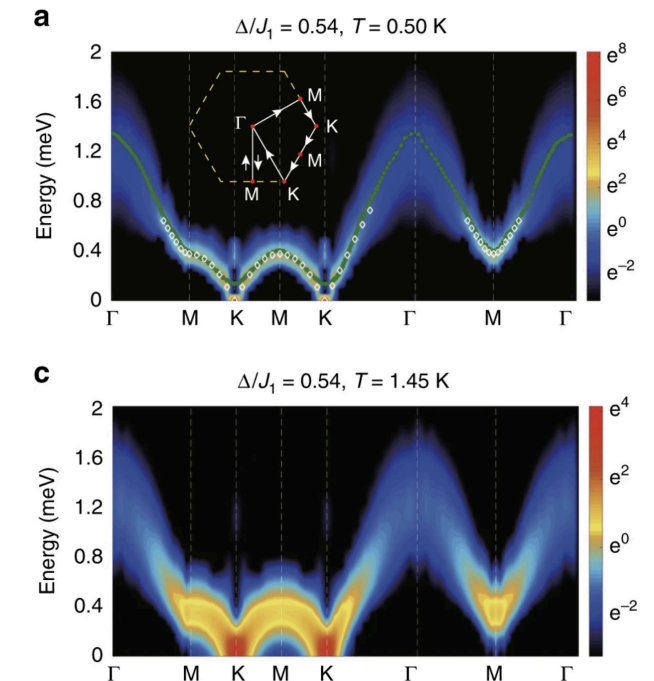
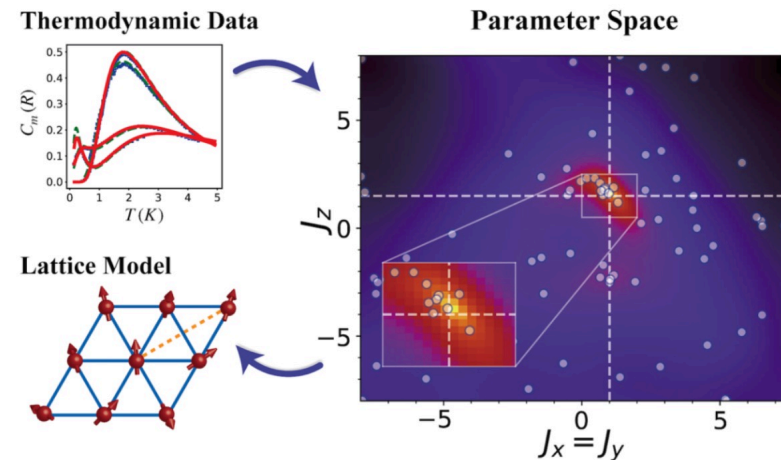
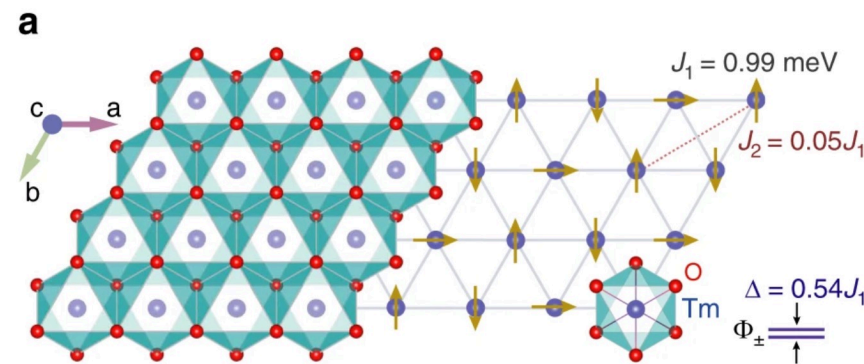
cooling ~ 8 kW (each ~ 2.4 kW)

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 (Magnesium) Ga (Gallium) O₄ (tetroxide) — TMGO

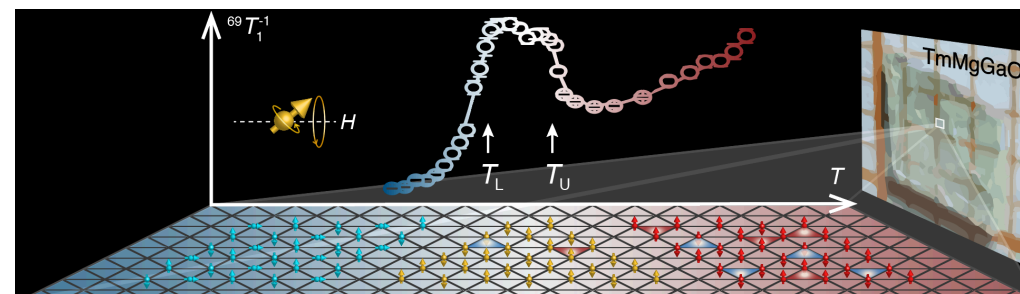
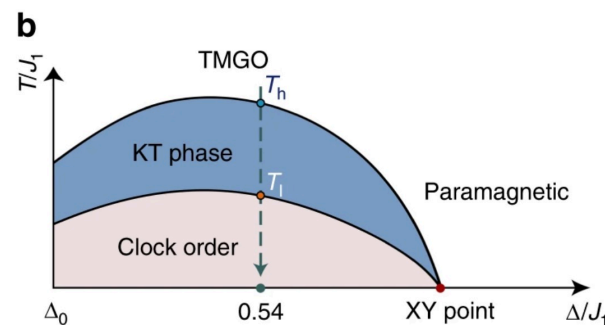


[Nature Communications 11, 1111 \(2020\)](#)

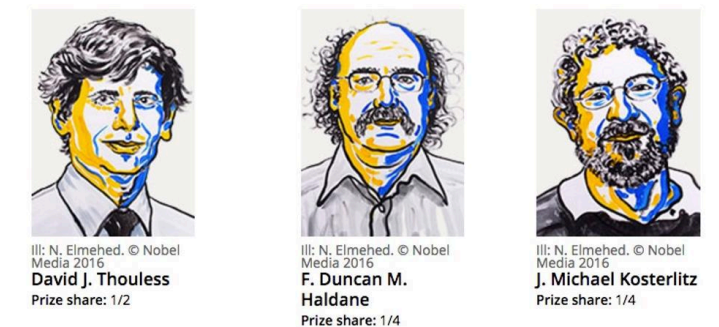
auto-gradient, Bayesian optimization

Confirming simulated calculations, quantum material research reveals topological KT phase

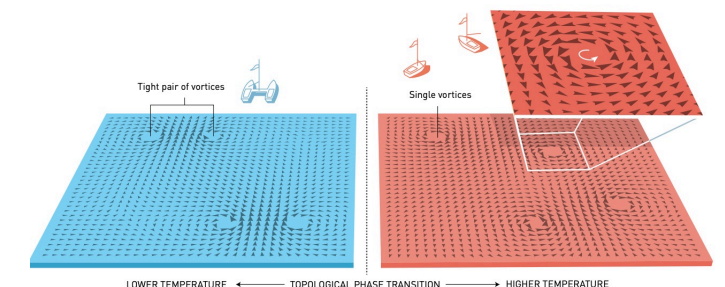
Nuclear magnetic resonance — MRI / CT scans



The Nobel Prize in Physics 2016



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



Computation in Quantum Physics



electric power transmission at high voltage

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



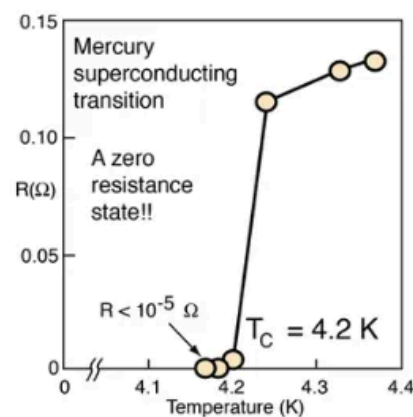
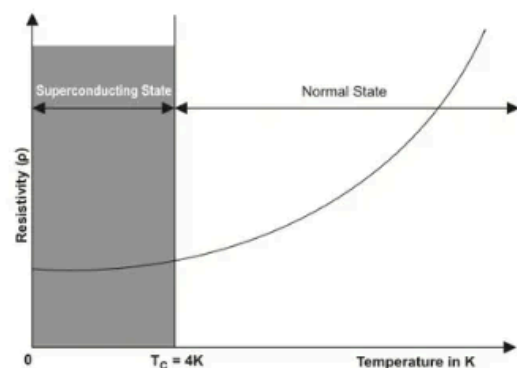
High speed rail



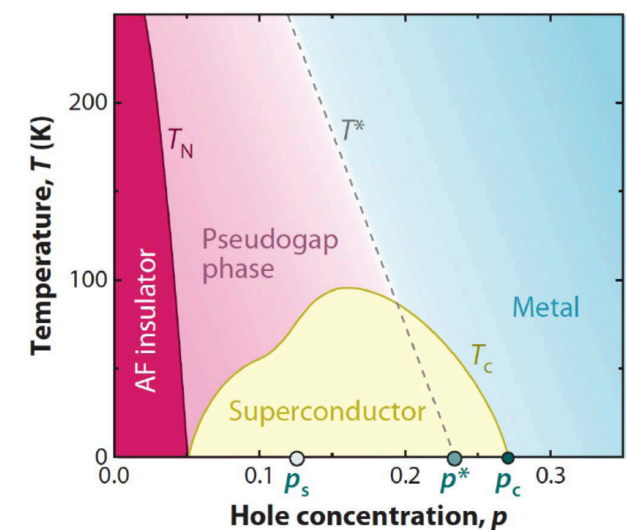
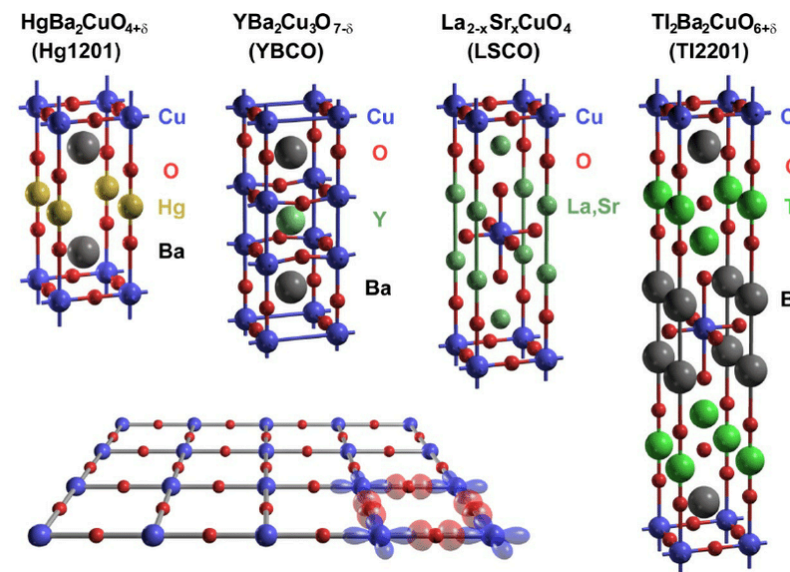
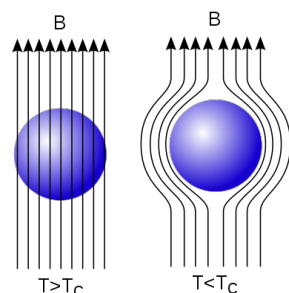
superconductors at $\sim -270^{\circ}\text{C}$

High-temperature superconductors at $\sim -100^{\circ}\text{C}$

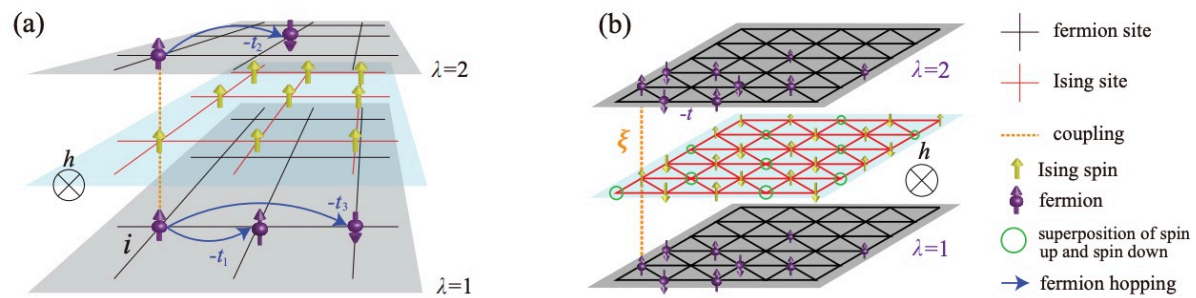
What is Superconductivity?



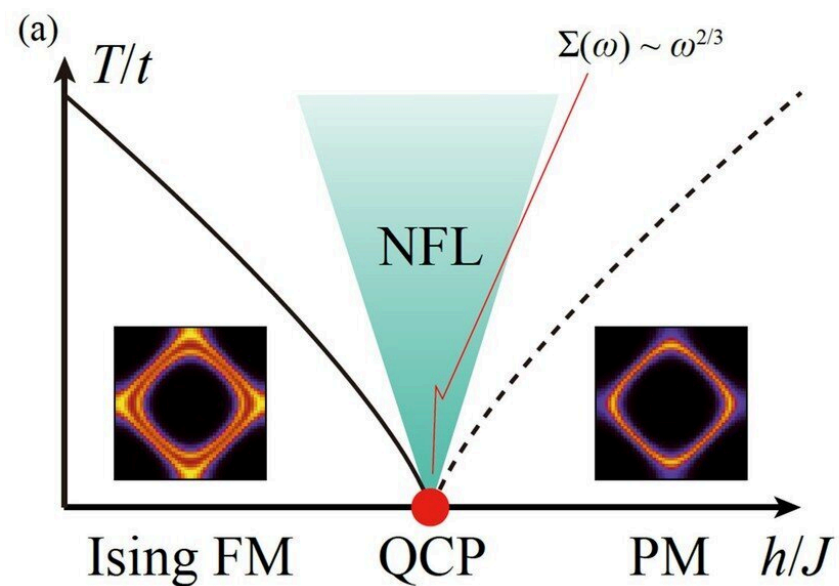
Dutch Physicist
Heike Kamerlingh Onnes in 1911



Understanding quantum critical Metals

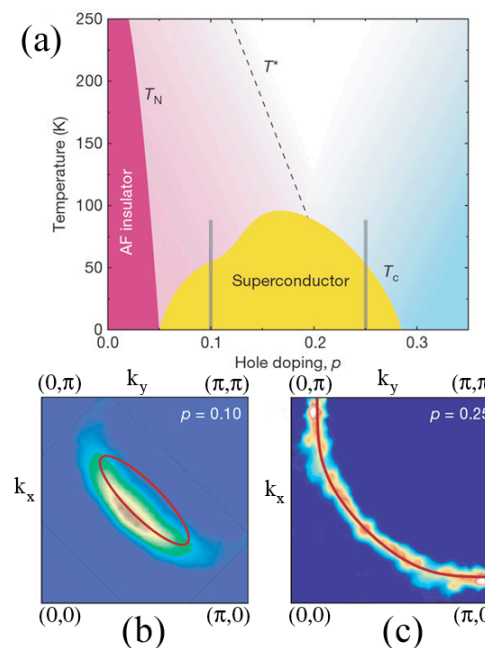


[PNAS 20, 116 \(34\) 16760-16767 \(2019\)](#)

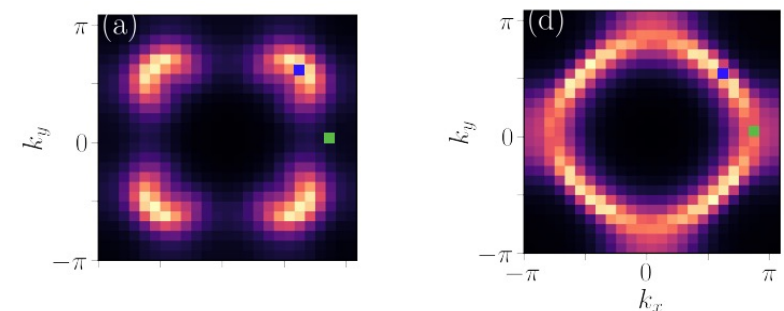


[npj Quantum Materials 5, 65 \(2020\)](#)

metals' awkward cousin is found

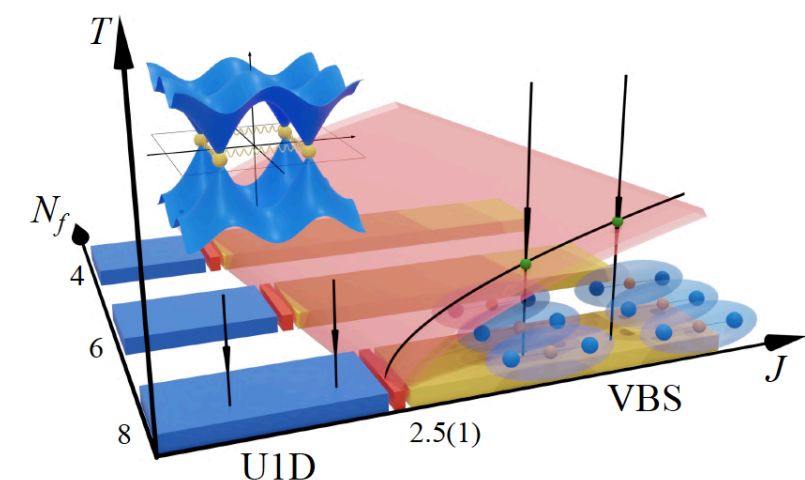
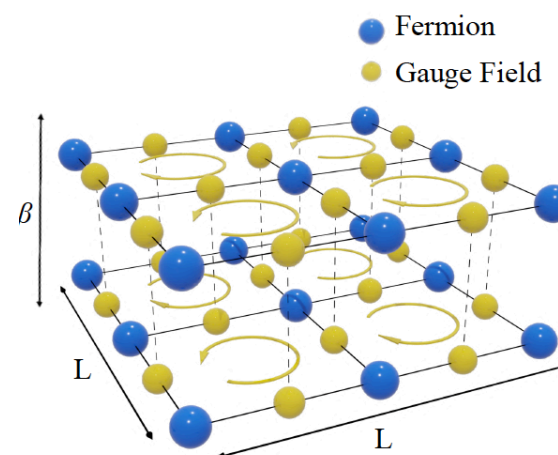


[Chin. Phys. Lett. 37 047103 \(2020\) Express Letters](#)



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

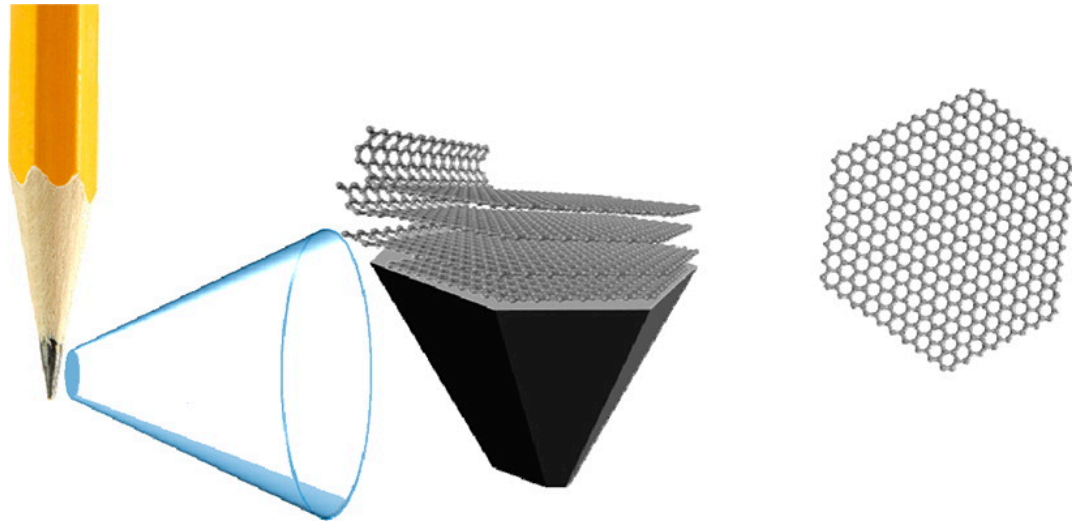
Parent State of quantum phases



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

Computation in graphene face masks

From graphite to graphene



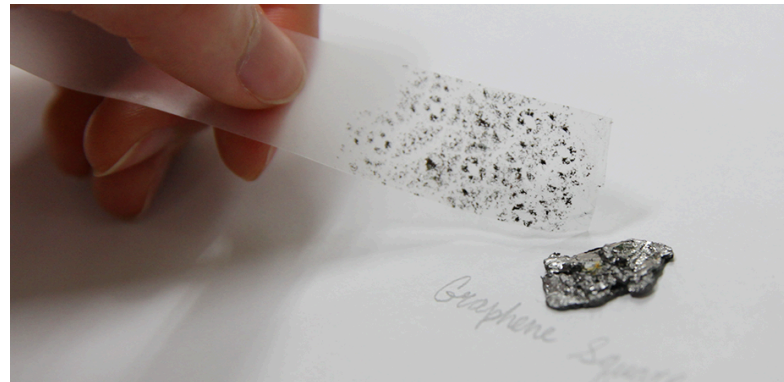
The Nobel Prize in Physics 2010



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



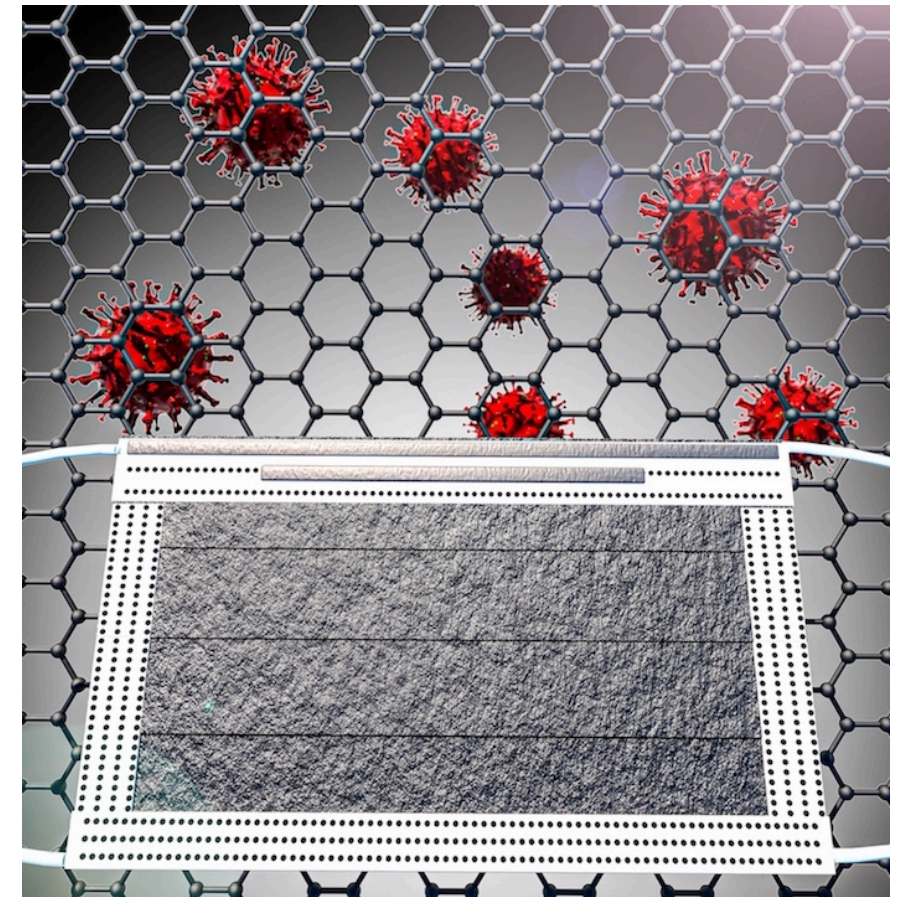
© The Nobel Foundation. Photo: U. Montan
Konstantin Novoselov
Prize share: 1/2



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.

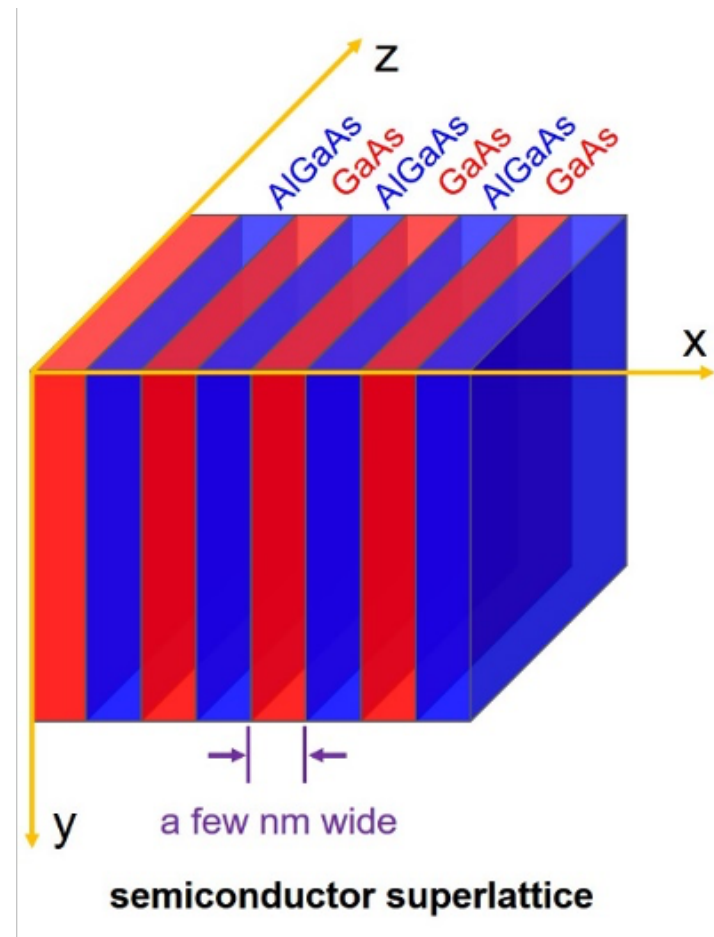


Graphene joins the fight against COVID-19



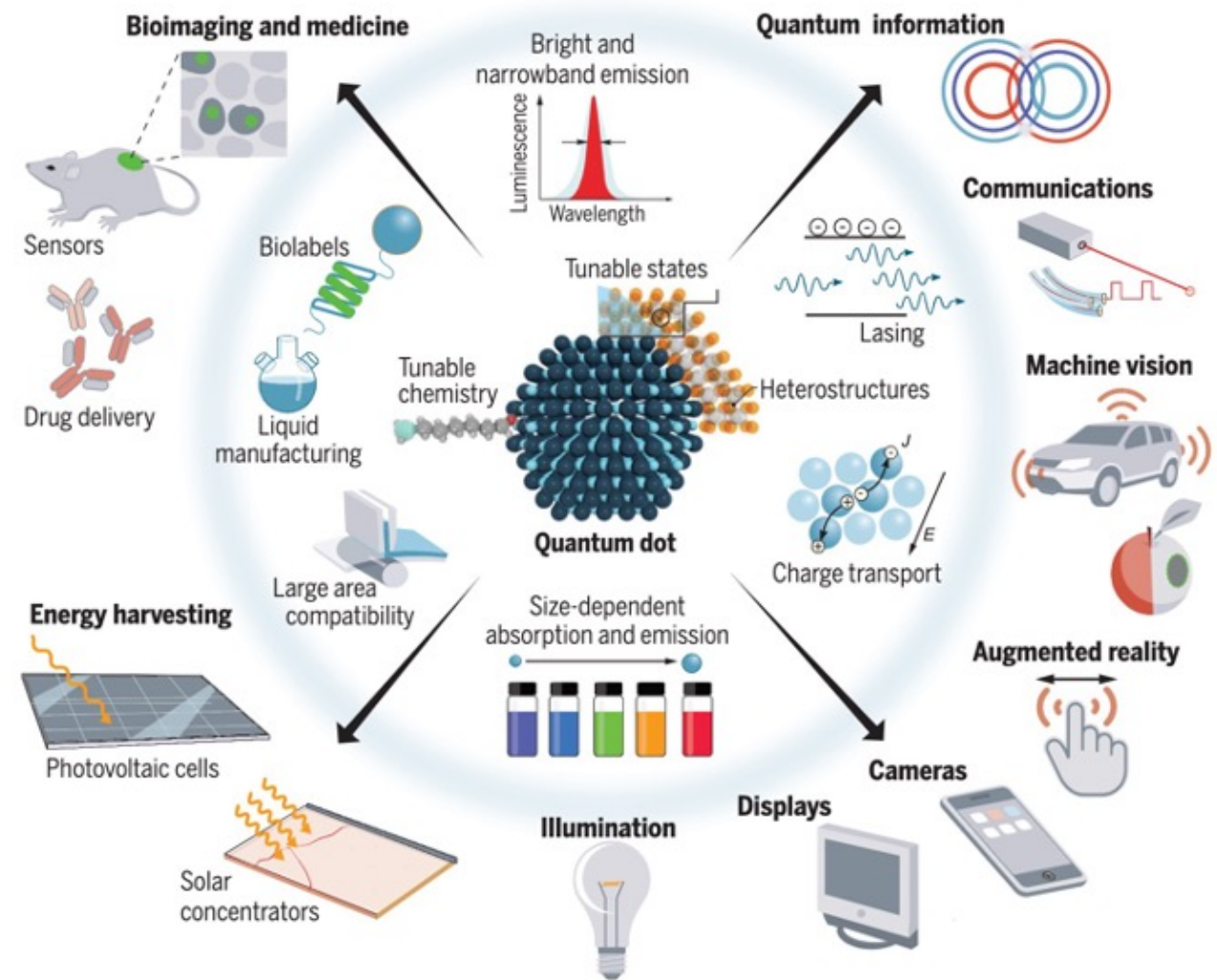
Superlattices are widely used as electric and optical devices

In semiconductor industry



Wikipedia

In semiconductor quantum dots / wires technologies

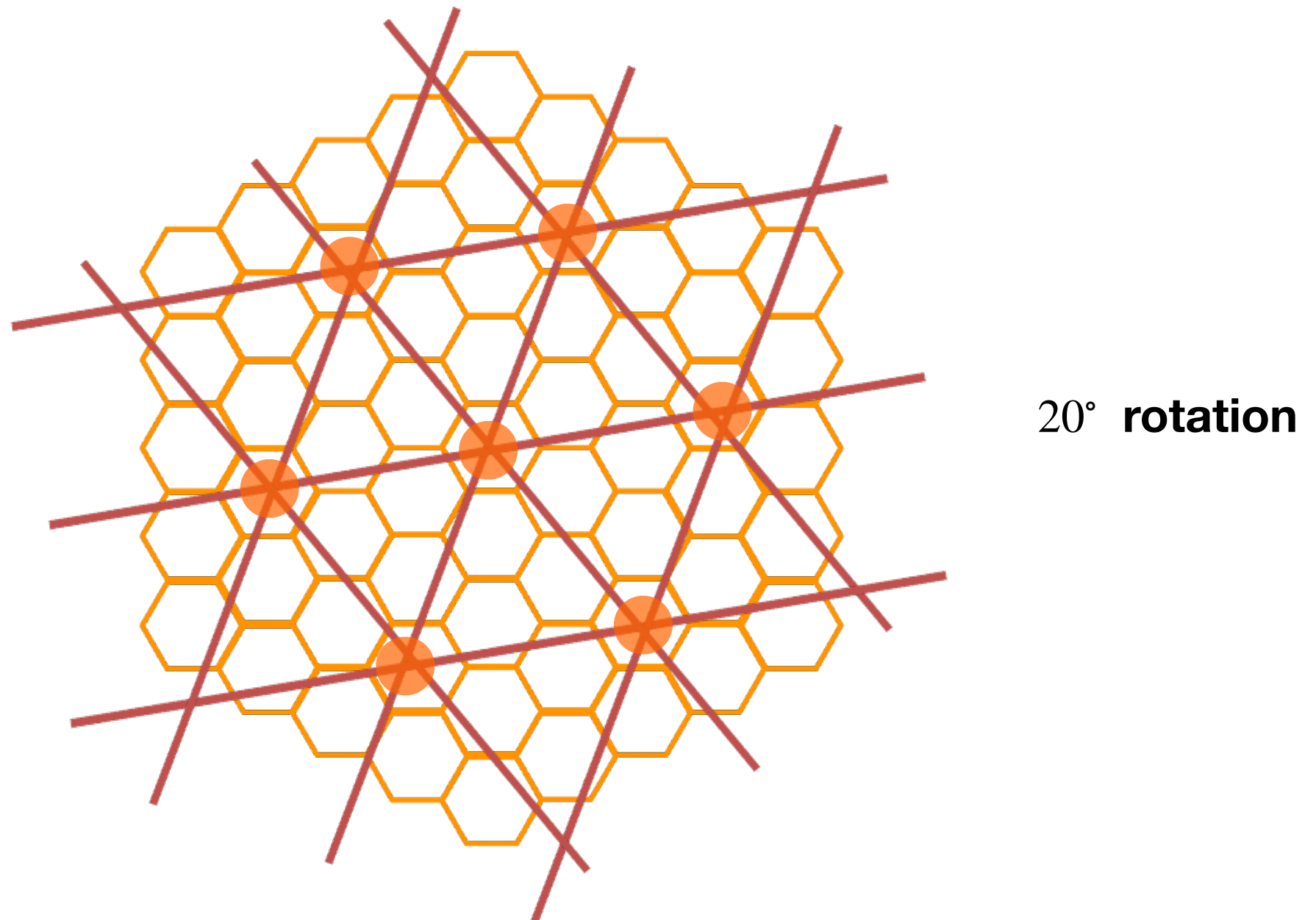


Garcia de Arquer et al., Science (2021)

- 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

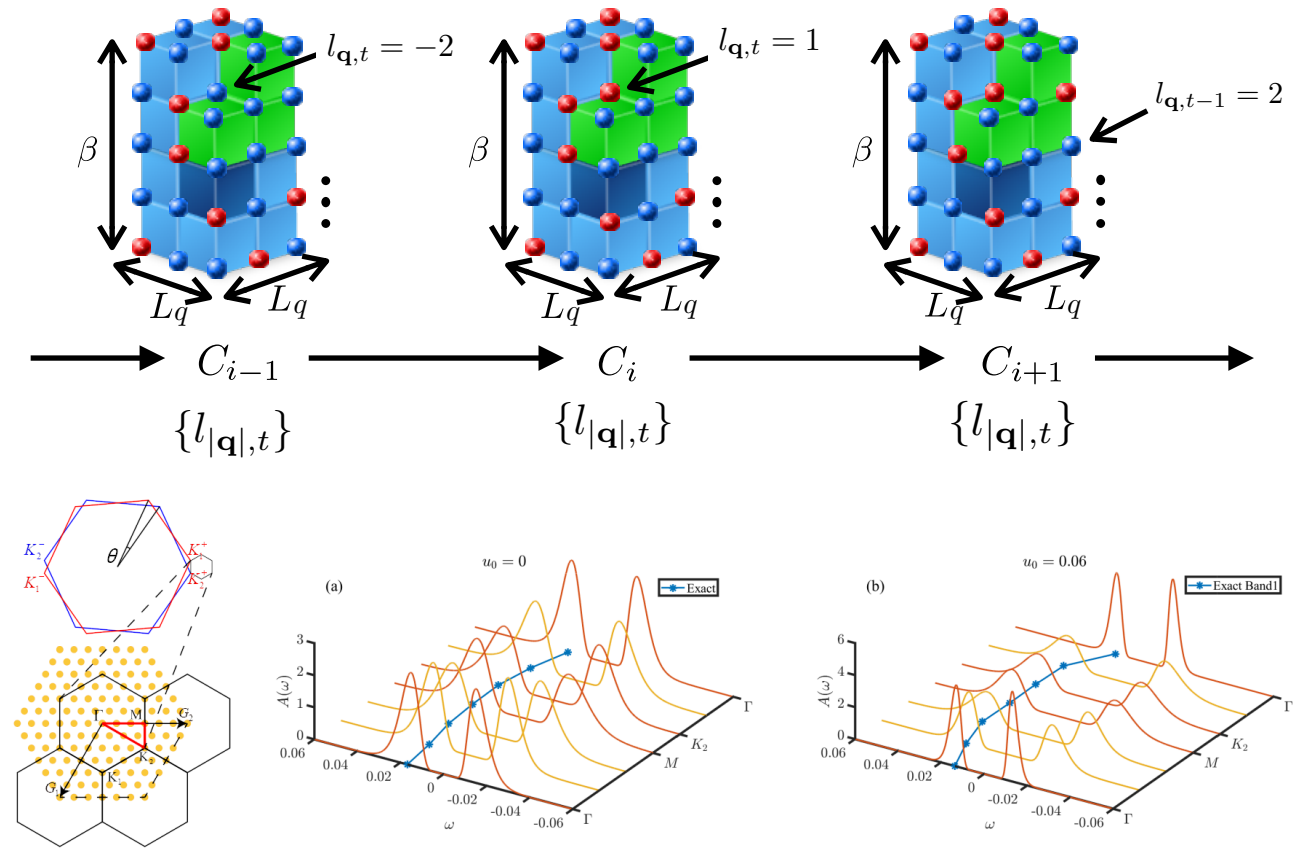
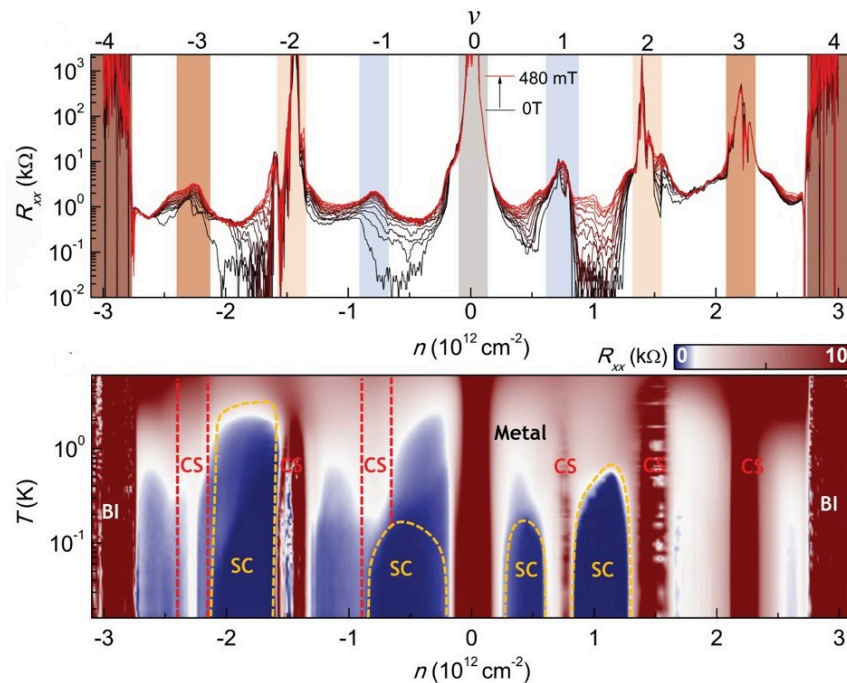
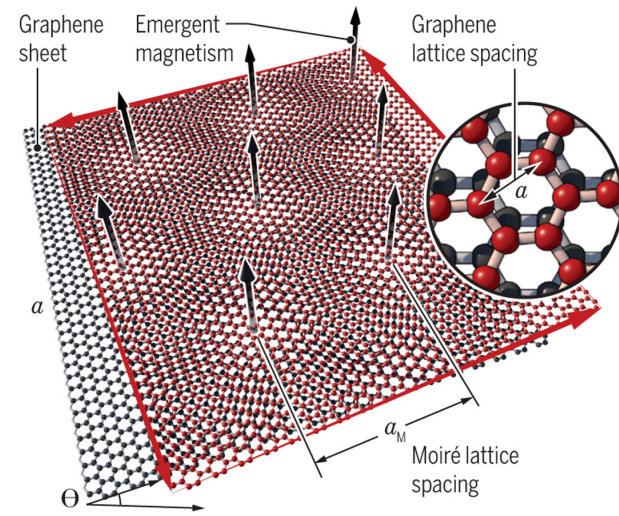


Computation in graphene face masks

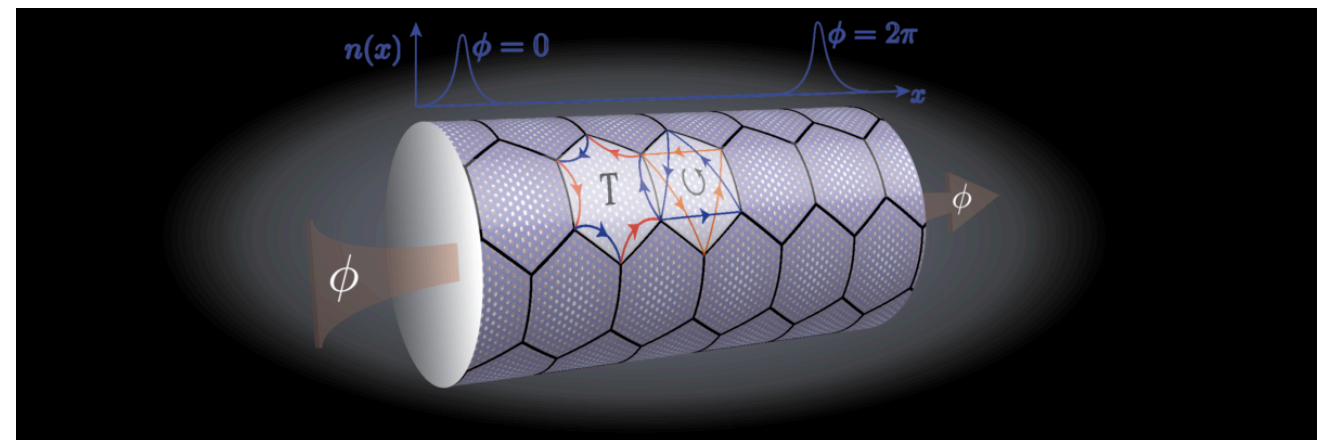
🌀 The Samadhi of magic angle twisted bilayer graphene (转角石墨烯的三昧)

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



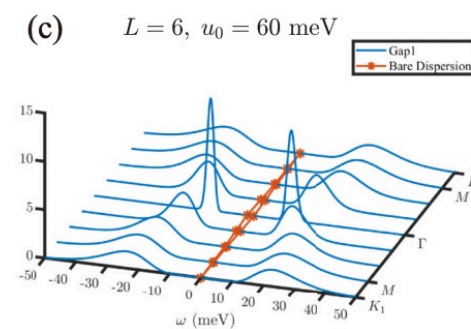
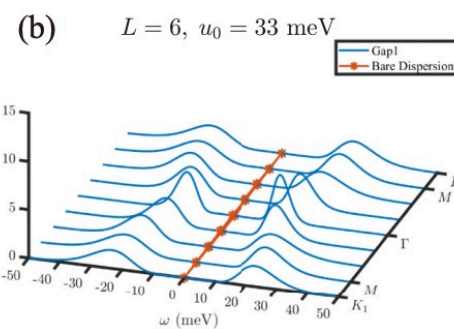
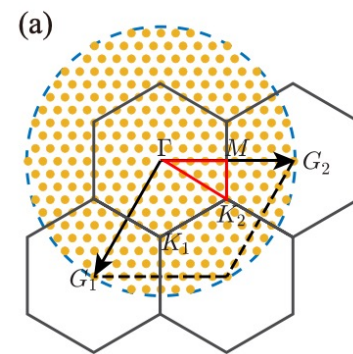
$$H = H_0 + H_{int}$$

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

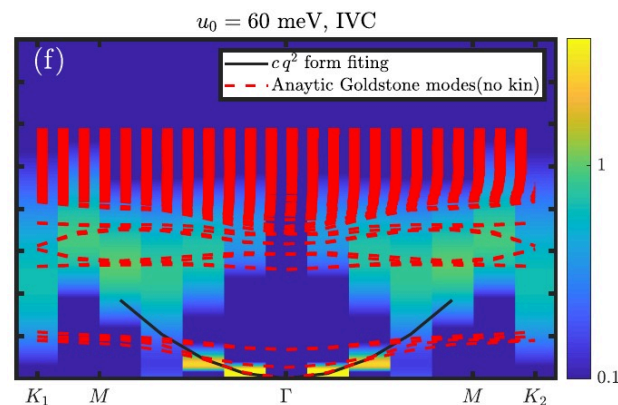
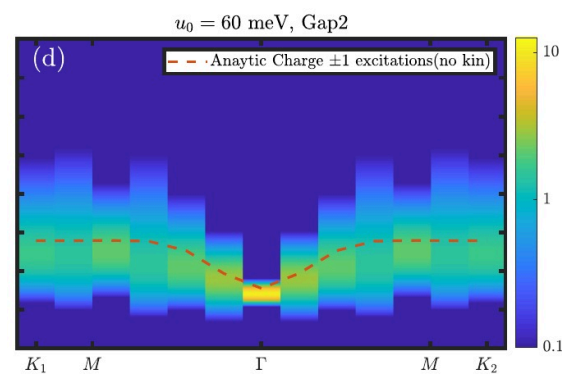
$$H_0 = \sum_m \sum_{\mathbf{k}, \tau, s} \epsilon(\mathbf{k}) d_{\mathbf{k}, m, \tau, s}^\dagger d_{\mathbf{k}, m, \tau, s}$$

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

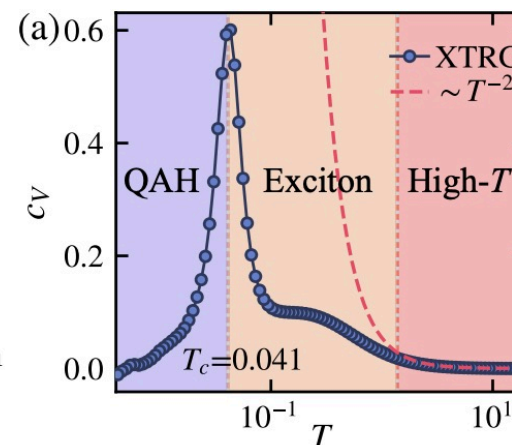
$$\delta \rho_{\mathbf{q} + \mathbf{G}} \sim \sum_{\mathbf{k} \in mBZ, m_1, m_2, \tau, s} \lambda_{m_1, m_2, \tau}(\mathbf{k}, \mathbf{k} + \mathbf{q} + \mathbf{G}) d_{\mathbf{k}, m_1, \tau, s}^\dagger d_{\mathbf{k} + \mathbf{q}, m_2, \tau, s}$$



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.

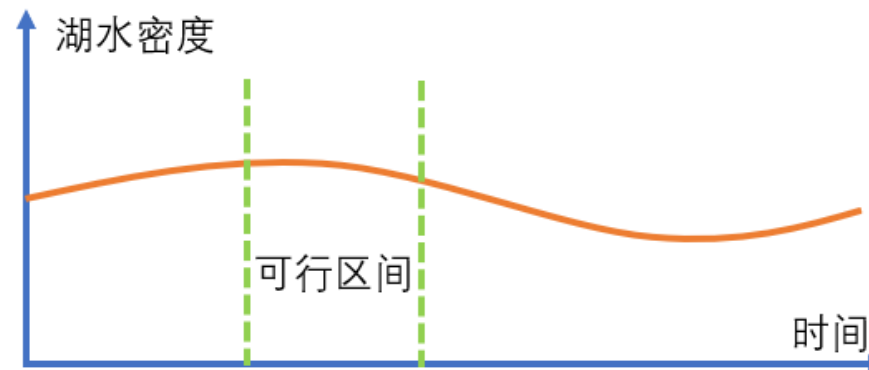
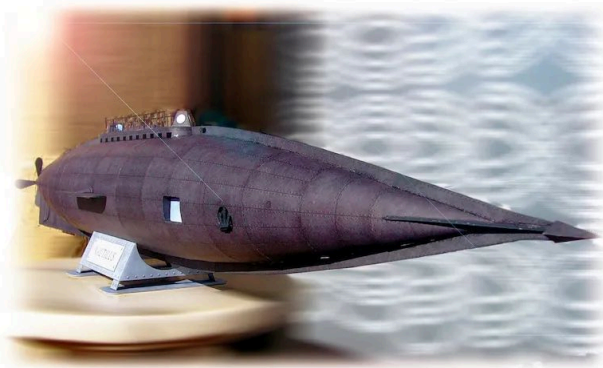
Bin Bin Chen & Zi Yang Meng
The University of Hong Kong



Xu Zhang

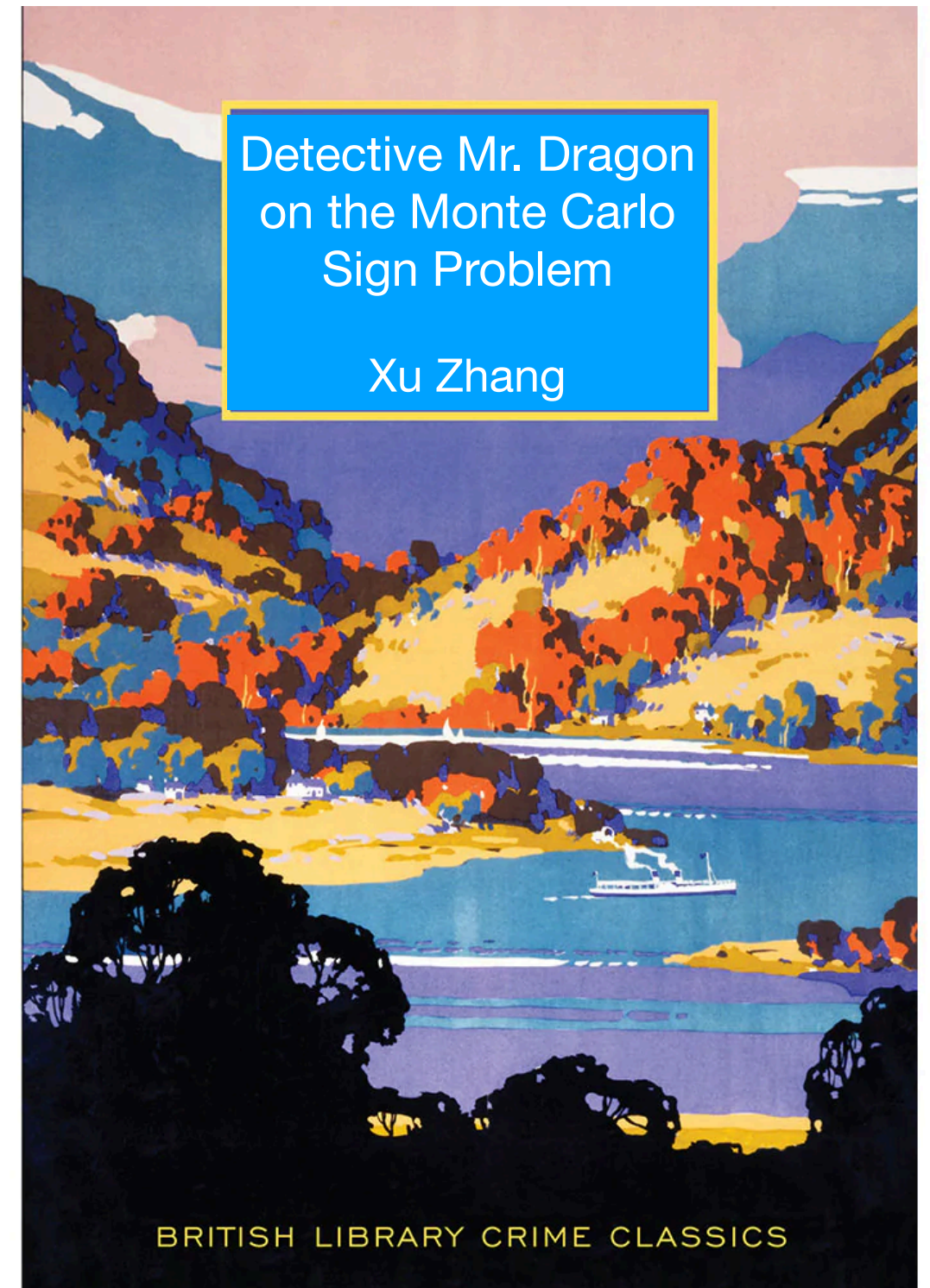


Caption Nemo and submarine Nautilus



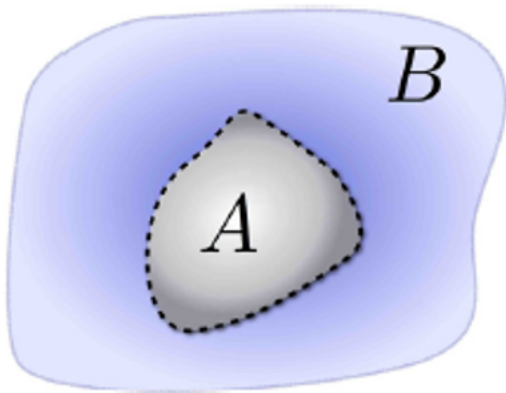
$$\langle \rho \rangle_{V_i} = \frac{\sum_i V_i \rho_i}{\sum_i V_i} = \frac{\frac{\sum_i |V_i| (\pm \rho_i)}{\sum_i |V_i|}}{\frac{\sum_i |V_i| (\pm 1)}{\sum_i |V_i|}} = \frac{\langle \pm \rho_i \rangle_{|V_i|}}{\langle \pm 1 \rangle_{|V_i|}}$$

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

J. Stat. Mech. (2004) P06002



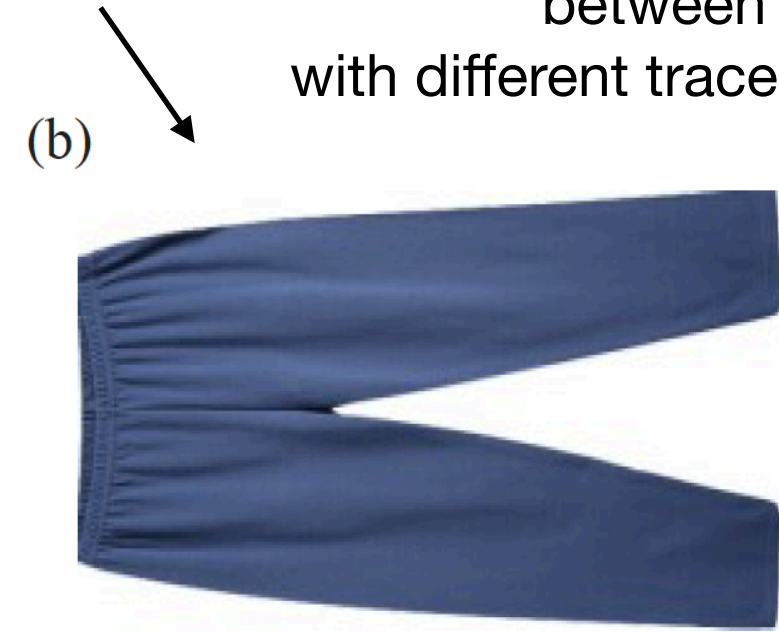
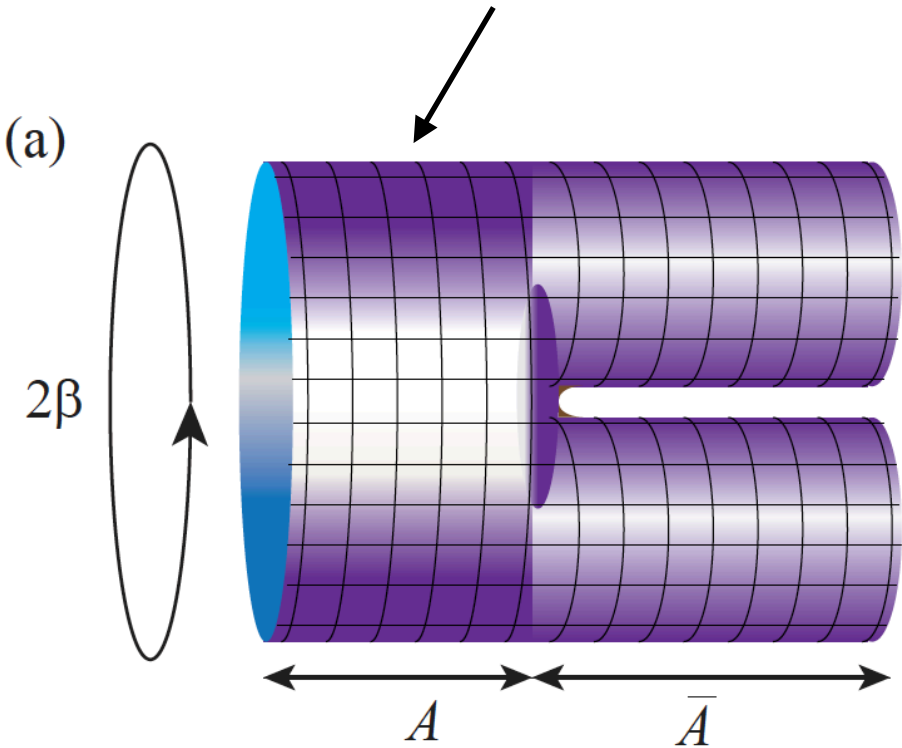
$$\rho = |\Psi\rangle\langle\Psi|$$

$$\rho_A = \text{Tr}_B \rho$$

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

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

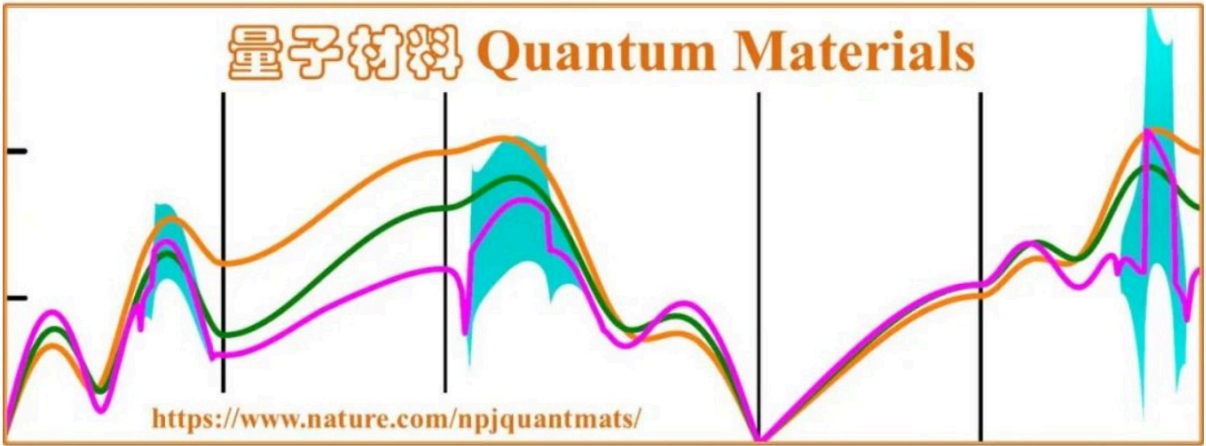
“ Qiu Ku is the $Z_A^{(2)}$ ”



(b)



Jiarui Zhao



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

$$S_A^{(2)} = -\ln(\text{Tr}_A(\rho_A^{(2)})) = -\ln\left(\frac{Z_A^{(2)}}{Z_\emptyset^{(2)}}\right) = \beta(F(Z_A^{(2)}) - F(Z_\emptyset^{(2)}))$$

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

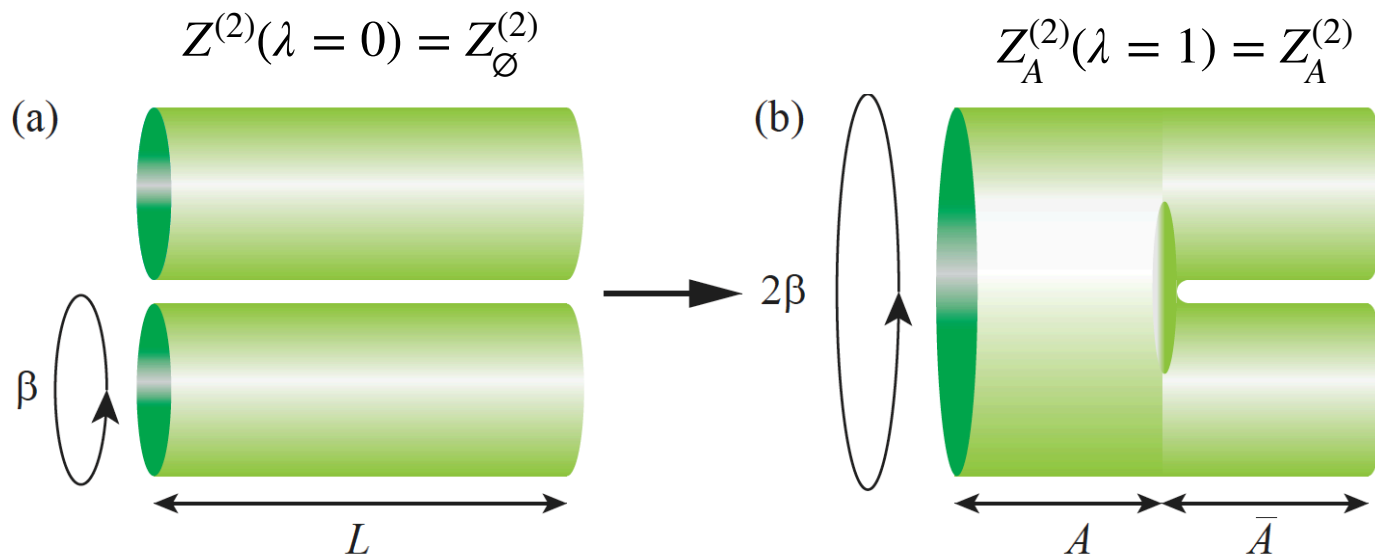
Incremental (Qiu Ku) method

📌 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)

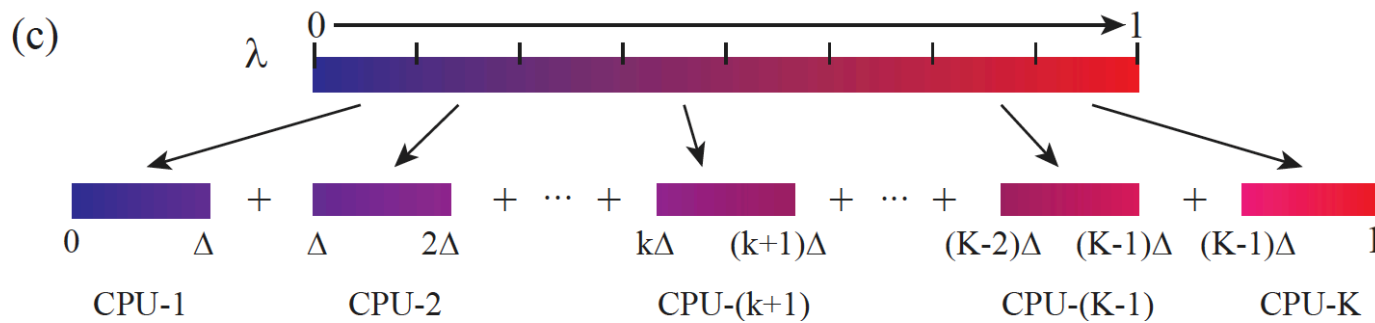
📌 Gaopei Pan, Yuan Da Liao, Weilun Jiang, Jonathan D'Emidio, **ZYM**, PRB 108, L081123 (2023)

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



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

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



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

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

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

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

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

Computation in Physics



Tycho Brahe

Measure positions of planets for 20 years (big data)



Johannes Kepler

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



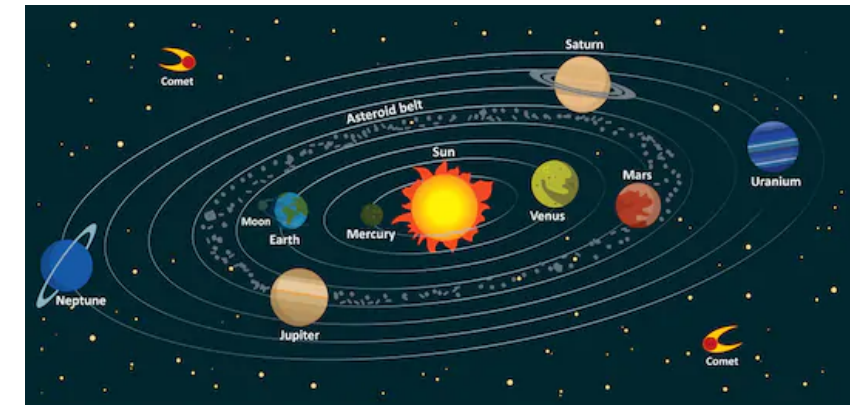
Issac Newton

Gravitation is the reason

$$F = GM_1M_2/r^2$$

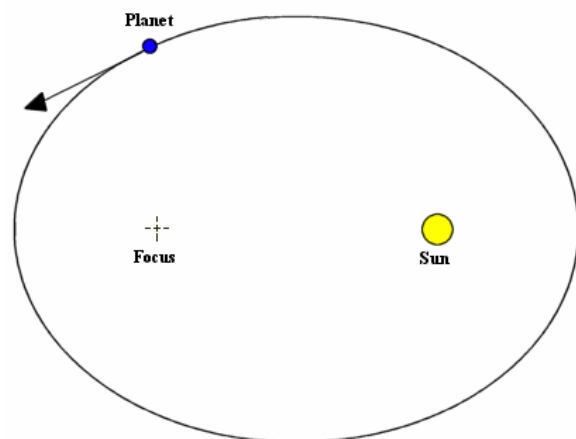
$$\dot{\vec{v}}(t) = \vec{a}(\vec{x}(t), \vec{v}(t), t)$$

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

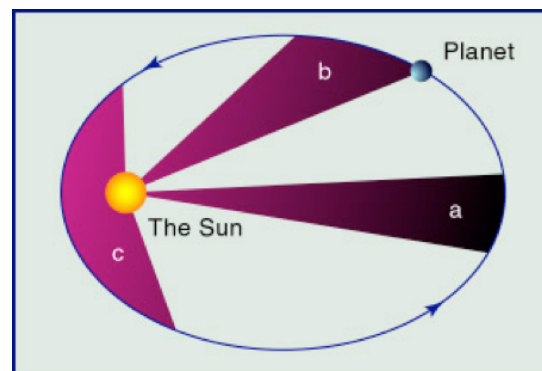


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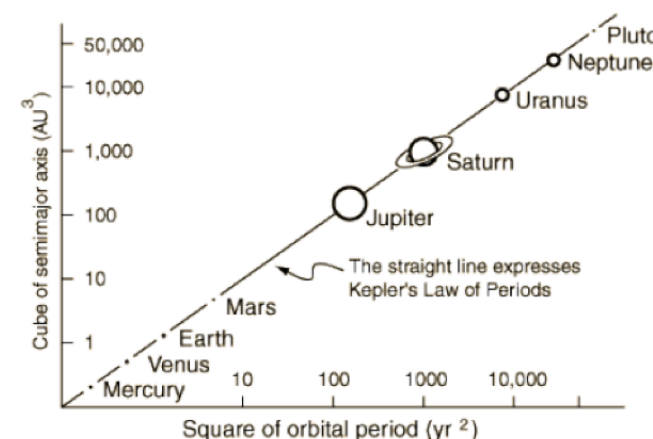
First law, ellipses



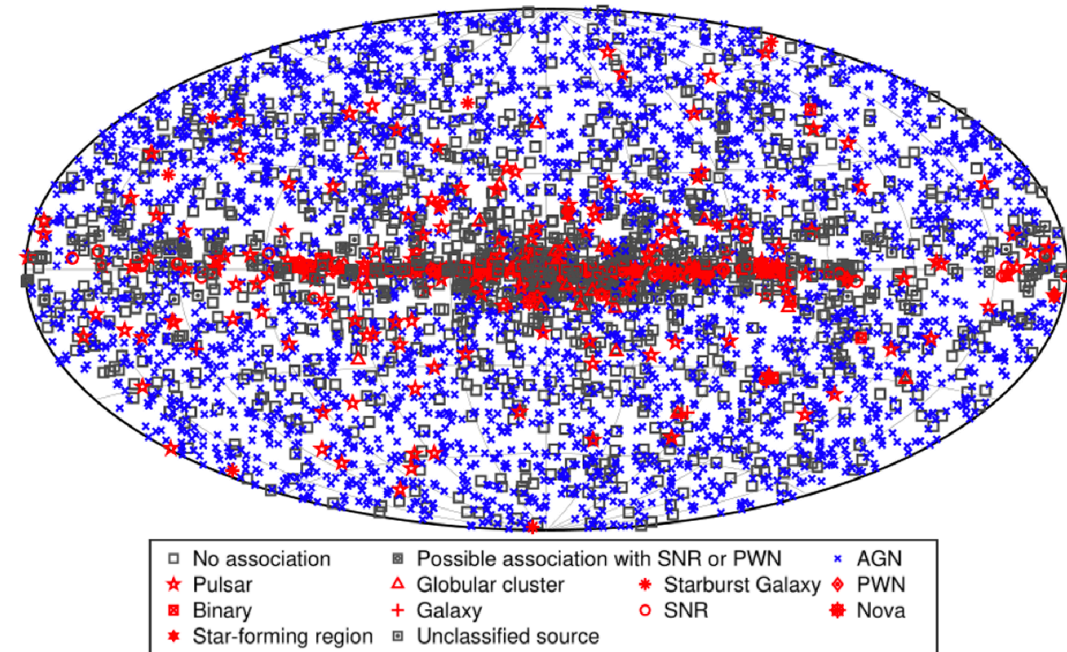
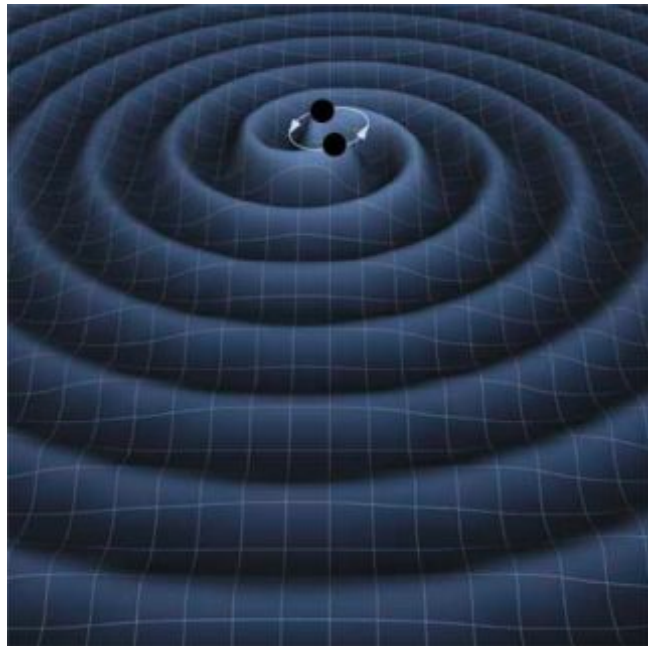
Second law, equal areas in equal time



Third law, $T^2 \sim D^3$



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

