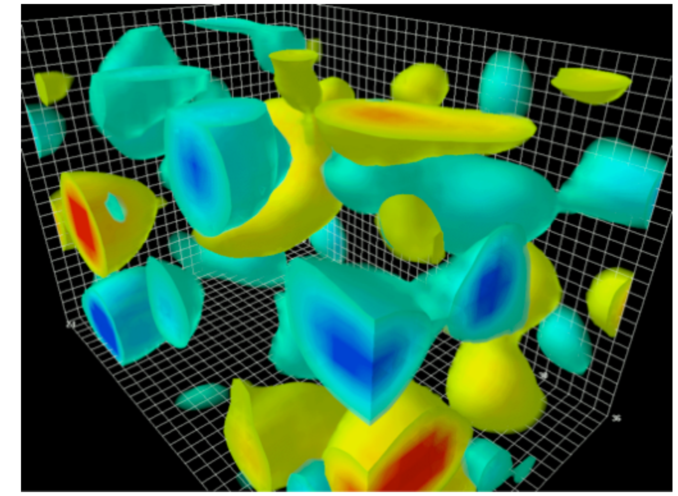
NuclearScience Computing CenteratCCNU

Introduction to hot and dense Lattice QCD



Heng-Tong Ding (丁亨通)
Central China Normal University, Wuhan

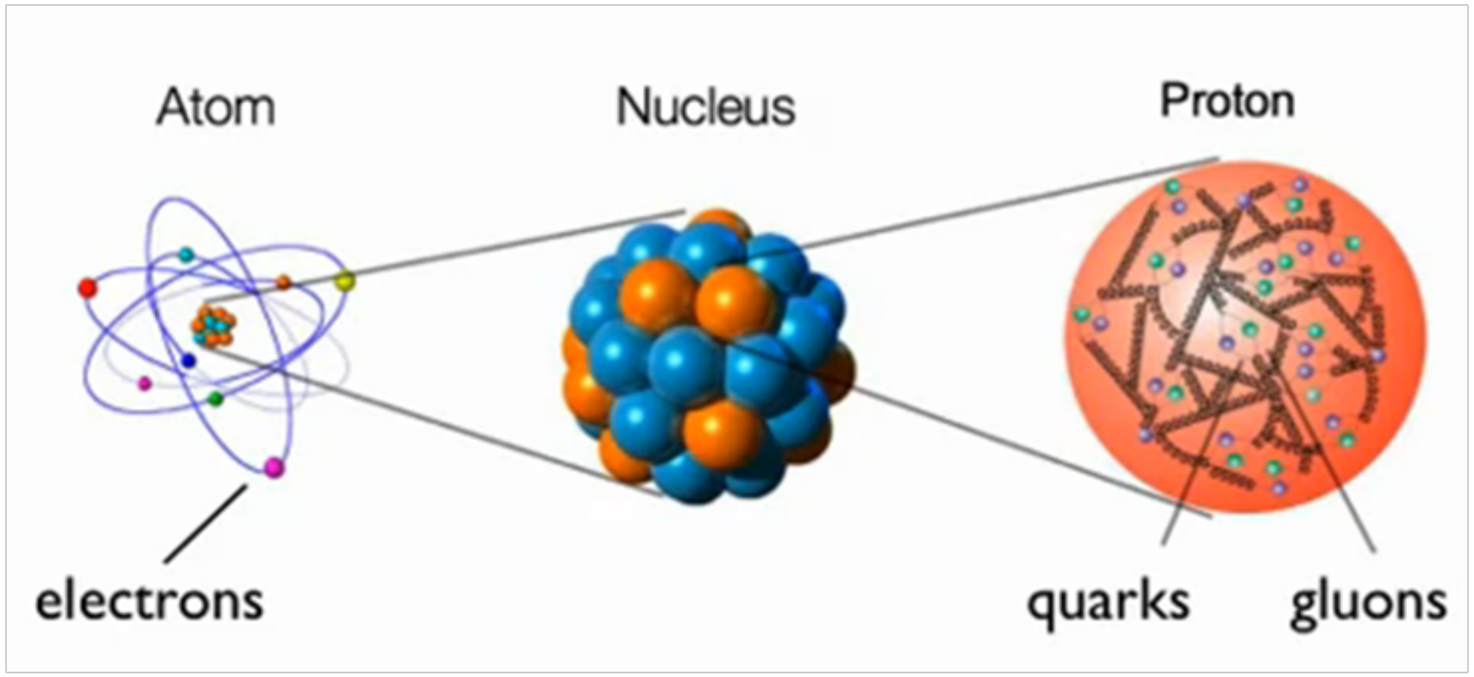
Email: hengtong.ding AT ccnu.edu.cn

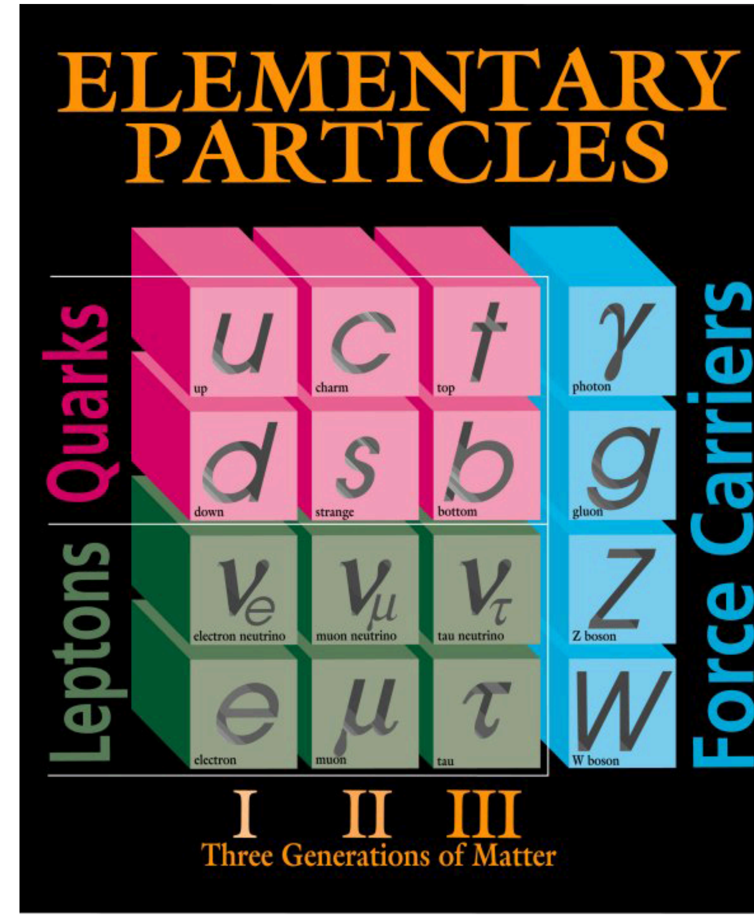
“量子计算与高能核物理交叉前沿讲习班”
华南师范大学,14-25 Nov. 2022

课程目标

- 介绍格点QCD基础，了解其非微扰定义
    - ✤ “Quantum Chromodynamics on the Lattice”, C. Gattringer & C. B. Lang, Springer 2010
    - ✤ “Lattice QCD for Novices”, G. Peter Lepage, arXiv:hep-lat/0506036
    - ✤ 格点量子色动力学导论，刘川，北京大学出版社, 2017
- 看懂有限温度密度格点QCD相关文献： famous plots
    - ✤ “Thermodynamics of strong-interaction matter from Lattice QCD”, 丁亨通, F. Karsch, S. Mukherjee, arXiv:1504.05274
    - ✤ Conference proceedings in the annual “lattice conference”
        - Lattice 2018, Michigan, USA
        - Lattice 2019, CCNU, Wuhan, China
        - Lattice 2021, MIT, USA
        - Lattice 2022, Bonn, Germany
        - …

夸克、胶子和强相互作用





mass of proton ~ 938 MeV

mass of u(d) quarks ~ 3 MeV

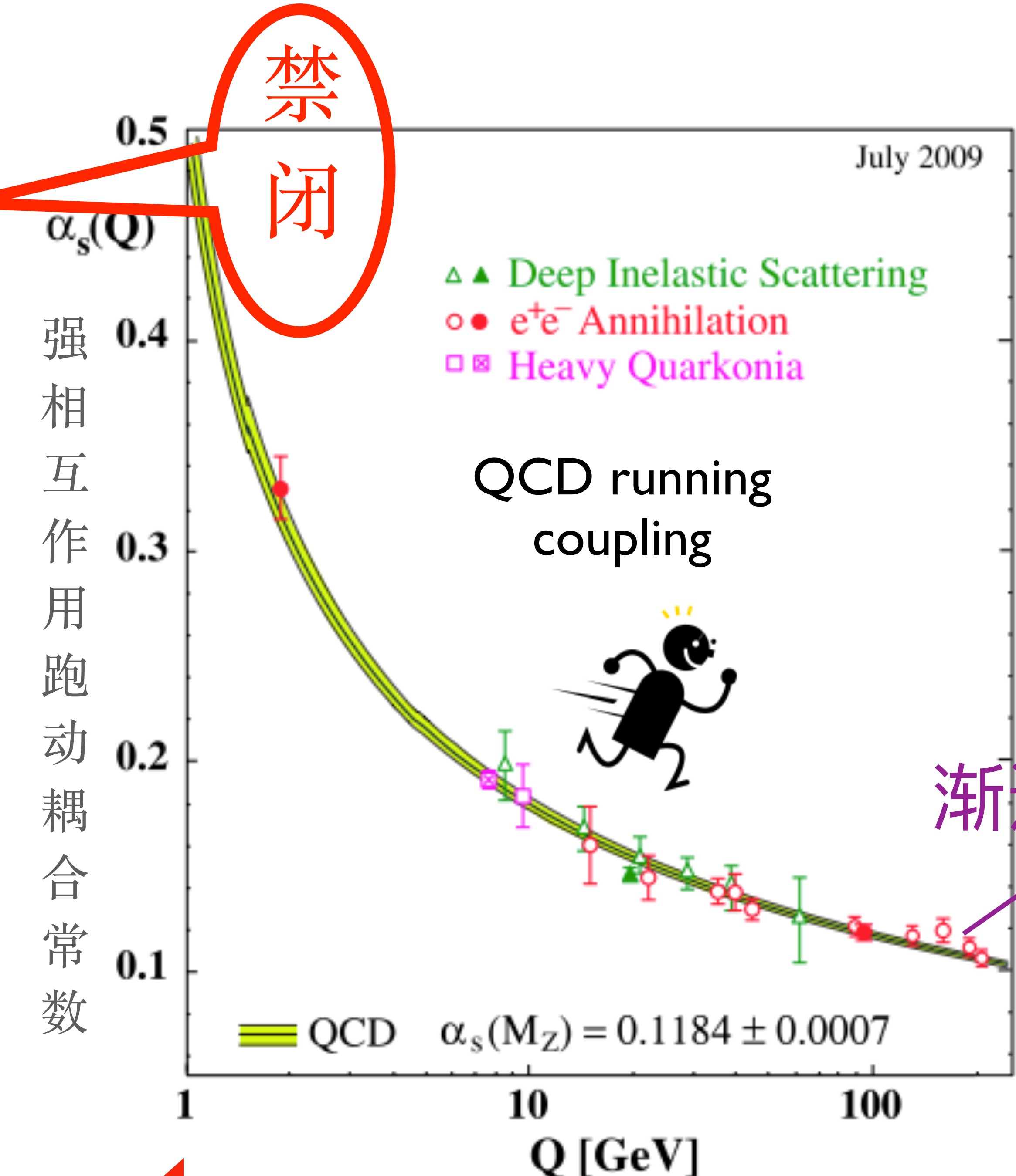
$m=E/c^2$

99% of the proton mass comes from the strong force

强相互作用特性：渐近自由与禁闭

Millennium Prize Problems

非微扰



David J. Gross H. David Politzer Frank Wilczek

2004

for the discovery of asymptotic freedom in the theory of the strong interaction

微扰展开，
收敛！

长距离，非微扰

短距离，微扰

Symmetries of QCD in the vacuum

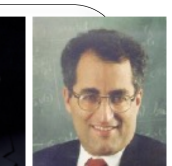
$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q}\left[i\gamma^{\mu}(\partial_{\mu} - igA_{\mu}) - m_q\right]q$$

Classical QCD symmetry (m_q=0)

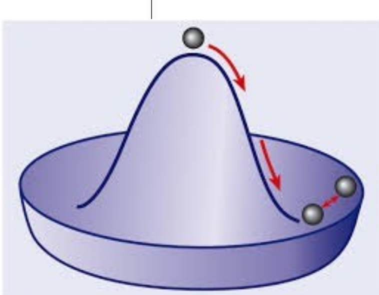
$$SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A$$


Quantum QCD vacuum (m_q=0)





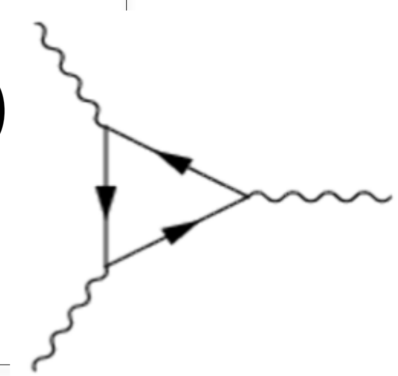
Chiral condensate:
spontaneous mass generation



$$\langle \bar{q}_R q_L \rangle \neq 0$$

Axial anomaly:
quantum violation of $U(1)_A$

$$\partial_{\mu} j_5^{\mu} = \frac{g^2 N_f}{16\pi^2} tr(\tilde{F}_{\mu\nu}F^{\mu\nu})$$



$$SU(N_f)_V \times U(1)_V$$

Lattice gauge theory

PHYSICAL REVIEW D VOLUME 10, NUMBER 8 15 OCTOBER 1974

从第一性原理出发
包含了体系所有（非）微扰性质

用来理解自然界中
为什么不存在自由的夸克

Confinement of quarks*

Kenneth G. Wilson

Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14850

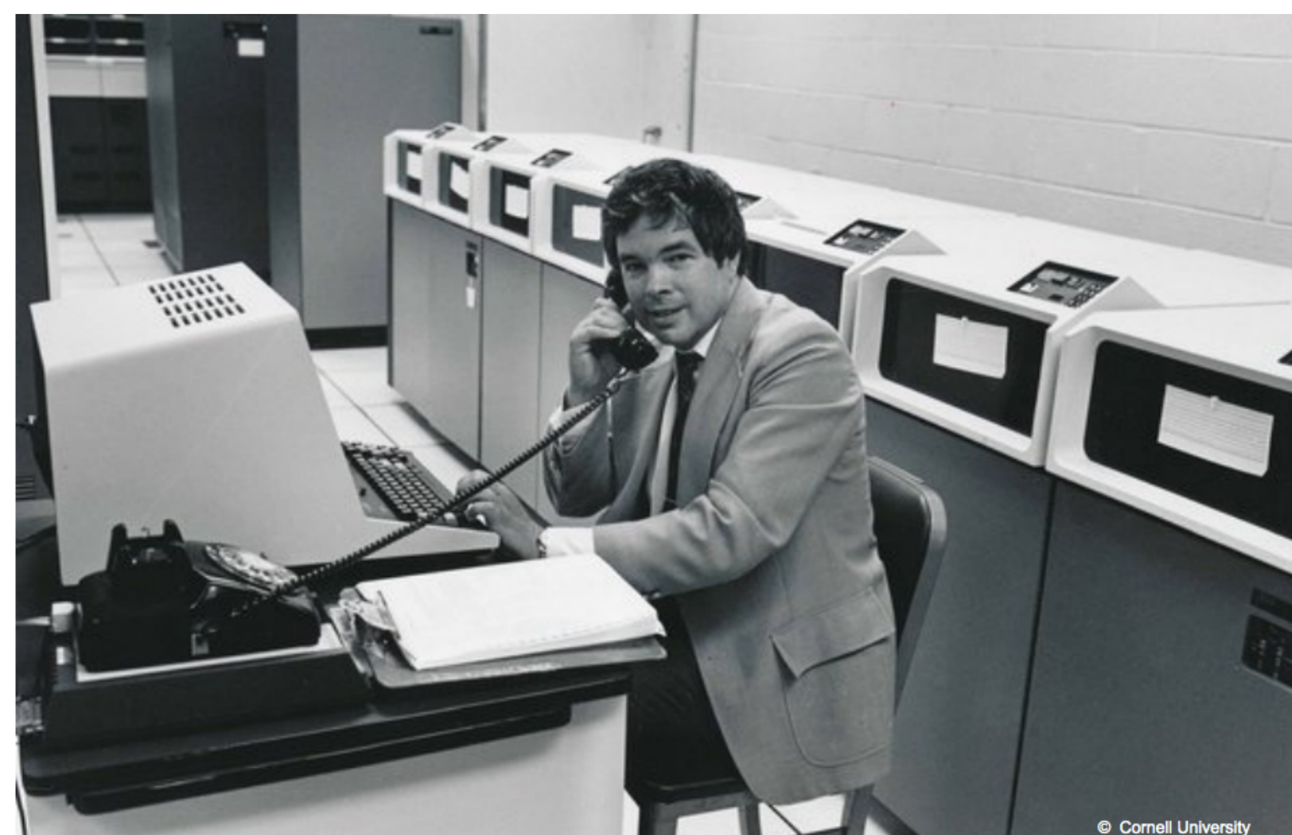
(Received 12 June 1974)

A mechanism for total confinement of quarks, similar to that of Schwinger, is defined which requires the existence of Abelian or non-Abelian gauge fields. It is shown how to quantize a gauge field theory on a discrete lattice in Euclidean space-time, preserving exact gauge invariance and treating the gauge fields as angular variables (which makes a gauge-fixing term unnecessary). The lattice gauge theory has a computable strong-coupling limit; in this limit the binding mechanism applies and there are no free quarks. There is unfortunately no Lorentz (or Euclidean) invariance in the strong-coupling limit. The strong-coupling expansion involves sums over all quark paths and sums over all surfaces (on the lattice) joining quark paths. This structure is reminiscent of relativistic string models of hadrons.

Kenneth G. Wilson
June 8, 1936 - June 15, 2013

for his theory for
critical phenomena
in connection with
phase transitions

1982



arXiv: hep-lat

https://arxiv.org/archive/hep-lat

arXiv.org

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- High Energy Physics - Lattice (**hep-lat** new, recent,
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- High Energy Physics - Theory (**hep-th** new, recent,
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- Nuclear Theory (**nucl-th** new, recent, search)
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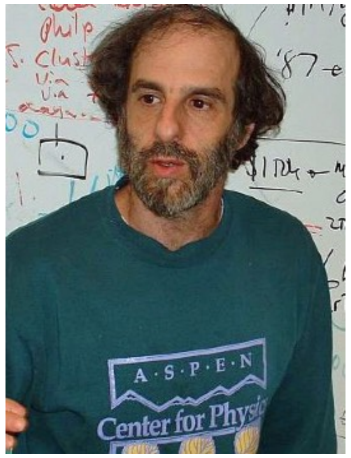


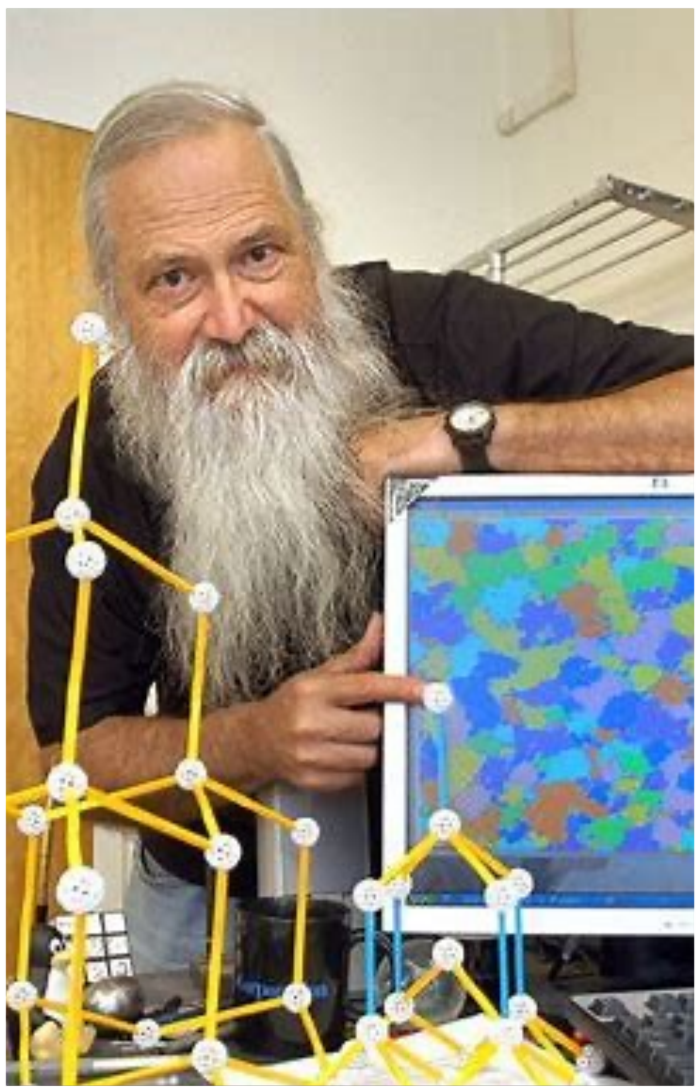
Paul Ginsparg
1955-

Known for Arxiv,
Ginsparg-Wilson equation…,
PhD student of K.G. Wilson

First numerical lattice simulations

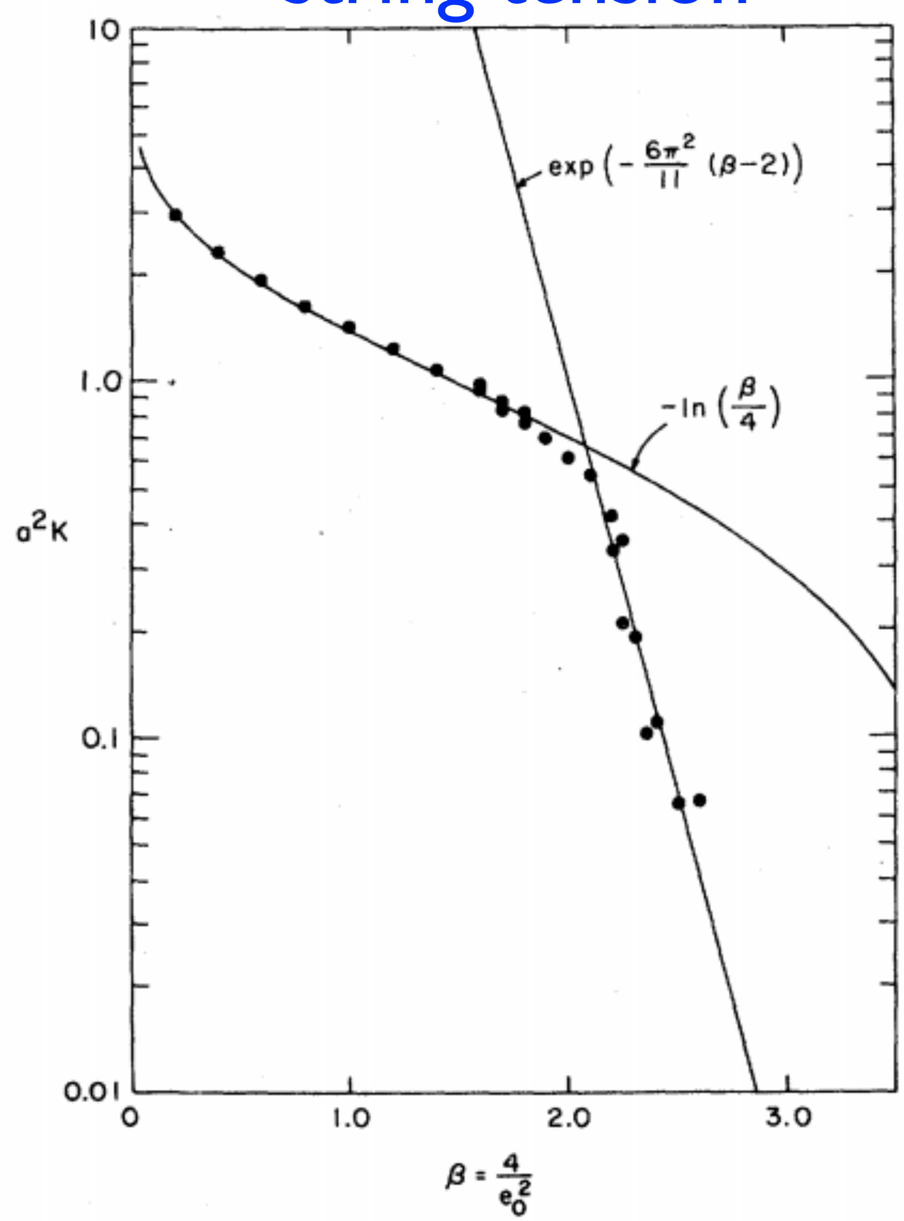
Spawned golden age in lattice QCD

M. Creutz, PRD 1980



Michale Creutz
@BNL

string tension



lattice gauge coupling

Michale Creutz
on the beach

VOLUME 47, NUMBER 25 PHYSICAL REVIEW LETTERS 21 DECEMBER 1981

Numerical Estimates of Hadronic Masses in a Pure SU(3) Gauge Theory

H. Hamber
Department of Physics, Brookhaven National Laboratory, Upton, New York 11973

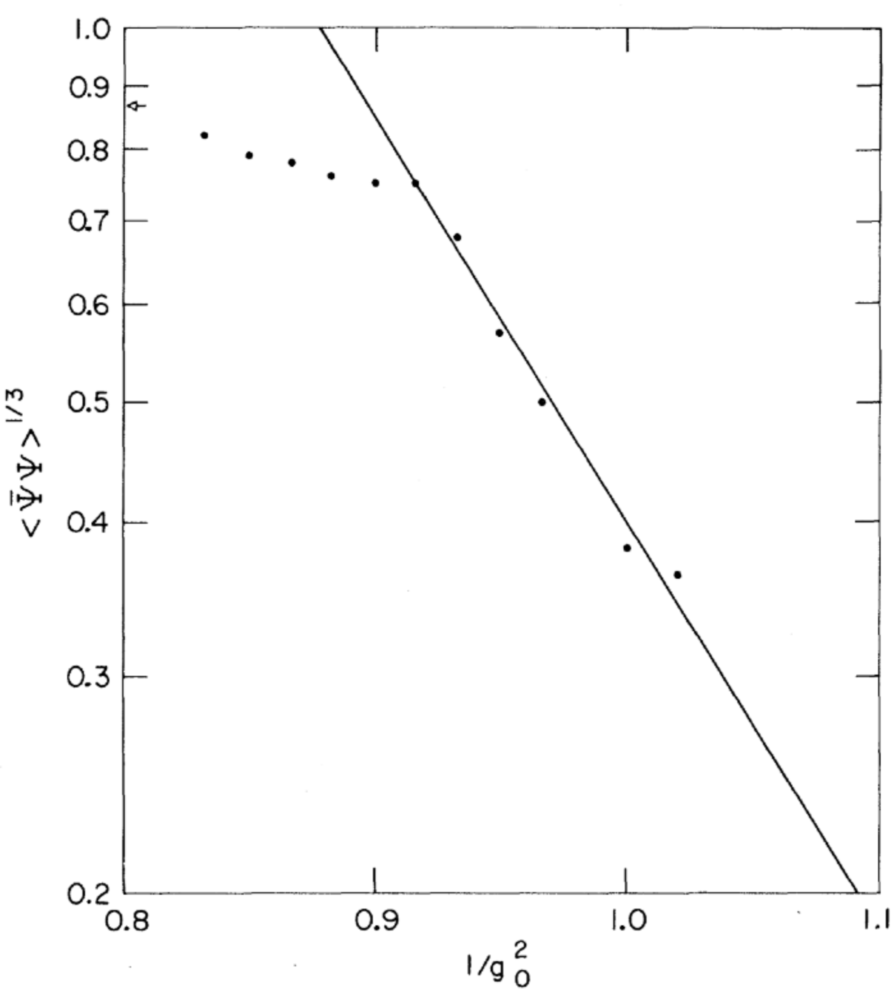
and

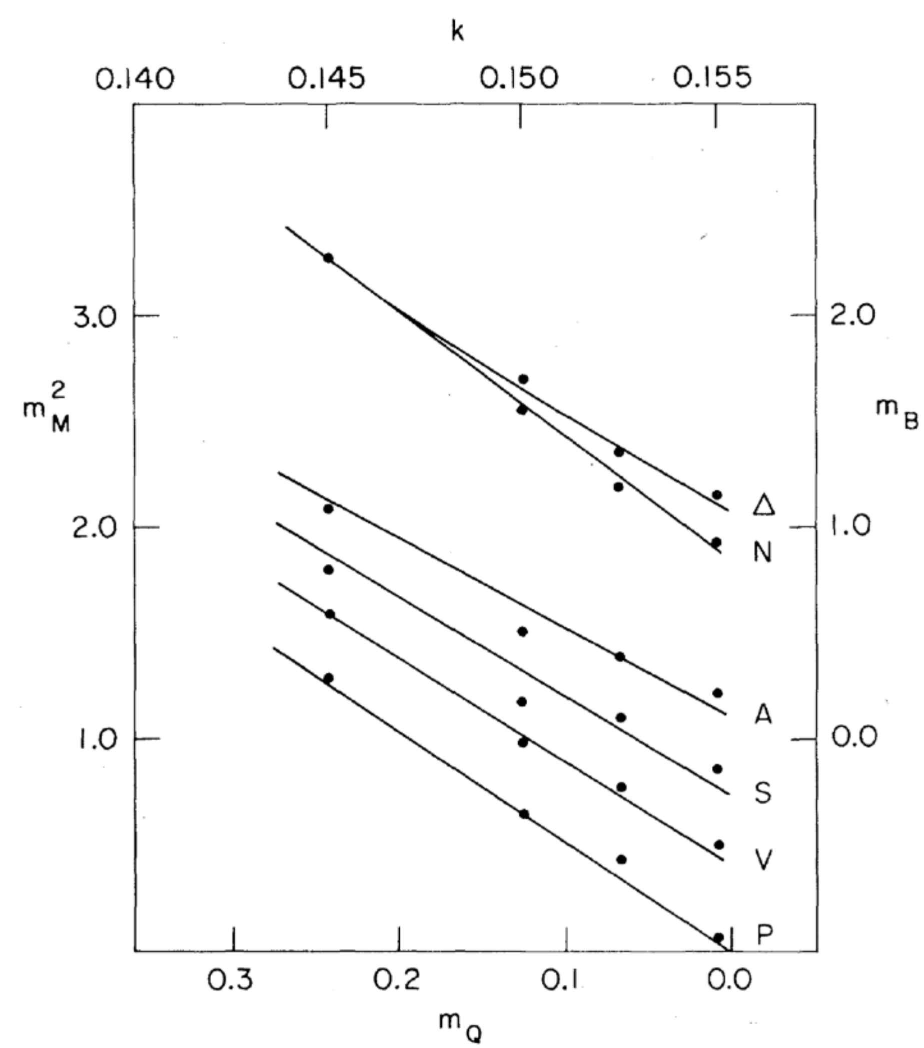
G. Parisi
Istituto Nazionale di Fisica Nucleare, Frascati, Italy, and Istituto di Fisica della Facoltà di Ingegneria, Rome, Italy

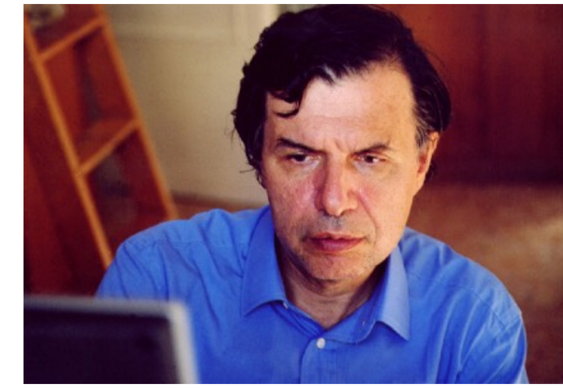
(Received 2 October 1981)

In lattice quantum chromodynamics, the hadronic mass spectrum is evaluated by computer simulations in the approximation where closed quark loops are neglected. Chiral symmetry is shown to be spontaneously broken and an estimate of the pion decay constant is given.

PACS numbers: 12.70.+q, 11.10.Np, 11.30.Jw, 12.40.Cc







Giorgio Parisi
1948-

2021

for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales

格点场论研究内容

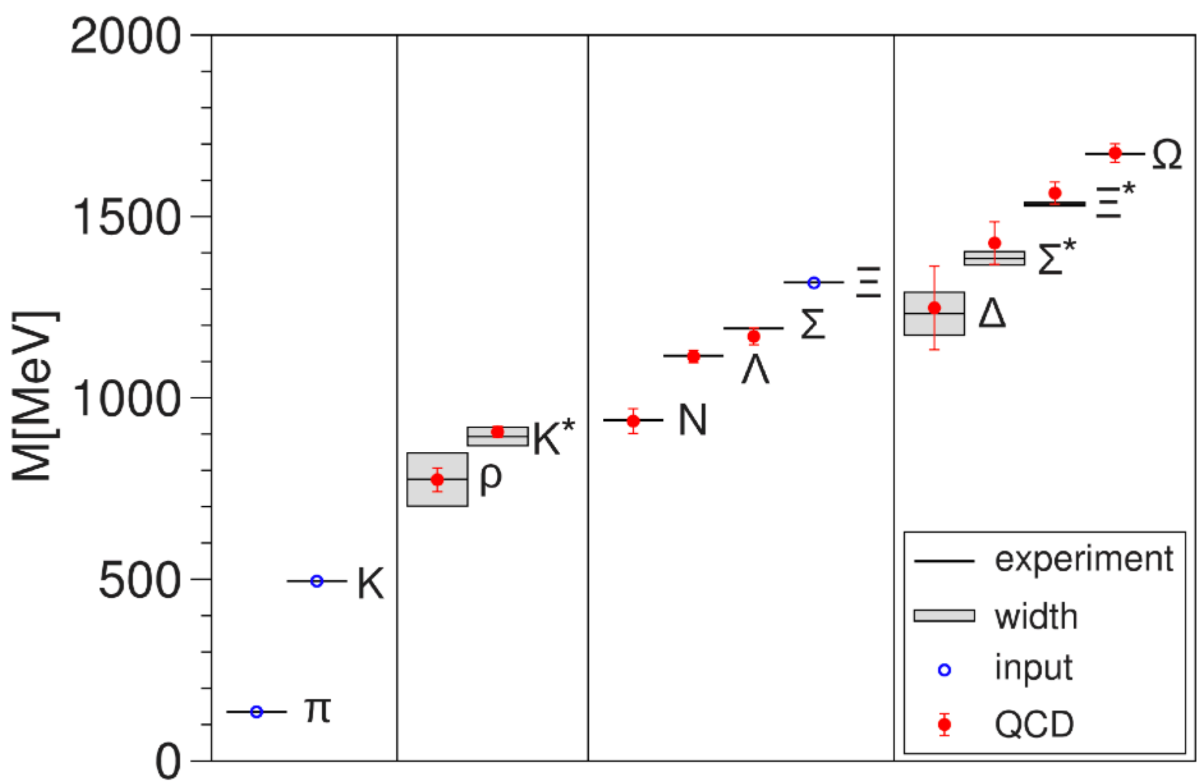
- Algorithms and Machines
- Applications Beyond QCD
- Chiral Symmetry
- Hadron Spectroscopy and Interactions
- Hadron Structure
- QCD at nonzero Temperature and Density
- Physics Beyond the Standard Model
- Standard Model Parameters and Renormalisation
- Theoretical Developments
- Vacuum Structure and Confinement
- Weak Decays and Matrix Elements
- Code Development

1. 算法和计算机
2. 超出QCD之外的应用
3. 手征对称性
4. 强子谱和相互作用
5. 强子结构
6. 有限温度密度QCD
7. 超出标准模型的物理
8. 标准模型参数和重整化
9. 理论进展
10. 真空结构和禁闭
11. 弱衰变和矩阵元
12. 代码研发

第39届国际格点年会(Lattice 2022)
http://lattice2022.uni-bonn.de/

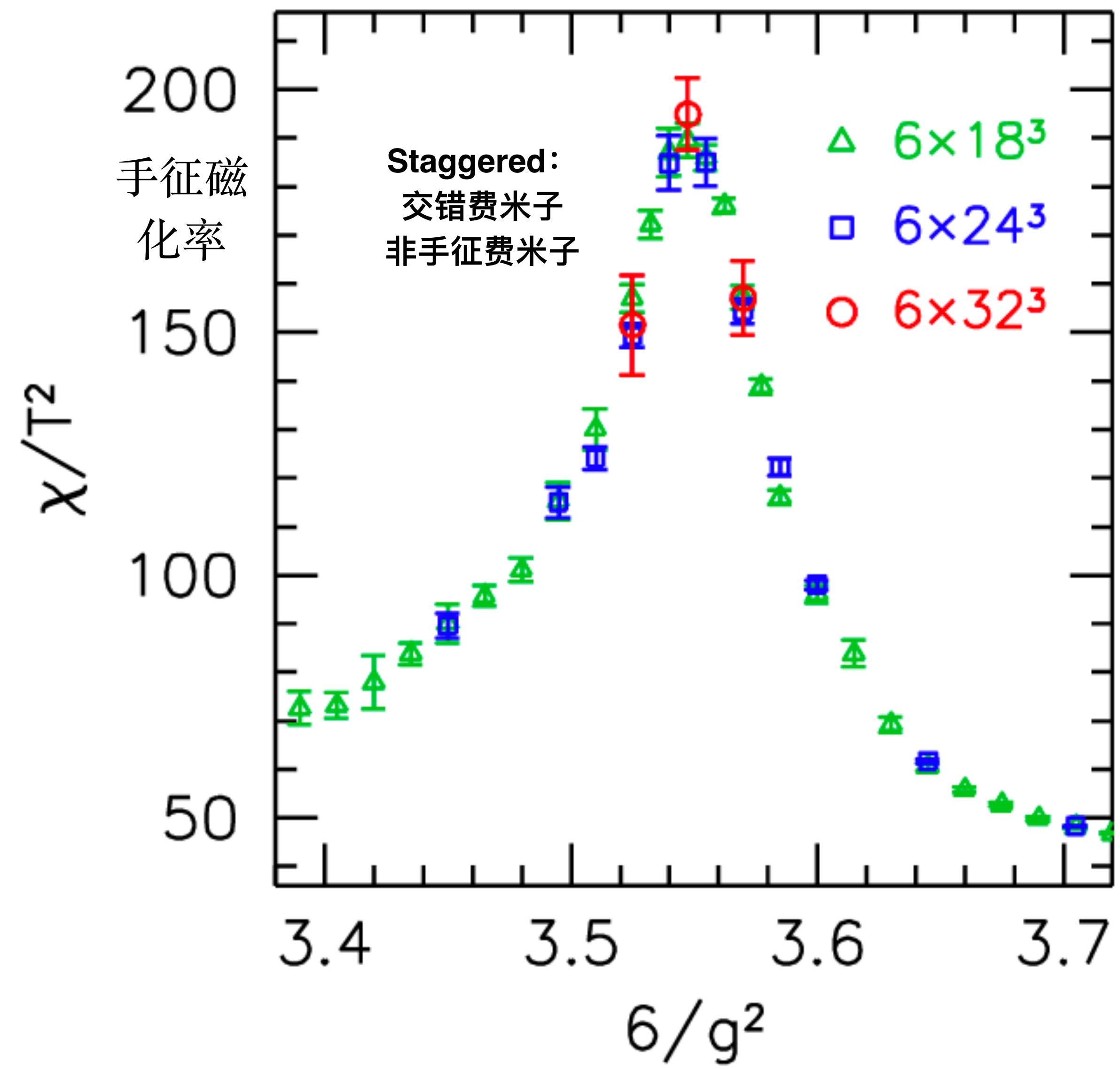
格点QCD里程碑式的进展

轻强子谱



S. Dürr et al., Science 322 (2008) 1224

强子相到夸克胶子等离子体相：
平滑过渡



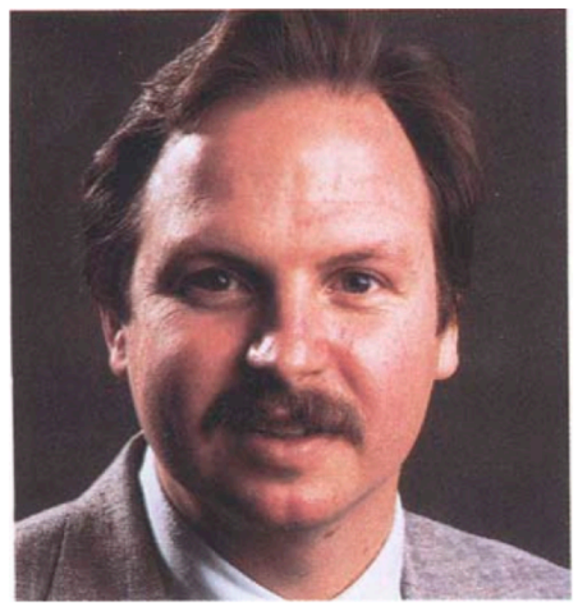
Y. Aoki et al., Nature 443 (2006) 675-678

更快的计算机 +更有效的算法 +更好物理分析方法

from The Hitchhiker's Guide to the Galaxy (2005) 《银河系漫游指南》

We are trying very hard to get the 256-node machine built and get good physics out of it.

—Norman Christ, Columbia



THINKING MACHINES

We've done a conjugate algorithm for QCD with dynamical fermions that is running on the CM-2 in excess of 1 gigaflop.

—John Richardson, Thinking Machines

FERMILAB

After the initial 16-node system is running, we'll go on to build a 256-processor machine with 5.0 gigaflops peak.

—Thomas Nash, Fermilab

Peter Batacan, New Computer Architectures for Lattice QCD, Computers in Physics 3, 17

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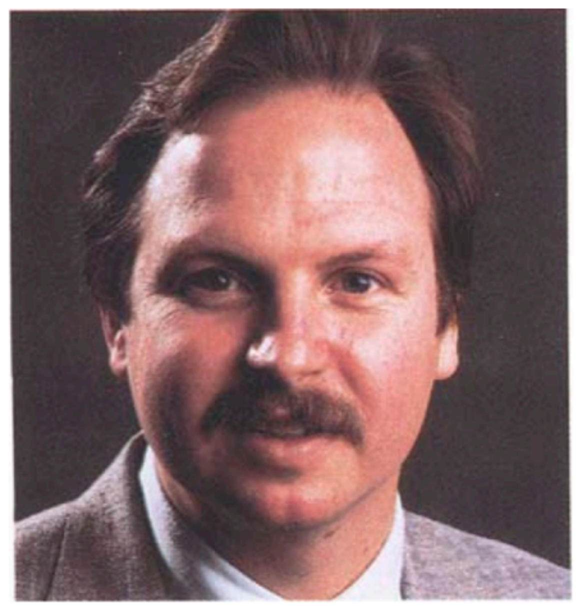
1989



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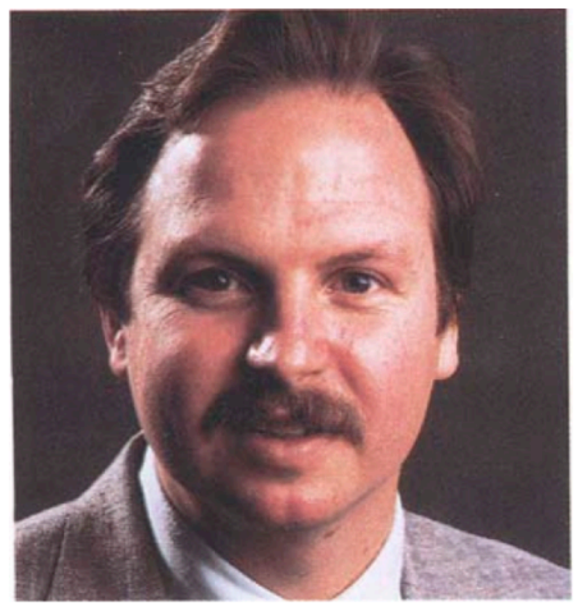

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Peter Batacan, New Computer Architectures for Lattice QCD, Computers in Physics 3, 17

QCDSP:

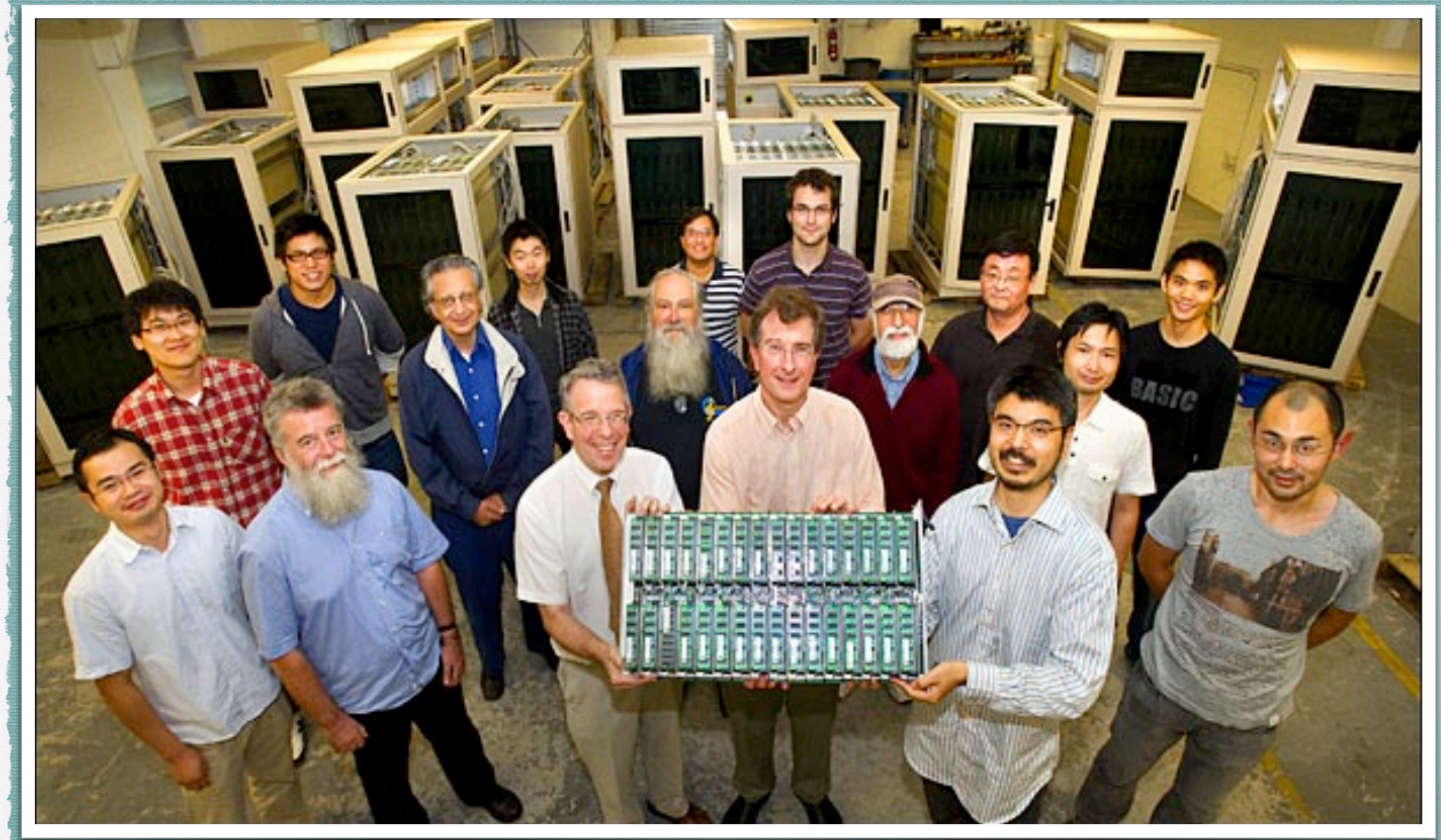
QCD on a digital Signal Processor

- 0.6 Tflops
- completed 1998
- Gordon Bell (戈登贝尔) Prize

QCDOC:

QCD On a Chip

- 10 Tflops
- completed 2005
- Parent of IBM Bluegene



QCDOC:
Quantum ChromoDynamics (QCD) On a Chip

capable of handling the complex calculations of QCD, the theory that describes the nature and interactions of the basic building blocks of the universe

Retirement of QCDOC in 2011at Brookhaven National Lab, NY, USA

https://www.bnl.gov/newsroom/news.php?a=22647

Available online at www.sciencedirect.com

ScienceDirect

Computer Physics Communications 177 (2007) 631–639

Computer Physics Communications

www.elsevier.com/locate/cpc

打游戏的显卡（GPU）
可以用来做科学计算！

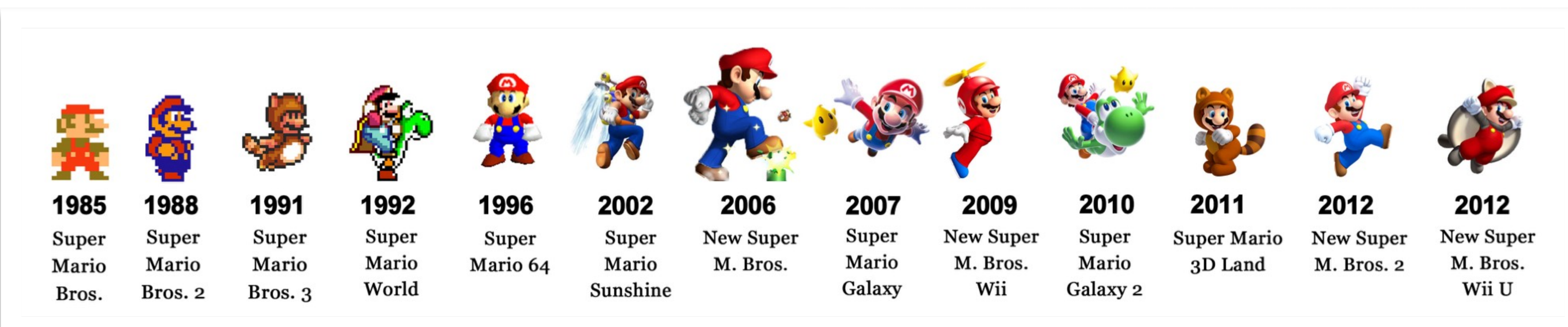
Lattice QCD as a video game

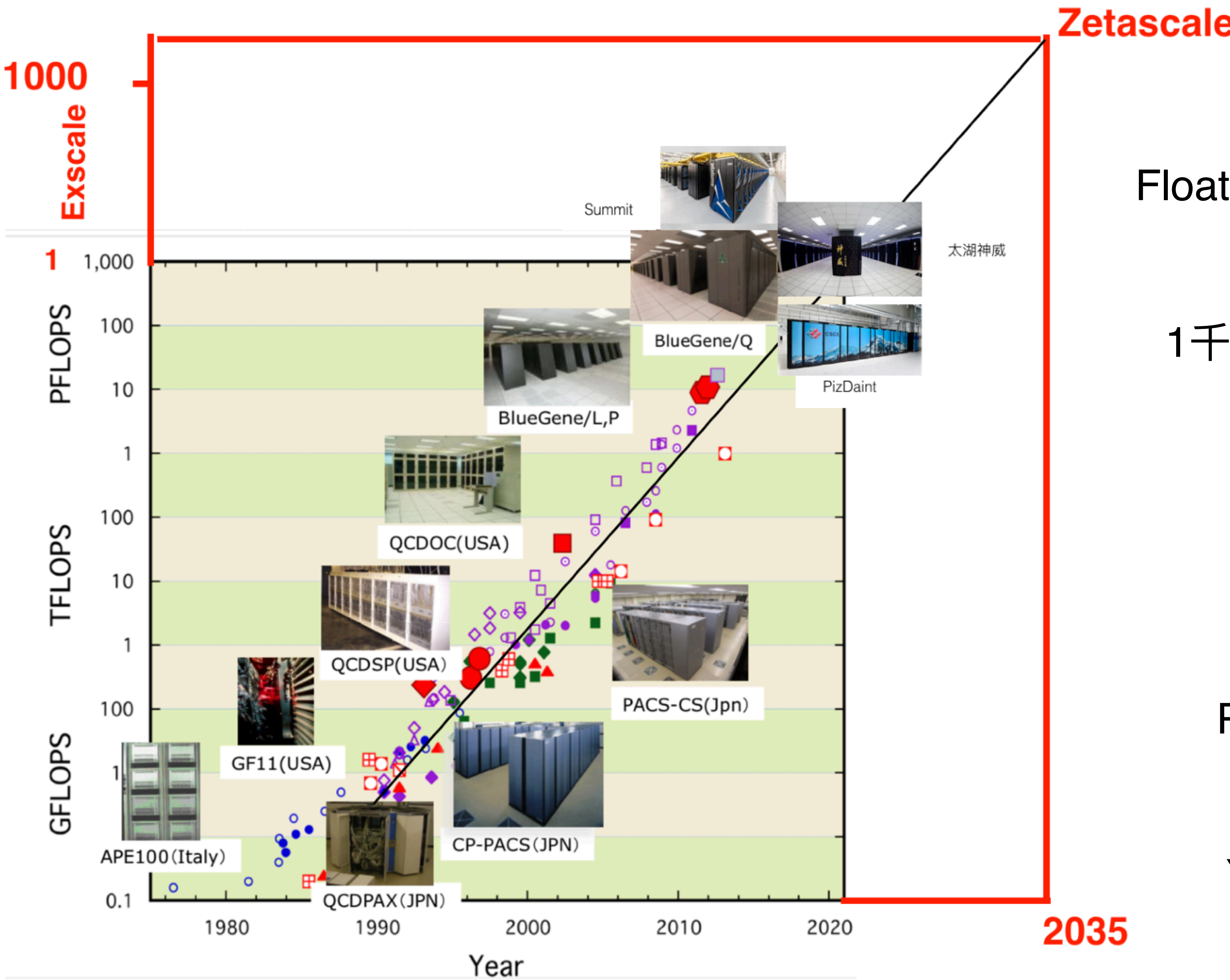
Győző I. Egri [a], Zoltán Fodor [a,b,c,*], Christian Hoelbling [b], Sándor D. Katz [a,b], Dániel Nógrádi [b], Kálmán K. Szabó [b]

[a] *Institute for Theoretical Physics, Eötvös University, Budapest, Hungary*
[b] *Department of Physics, University of Wuppertal, Germany*
[c] *Department of Physics, University of California, San Diego, USA*

Received 2 February 2007; received in revised form 29 May 2007; accepted 7 June 2007

Available online 15 June 2007





Flops/s:

Floating operations per second

PFlops/s:

1千万亿(10^{15})次浮点运算每秒

Kilo(Thousand): 10^3
Mega(Million): 10^6
Giga(Billion): 10^9
Tera(Trillion): 10^{12}
Peta(Quadrillion): 10^{15}
Exa(Quintillion): 10^{18}
Zeta(Sextillion): 10^{21}
Yotta(Septillion): 10^{24}

based on A. Ukawa, 2013 HPC summer school

格点量子色动力学在中国

陈 莹[1] 丁亨通[2] 冯 旭[3] 傅子文[4] 宫 明[1] 桂龙成[5] 苏 宁[6]
刘 川[3] 刘柳明[7] 刘玉斌[8] 刘朝峰[1] 马建平[9] 孙 鹏[10]
吴佳俊[11] 吴良凯[12] 杨一玻[9] 张剑波[13]

(1. 中国科学院高能物理研究所 100049;2. 华中师范大学粒子物理研究所 430079;3. 北京大学物理学院 100871;4. 四川大学原子核科学技术研究所 610064;5. 湖南师范大学物理与电子科学学院 410081; 6. 西安工业大学理学院 710021;7. 中国科学院近代物理研究所 730000;8. 南开大学物理科学学院 300071;9. 中国科学院理论物理研究所 100190;10. 南京师范大学物理科学与技术学院 210023;11. 中国科学院大学物理科学学院 100049;12. 江苏大学理学院 212013;13. 浙江大学物理系 310027)

1. 格点量子色动力学概述

经过多年努力,人们已经成功地将自然界四种基本相互作用(强、弱、电磁、引力)中的前三种统一在量子场论的框架之中,即粒子物理的标准模型(Standard Model, SM)。该模型中关于强相互作用部分的基本理论是量子色动力学(Quantum Chromodynamics,QCD),它在高能区和低能区呈现出迥然不同的特性:在高能区QCD呈现出渐近自由(asymptotic freedom)和部分可微扰的特性;在低能区则展现出手征对称性破缺和色禁闭等非微扰特性。由于QCD在低能区(通常指几个GeV以下)具有非常强的非微扰特性,因此研究这个能区的物理必须利用非微扰的量子场论方法。目前已知最系统的非微扰理论方法就是格点QCD,如图1所示。

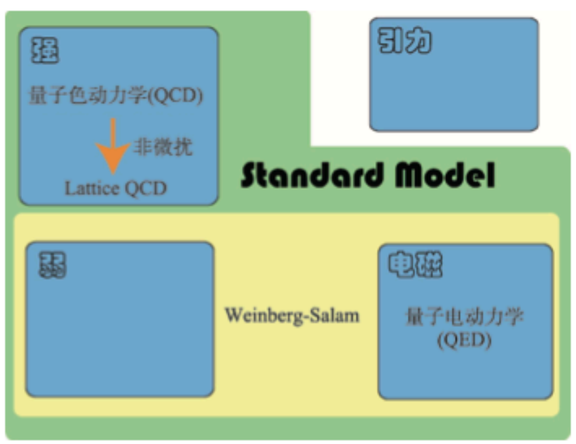


图 1 格点QCD在标准模型中的相对位置的示意图

格点QCD从第一性原理出发,将QCD的基本自由度定义在离散的四维欧氏时空格子上。如图2所示,夸克和反夸克场被定义在格点上,而规范场则定义在相邻两格点间的链接上。超立方格子的体积为$(N_s a)^3 \times (N_t a)$,其中格点间距a和空间方向上长度$N_s a$提供了量子场论的紫外和红外截断。利用路径积分量子化进行表述,格点QCD形式上类似于一个统计物理模型。如果将所有的场变量集中

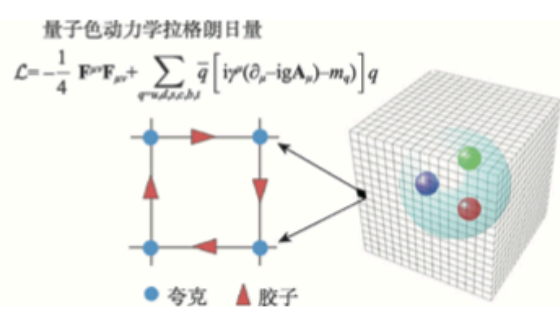


图2 格点QCD中,夸克和反夸克场被定义在格点上,而规范场则定义在相邻两格点间的链接上

解QCD的非微扰性质。同时,将这些结果联系到唯象研究,也需要相关的解析微扰重整化和匹配计算。此外,格点QCD与有效场论、粒子物理唯象学和少体核物理等学科也有交叉和互鉴的关系。

主要挑战:我们看到,格点QCD研究的方向涉及与强相互作用相关的粒子物理、核物理、计算机科学等学科的方方面面。格点QCD多年来已经在上述研究方向取得了诸多成就,但是依然存在一些尚未彻底征服的核心挑战,例如符号问题和含时问题。

Monte Carlo方法本质上是一种基于概率的数值方法,概率必须是正定的。因此,Monte Carlo方法无法有效抽样具有复的"概率"的场的位型空间。这就是著名的符号问题。这类问题会出现在有限密度格点QCD问题中。类似的,如果需要计算明显含时的问题,这时候会涉及到复的函数的数值积分问题,也无法进行有效的MonteCarlo数值计算。

格点QCD多年的发展之中,曾经也有过不少物理量被认为是复"概率"的问题,因此无法利用格点QCD进行有效的处理。但是不少问题后来实际上部分地被解决了。例如在有限密度下的格点QCD研究中,可以通过计算密度为零时的泰勒展开系数来规避符号问题。再例如强子之间的散射问题,通过计算两个强子的能量,可以间接地抽取出相应的两个强子的散射相移,从而不必计算两个强子的具体散射过程。最近的例子是PDF的格点计算,通过计算类似的空间关联函数,然后利用所谓大动量展开有效理论,将其匹配到涉及光锥坐标的PDF。但是,这类问题到目前为止还没有通用而非常有效的方法,尽管人们仍在尝试。

从业人员:格点QCD研究领域目前在全球范围内,约有三百余名专业研究人员(仅包括正/副教授或相当级别的固定职位)活跃在这一研究方向上。其中,在美国约有150名,欧洲约100名,日本约有40名。

中国的格点QCD研究最早是从20世纪80年代初开始的,距K.G. Wilson提出格点规范理论并不远。李政道先生对格点规范理论有浓厚的兴趣,认为其在强相互作用研究方面有很大的发展前景并着力组织和培养中国的格点研究队伍。中国也逐渐形成了以李文铸(浙江大学)、郭硕鸿(中山大学)、冼鼎昌(中科院高能所)、吴济民(中科院高能所)、陈天伦(南开大学)、郑希特(四川大学)等老一辈科学家为代表的第一代格点研究队伍。他们在进行格点理论研究和探索的同时,也为中国培养了一批格点研究人才,如朱允伦(北京大学)、董绍静(浙江大学)、季达人(浙江大学)、应和平(浙江大学)、张剑波(浙江大学)、赵佩英(中科院高能所)和罗向前(中山大学)等。但是,受国内当时的计算条件的限制,中国格点研究在数值模拟方面发展相对缓慢,除少数人员赴国外合作研究和学习外,研究队伍没有迅速壮大。

随着国内计算条件的改善,本世纪初中国逐渐开始开展格点QCD的数值模拟研究。2005年,马建平(中科院理论所)、刘川(北京大学)、刘玉斌(南开大学)、张剑波(浙江大学)和陈莹(中科院高能所)等发起成立了中国的格点研究组织——中国格点合作组(China Lattice QCD Collaboration, 简称CLQCD),开展了卓有成效的格点数值模拟研究。这些年来,中国格点组的主要研究内容是奇特强子态,在胶球、XYZ粒子性质方面做了不少工作,取得了一些国际影响。近些年来,一批在国际上崭露头角的优秀年轻研究人员回国,大大充实了国内的格点QCD研究力量。他们包括刘朝峰(中科院高能所)、丁亨通(华中师范大学)、宫明(中科院高能所)、冯旭(北京大学)、刘柳明(中科院近物所)、杨一玻(中科院理论所)等,研究兴趣涵盖强子谱学、强子结构、QCD相变、高精度前沿、软件架构研发等方面,并与国际上重要的格点研究团队有密切的合作关系。目前,国内已经形成以中青年研究人员为骨干的研究队伍,具有一定规模并于2009年(北京大学)和2019年(华中师范大学)两次承办国际格点场论大会。

计算资源:

以产生典型的$64^3 \times 128$体积的蒙特卡洛规范场组态并进行物理计算为例,需要每年数亿CPU核小

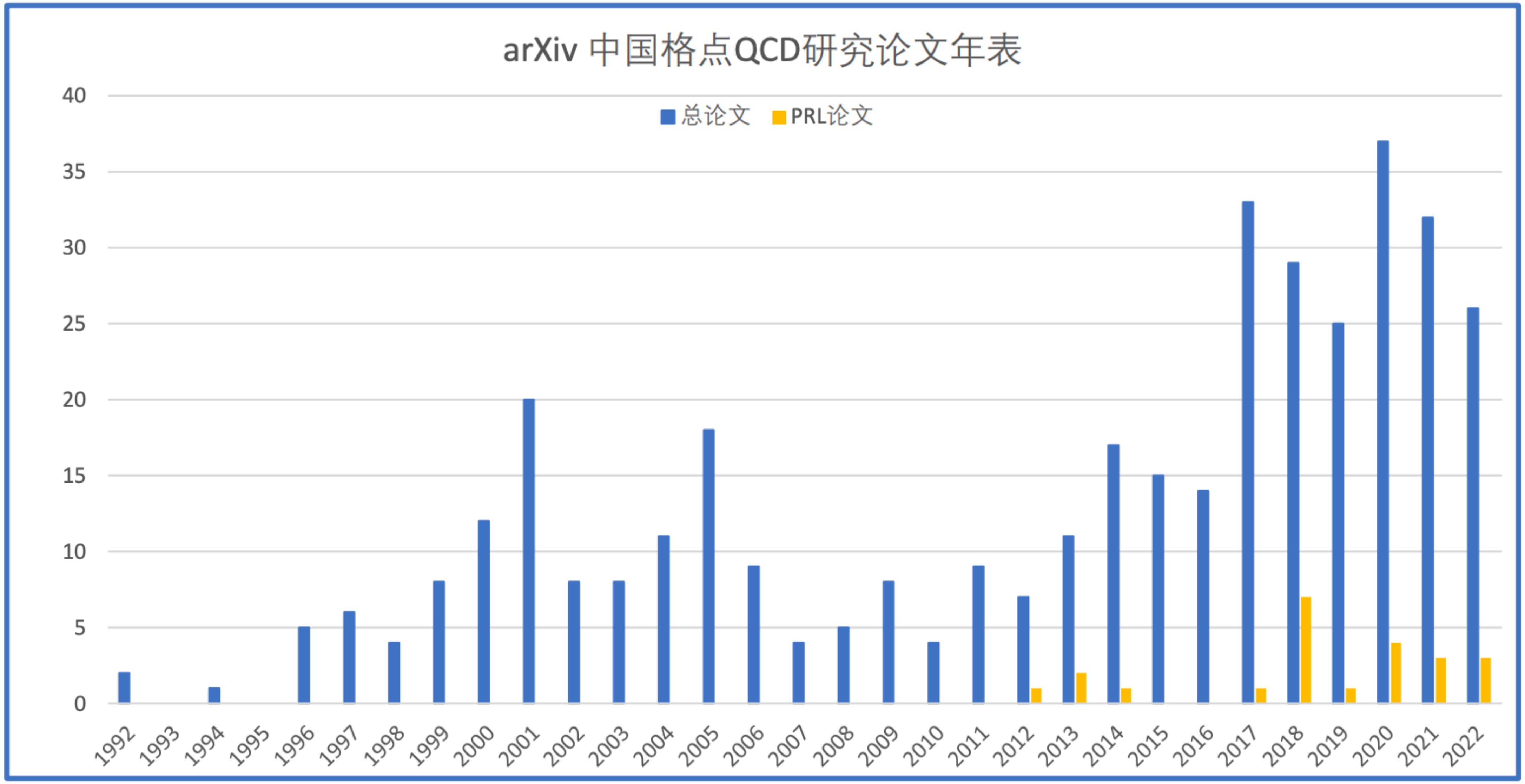
https://mp.weixin.qq.com/s/wI0oQpNYWE_rD0TUazFOgA

Lattice年会：格点场论领域最高级别会议

第27届, 2009年7月26-31日@北京大学，北京
第37届, 2019年6月16-22日@华中师范大学，武汉

Lattice 2019: 340余人参会

主办单位：华中师范大学
协办单位：北京大学, 清华大学, 南开大学, 浙江大学, 四川大学, 湖南师范大学, 江苏大学, 西安工业大学, 台湾交通大学, 中科院高能物理研究所，中科院近代物理研究所, 中科院理论物理研究所



CLQCD
China LQCD
中国格点合作组

国内网络还不发达

筚路蓝缕

蓬勃发展

arXiv 的 hep-lat 每年文章数大致400-600篇

陈莹，第二届中国格点QCD研讨会, 2022.10.7-10

https://indico-tdli.sjtu.edu.cn/event/1198/contributions/5265/attachments/2250/3443/pdf

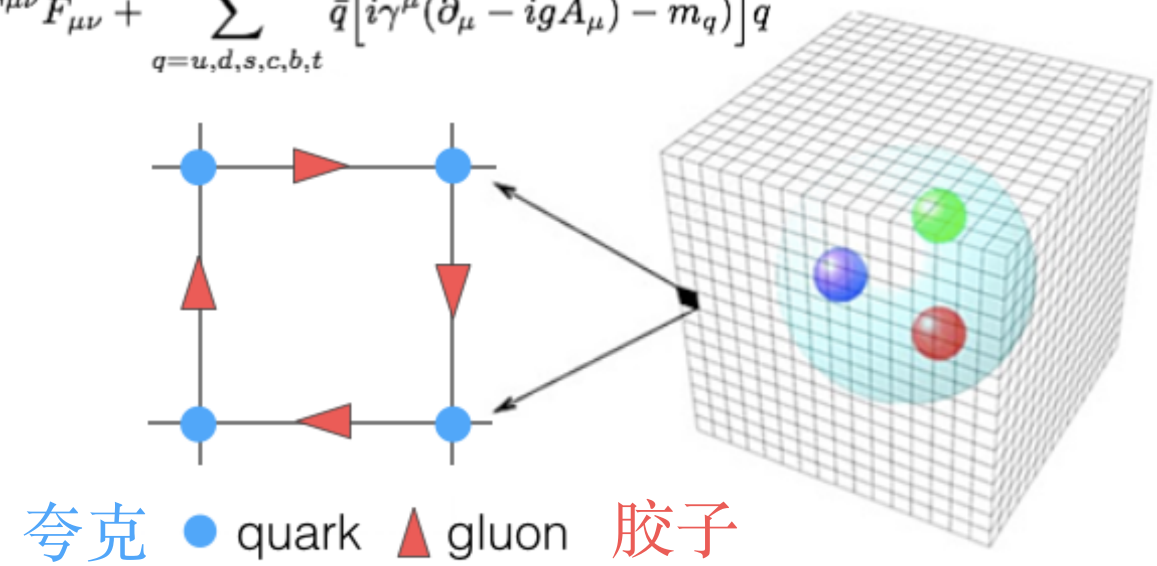
Lattice QCD (格点量子色动力学)

唯一的从第一性原理出发的(从头开始算)

用来研究QCD长程非微扰的理论方法

QCD Lagrangian 量子色动力学拉格朗日量

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q}\left[i\gamma^\mu(\partial_\mu - igA_\mu) - m_q\right]q$$



- 将时空离散化为有一定间距的格子：虚时的欧几里得空间！
- 夸克放在点上，胶子作为点与点之间的连线
- 将作用力量（拉格朗日量相关）离散化，定义路径积分的量度
- 定义可观测的物理量

Two key equations in Lattice field theory

- Euclidean correlator: Useful to extract matrix elements of operators and the energy spectrum of the theory (Interpretation)

$$\lim_{T\to\infty}\frac{1}{Z_T}\mathrm{Tr}[e^{-(T-t)\hat{H}}\,\hat{O}_2\,e^{-t\hat{H}}\,\hat{O}_1]=\sum_n\langle 0|\hat{O}_2|n\rangle\langle n|\hat{O}_1|0\rangle\,e^{-tE_n}$$

partition function: $Z_T=\mathrm{Tr}[e^{-T\hat{H}}]$

- Path integral formalism used to be evaluated numerically on the lattice (Computation)

$$\frac{1}{Z_T}\mathrm{Tr}[e^{-(T-t)\hat{H}}\,\hat{O}_2\,e^{-t\hat{H}}\,\hat{O}_1]=\frac{1}{Z_T}\int\mathcal{D}[\Phi]e^{-S_E[\Phi]}\,O_2[\Phi(.,t)]\,O_1[\Phi(.,0)]$$

Euclidean correlators

$$\langle O_2(t)\, O_1(0)\rangle_T = \frac{1}{Z_T}\,\mathrm{tr}\left[\mathrm{e}^{-(T-t)\widehat{H}}\,\widehat{O}_2\,\mathrm{e}^{-t\widehat{H}}\,\widehat{O}_1\right] \qquad Z_T = \sum_n \langle n|\mathrm{e}^{-T\,\widehat{H}}|n\rangle = \sum_n \mathrm{e}^{-T\,E_n}$$

$$\langle O_2(t)\, O_1(0)\rangle_T = \frac{1}{Z_T}\sum_{m,n}\langle m|\mathrm{e}^{-(T-t)\,\widehat{H}}\widehat{O}_2|n\rangle\langle n|\mathrm{e}^{-t\,\widehat{H}}\,\widehat{O}_1|m\rangle$$

$$= \frac{1}{Z_T}\sum_{m,n}\mathrm{e}^{-(T-t)\,E_m}\,\langle m|\widehat{O}_2|n\rangle\,\mathrm{e}^{-t\,E_n}\,\langle n|\widehat{O}_1|m\rangle$$

$$E_0 \le E_1 \le E_2 \cdots$$

$$\Delta E_n = E_n - E_0$$

$$= \frac{\sum_{m,n}\langle m|\widehat{O}_2|n\rangle\,\langle n|\widehat{O}_1|m\rangle\,\mathrm{e}^{-t\,\Delta E_n}\,\mathrm{e}^{-(T-t)\,\Delta E_m}}{1+\mathrm{e}^{-T\,\Delta E_1}+\mathrm{e}^{-T\,\Delta E_2}+\ldots}$$

$$\lim_{T\to\infty}\langle O_2(t)\, O_1(0)\rangle_T = \sum_n \langle 0|\widehat{O}_2|n\rangle\langle n|\widehat{O}_1|0\rangle\,\mathrm{e}^{-t\,E_n}$$

Determine the mass spectrum of e.g. proton

$$\lim_{T\to\infty}\langle O_p(t)\,O_p(0)^\dagger\rangle_T = |\langle p|\widehat{O}_p^\dagger|0\rangle|^2\,\mathrm{e}^{-t\,E_p} + |\langle p'|\widehat{O}_p^\dagger|0\rangle|^2\,\mathrm{e}^{-t\,E_{p'}}+\ldots$$

Path integral for a scalar field theory

- Lagrangian $$L(\Phi, \partial_\mu \Phi) = \frac{1}{2}(\partial_\mu \Phi)(\partial^\mu \Phi) - \frac{m^2}{2}\Phi^2 - V(\Phi)$$

Hamiltonian operator
$$\hat{H} = \int d^3x \left(\underbrace{\frac{1}{2}\hat{\Pi}(\boldsymbol{x})^2}_{\hat{H}_0} + \underbrace{\frac{1}{2}\left(\nabla\hat{\Phi}(\boldsymbol{x})\right)^2 + \frac{m^2}{2}\hat{\Phi}(\boldsymbol{x})^2 + V\left(\hat{\Phi}(\boldsymbol{x})\right)}_{\hat{U}} \right)$$

Discretization in time: $T = N_T\, \epsilon$

ϵ**:** spacing in the temporal direction

Trotter formula: $e^{A+B} = \lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n$, $\hat{W}_\epsilon = e^{-\epsilon\hat{U}/2}e^{-\epsilon\hat{H}_0}e^{-\epsilon\hat{U}/2}$

$$Z_T = \int \mathcal{D}\Phi_0 \langle \Phi_0 | e^{-T\hat{H}} | \Phi_0 \rangle = \lim_{N_T\to\infty} \int \mathcal{D}\Phi_0 \langle \Phi_0 | \widehat{W}_\varepsilon^{\,N_T} | \Phi_0 \rangle$$

Discretization in 3D-space: $\boldsymbol{x} \quad \Rightarrow \quad a\,\boldsymbol{n}\,, \quad n_i = 0, 1, \ldots, N-1 \quad \text{for} \quad i = 1, 2, 3$

a: spacing in the spatial direction

$$\partial_j \hat{\Phi}(\boldsymbol{x}) = \frac{\hat{\Phi}(\boldsymbol{n}+\hat{j}) - \hat{\Phi}(\boldsymbol{n}-\hat{j})}{2a} + \mathcal{O}(a^2)$$

$$\hat{U} = a^3 \sum_{\boldsymbol{n}\in\Lambda_3}\left(\frac{1}{2}\sum_{j=1}^{3}\left(\frac{\hat{\Phi}(\boldsymbol{n}+\hat{j}) - \hat{\Phi}(\boldsymbol{n}-\hat{j})}{2a}\right)^2 + \frac{m^2}{2}\hat{\Phi}(\boldsymbol{n})^2 + V\left(\hat{\Phi}(\boldsymbol{n})\right)\right)$$

$$\hat{H}_0 = a^3 \sum_{\boldsymbol{n}\in\Lambda_3}\frac{1}{2}\left(-\frac{\mathrm{i}}{a^3}\frac{\partial}{\partial\Phi(\boldsymbol{n})}\right)^2 = -\frac{1}{2a^3}\sum_{\boldsymbol{n}\in\Lambda_3}\frac{\partial^2}{\partial\Phi(\boldsymbol{n})^2}$$

$$Z_T = \int \mathcal{D}\Phi_0 \, \langle \Phi_0 | e^{-T\hat{H}} | \Phi_0 \rangle = \lim_{N_T \to \infty} \int \mathcal{D}\Phi_0 \, \langle \Phi_0 | \widehat{W}_\varepsilon{}^{N_T} | \Phi_0 \rangle$$

$$= \int \mathcal{D}\Phi_0 \, \ldots \, \mathcal{D}\Phi_{N_T-1} \, \langle \Phi_0 | \widehat{W}_\varepsilon | \Phi_{N_T-1} \rangle \langle \Phi_{N_T-1} | \widehat{W}_\varepsilon | \Phi_{N_T-2} \rangle \, \ldots \, \langle \Phi_1 | \widehat{W}_\varepsilon | \Phi_0 \rangle$$

periodic boundary condition is used

$$\langle \boldsymbol{\Phi}_{i+1} | \widehat{W}_\varepsilon | \boldsymbol{\Phi}_i \rangle = \langle \boldsymbol{\Phi}_{i+1} | \mathrm{e}^{-\varepsilon \hat{U}/2} \mathrm{e}^{-\varepsilon \hat{H}_0} \mathrm{e}^{-\varepsilon \hat{U}/2} | \boldsymbol{\Phi}_i \rangle$$

$$= \mathrm{e}^{-\varepsilon\, U[\boldsymbol{\Phi}_{i+1}]/2} \, \langle \boldsymbol{\Phi}_{i+1} | \mathrm{e}^{-\varepsilon \hat{H}_0} | \boldsymbol{\Phi}_i \rangle \, \mathrm{e}^{-\varepsilon\, U[\boldsymbol{\Phi}_i]/2}$$

$$= C^{N^3} \mathrm{e}^{-\varepsilon\, U[\boldsymbol{\Phi}_i]/2 \, - a^3/(2\varepsilon) \sum_{\boldsymbol{n}} (\boldsymbol{\Phi}(\boldsymbol{n})_i - \boldsymbol{\Phi}(\boldsymbol{n})_{i+1})^2 \, - \, \varepsilon\, U[\boldsymbol{\Phi}_{i+1}]/2}$$

$$= C^{N^3 N_T} \int \mathcal{D}\Phi_0 \, \ldots \, \mathcal{D}\Phi_{N_T-1} \, \mathrm{e}^{-S_E[\Phi]}$$

Euclidean Action In discretized Space-time

$$S_E[\Phi] = \frac{1}{2} \sum_{j=0}^{N_T-1} a^3 \sum_{\boldsymbol{n} \in \Lambda_3} \frac{1}{\varepsilon} \left(\Phi(\boldsymbol{n})_{j+1} - \Phi(\boldsymbol{n})_j \right)^2 + \varepsilon \sum_{j=0}^{N_T-1} U[\Phi_j]$$

Euclidean Action In discretized Space-time

$$S_E[\Phi] = \frac{1}{2}\sum_{j=0}^{N_T-1} a^3 \sum_{\boldsymbol{n}\in\Lambda_3} \frac{1}{\varepsilon}\left(\Phi(\boldsymbol{n})_{j+1} - \Phi(\boldsymbol{n})_j\right)^2 + \varepsilon \sum_{j=0}^{N_T-1} U[\Phi_j]$$

In a compact 4D-space, the action becomes

$$S_E[\Phi] = \varepsilon a^3 \sum_{(\boldsymbol{n},n_4)\in\Lambda} \left(\frac{1}{2}\left(\frac{\Phi(\boldsymbol{n},n_4+1) - \Phi(\boldsymbol{n},n_4)}{\varepsilon}\right)^2 + \frac{1}{2}\sum_{j=1}^{3}\left(\frac{\Phi(\boldsymbol{n}+\hat{j},n_4) - \Phi(\boldsymbol{n}-\hat{j},n_4)}{2a}\right)^2 + \frac{m^2}{2}\Phi(\boldsymbol{n},n_4)^2 + V\left(\Phi(\boldsymbol{n},n_4)\right)\right)$$

Discretization error: $f(x \pm \epsilon) = f(x) \pm \epsilon f'(\epsilon) + \epsilon^2 f''(\epsilon)/2 \pm \epsilon^3 f'''(\epsilon)/6 + \cdots$

Forward difference: $\dfrac{f(x+\epsilon) - f(x)}{\epsilon} = f'(x) + \mathcal{O}(\epsilon)$

Central difference: $\dfrac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon} = f'(x) + \mathcal{O}(\epsilon^2)$

Partition function & correlators

Partition function:

$$Z_T^\varepsilon = C^{N^3 N_T} \int \mathcal{D}[\Phi]\, \mathrm{e}^{-S_E[\Phi]}\ , \quad \mathcal{D}[\Phi] = \prod_{(\boldsymbol{n},n_4)\in\Lambda} \mathrm{d}\,\Phi(\boldsymbol{n},n_4)$$

Correlation function:

$$\langle O_2(t)\, O_1(0)\rangle_T^\varepsilon = \frac{C^{N^3 N_T}}{Z_T^\varepsilon} \int \mathcal{D}[\Phi]\, \mathrm{e}^{-S_E[\Phi]}\, O_2[\Phi(.\,,n_t)]\, O_1[\Phi(.\,,0)]$$

- Functionals $O_2[\Phi(\,.\,,n_t)]$ and $O_1[\Phi(.,0)]$: lattice transcripts of operators $\hat{O}_2$ and $\hat{O}_1$ in the Hilbert space
- $O_2[\Phi(\,.\,,n_t)]$, $O_1[\Phi(.,0)]$ and $S_E[\Phi]$ are numbers but not operators
- Trivial factor $C^{N^3 N_T}$ cancels out in the correlation function

格点上的标量场

- 第一步: 连续的闵氏空间 ⇒ 离散的4D欧氏空间，格点间距为a；自由度 ⇒ 位于格点上的经典场变量$\mathbf{\Phi}$
- 第二步: 将欧氏空间的作用量 $S_E(\Phi)$ 离散化，并确认在$a \to 0$时能回到其在连续空间中的值。
- 第三步：关联函数中的算符转化为泛函：场算符⇒经典的格点场变量
- 第四步：在格点场组态上计算泛函从而得到关联函数。考虑所有可能出现的格点场组态，权重因子为玻尔兹曼因子$\exp(-S_E(\Phi))$

Brief review of QCD

Fermion action

$$S_F[\psi,\overline{\psi},A] = \sum_{f=1}^{N_f} \int \mathrm{d}^4x\, \overline{\psi}^{(f)}(x) \left(\gamma_\mu \left(\partial_\mu + \mathrm{i}\, A_\mu(x)\right) + m^{(f)}\right) \psi^{(f)}(x)$$

$$= \sum_{f=1}^{N_f} \int \mathrm{d}^4x\, \overline{\psi}^{(f)}(x)_{\substack{\alpha\\c}} \Big((\gamma_\mu)_{\alpha\beta} \left(\delta_{cd}\partial_\mu + \mathrm{i}\, A_\mu(x)_{cd}\right) + m^{(f)}\delta_{\alpha\beta}\delta_{cd} \Big) \psi^{(f)}(x)_{\substack{\beta\\d}}$$

α, β: Dirac index, 1,2,3,4   μ: Lorentz index, 1,2,3,4   c,d: color index, 1,2,3

Gauge action

$$S_G[A] = \frac{1}{2\,g^2} \int \mathrm{d}^4x\ \mathrm{tr}\left[F_{\mu\nu}(x)F_{\mu\nu}(x)\right] = \frac{1}{4\,g^2} \sum_{i=1}^{8} \int \mathrm{d}^4x\, F_{\mu\nu}^{(i)}(x) F_{\mu\nu}^{(i)}(x)$$

$$F_{\mu\nu}^{(i)}(x) = \partial_\mu A_\nu^{(i)}(x) - \partial_\nu A_\mu^{(i)}(x) - f_{ijk} A_\mu^{(j)}(x) A_\nu^{(k)}(x)$$

Invariant under gauge transformations:

$$\psi(x) \to \psi'(x) = \Omega(x)\psi(x), \quad \overline{\psi}(x) \to \overline{\psi}'(x) = \overline{\psi}(x)\Omega(x)^\dagger$$

$$A_\mu(x) \to A'_\mu(x) = \Omega(x)A_\mu(x)\Omega(x)^\dagger + \mathrm{i}\left(\partial_\mu \Omega(x)\right)\Omega(x)^\dagger$$

SU(3) matrix:

$$\Omega(x)^\dagger = \Omega(x)^{-1}$$

$$\det \Omega(x) = 1$$

Discretization of the fermion action

- Free fermion action (A =0):

$$S_F^0[\psi,\overline{\psi}] = \int \mathrm{d}^4x\, \overline{\psi}(x)\,(\gamma_\mu \partial_\mu + m)\,\psi(x)$$

$$\partial_\mu \psi(x) \;\rightarrow\; \frac{1}{2a}\left(\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})\right)$$

$$S_F^0[\psi,\overline{\psi}] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})}{2a} \;+\; m\,\psi(n) \right)$$

- Not gauge invariant:

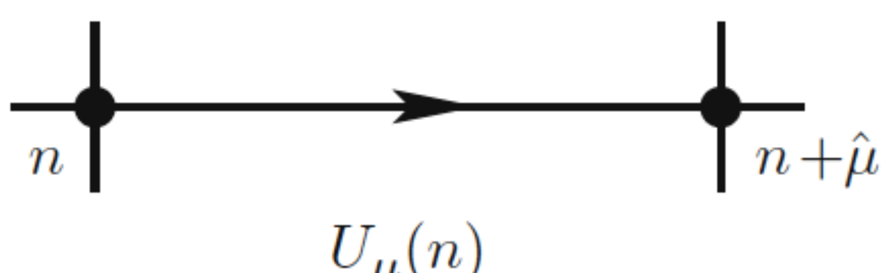
$$\psi(x) \rightarrow \psi'(x) = \Omega(x)\psi(x) \qquad \overline{\psi}(x) \rightarrow \overline{\psi}'(x) = \overline{\psi}(x)\Omega(x)^\dagger$$

$$\overline{\psi}(n)\psi(n+\hat{\mu}) \rightarrow \overline{\psi}'(n)\,\psi'(n+\hat{\mu}) = \overline{\psi}(n)\,\Omega(n)^\dagger\,\Omega(n+\hat{\mu})\,\psi(n+\hat{\mu})$$

- Introduction of a gauge link：

$$\overline{\psi}'(n)\,U'_\mu(n)\,\psi'(n+\hat{\mu}) \;=\; \overline{\psi}(n)\,\Omega(n)^\dagger\,U'_\mu(n)\,\Omega(n+\hat{\mu})\,\psi(n+\hat{\mu})$$

$$U_\mu(n) \;\rightarrow\; U'_\mu(n) = \Omega(n)\,U_\mu(n)\,\Omega(n+\hat{\mu})^\dagger$$



$$U_\mu(n) = \exp\left(\mathrm{i}\,aA_\mu(n)\right)$$

Doubler problem & Wilson fermion action

Naïve fermion action: $$S_F[\psi,\overline{\psi},U] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(n)\psi(n+\hat{\mu}) - U_{-\mu}(n)\psi(n-\hat{\mu})}{2a} + m\,\psi(n) \right)$$

$$S_F[\psi,\overline{\psi},U] = a^4 \sum_{n,m\in\Lambda} \sum_{a,b,\alpha,\beta} \overline{\psi}(n)_{\substack{\alpha\\a}} D(n|m)_{\substack{\alpha\beta\\ab}} \psi(m)_{\substack{\beta\\b}}$$

$$D(n|m)_{\substack{\alpha\beta\\ab}} = \sum_{\mu=1}^{4} (\gamma_\mu)_{\alpha\beta} \frac{U_\mu(n)_{ab}\,\delta_{n+\hat{\mu},m} - U_{-\mu}(n)_{ab}\,\delta_{n-\hat{\mu},m}}{2a} + m\,\delta_{\alpha\beta}\,\delta_{ab}\,\delta_{n,m}$$

Propagator: $$\widetilde{D}(p)^{-1}\Big|_{m=0} = \frac{-\mathrm{i}a^{-1}\sum_\mu \gamma_\mu \sin(p_\mu a)}{a^{-2}\sum_\mu \sin(p_\mu a)^2} \xrightarrow{a\to 0} \frac{-\mathrm{i}\sum_\mu \gamma_\mu p_\mu}{p^2}$$

$$\frac{sin(p_\mu a)}{a} \to p_\mu$$

physical poles: $p = (0,\, 0,\, 0,\, 0)$

unwanted poles,doublers: $p = (\pi/a, 0, 0, 0)\ ,\ (0, \pi/a, 0, 0)\ ,\ \ldots\ ,(\pi/a, \pi/a, \pi/a, \pi/a)$

Wilson fermion matrix: $$\widetilde{D}(p) = m\mathbb{1} + \frac{\mathrm{i}}{a}\sum_{\mu=1}^{4} \gamma_\mu \sin(p_\mu a) + \mathbb{1}\frac{1}{a}\sum_{\mu=1}^{4}(1-\cos(p_\mu a))$$

Wilson term

Wilson term vanishes when p_μ =0 and gives an extra mass l/a (infinity at a=0)

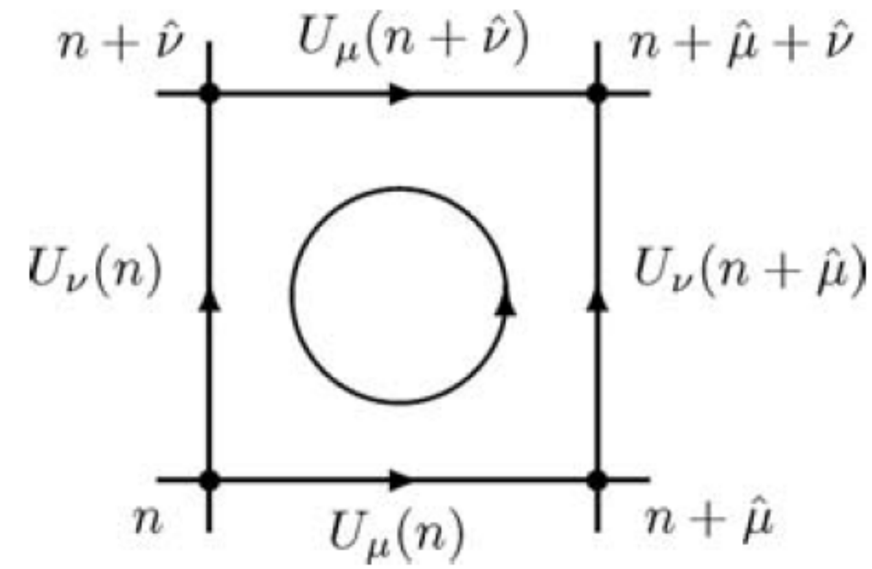
Wilson fermion action: $$S_F[\psi,\overline{\psi},U] = \sum_{f=1}^{N_f} a^4 \sum_{n,m\in\Lambda} \overline{\psi}^{(f)}(n)\, D^{(f)}(n|m)\, \psi^{(f)}(m)$$

$$D^{(f)}(n|m)_{\substack{\alpha\beta\\ab}} = \left(m^{(f)} + \frac{4}{a}\right)\delta_{\alpha\beta}\,\delta_{ab}\,\delta_{n,m} - \frac{1}{2a}\sum_{\mu=\pm1}^{\pm4}(\mathbb{1}-\gamma_\mu)_{\alpha\beta}\,U_\mu(n)_{ab}\,\delta_{n+\hat{\mu},m}$$

Wilson gauge action

Plaquette: $U_{\mu\nu}(n) = U_\mu(n)\, U_\nu(n+\hat{\mu})\, U_{-\mu}(n+\hat{\mu}+\hat{\nu})\, U_{-\nu}(n+\hat{\nu})$

smallest Wilson loop that is gauge invariant



Wilson gauge action:

$$S_G[U] = \frac{2}{g^2} \sum_{n\in\Lambda} \sum_{\mu<\nu} \mathrm{Re}\ \mathrm{tr}\left[\mathbb{1} - U_{\mu\nu}(n)\right]$$

Problem: Derive the gauge action in the continuum limit with an order a^2 correction

$$S_G[U] = \frac{a^4}{2\,g^2} \sum_{n\in\Lambda} \sum_{\mu,\nu} \mathrm{tr}[F_{\mu\nu}(n)^2] + \mathcal{O}(a^2)$$

The above the above equation can be obtained with the help of

$$U_\mu(n) = \exp\left(\mathrm{i}\, a A_\mu(n)\right), \quad \exp(A)\,\exp(B) = \exp\left(A + B + \frac{1}{2}[A,B] + \cdots\right)$$

Staggered fermions (交错费米子)

Naïve fermions: $$S_F[\psi,\overline{\psi}] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})}{2a} + m\,\psi(n) \right)$$

staggered transformation: $$\psi(n) = \gamma_1^{n_1}\,\gamma_2^{n_2}\,\gamma_3^{n_3}\,\gamma_4^{n_4}\,\psi(n)' \,, \quad \overline{\psi}(n) = \overline{\psi}(n)'\,\gamma_4^{n_4}\,\gamma_3^{n_3}\,\gamma_2^{n_2}\,\gamma_1^{n_1}$$

$$\overline{\psi}(n)\,\gamma_3\,\psi(n\pm\hat{3}) = (-1)^{n_1+n_2}\,\overline{\psi}(n)'\mathbb{1}\psi(n\pm\hat{3})'$$

$$S_F\left[\psi',\overline{\psi}'\right] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n)'\mathbb{1} \left(\sum_{\mu=1}^{4} \eta_\mu(x) \frac{\psi(n+\hat{\mu})' - \psi(n-\hat{\mu})'}{2\,a} + m\,\psi(n)' \right)$$

$$\eta_1(n) = 1 \,,\; \eta_2(n) = (-1)^{n_1} \,,\; \eta_3(n) = (-1)^{n_1+n_2} \,,\; \eta_4(n) = (-1)^{n_1+n_2+n_3}$$

staggered fermion action: keeping 1 of 4 identical Dirac components

$$S_F[\chi,\overline{\chi}] = a^4 \sum_{n\in\Lambda} \overline{\chi}(n) \left(\sum_{\mu=1}^{4} \eta_\mu(x) \frac{U_\mu(n)\chi(n+\hat{\mu}) - U_\mu^\dagger(n-\hat{\mu})\chi(n-\hat{\mu})}{2\,a} + m\chi(n) \right)$$

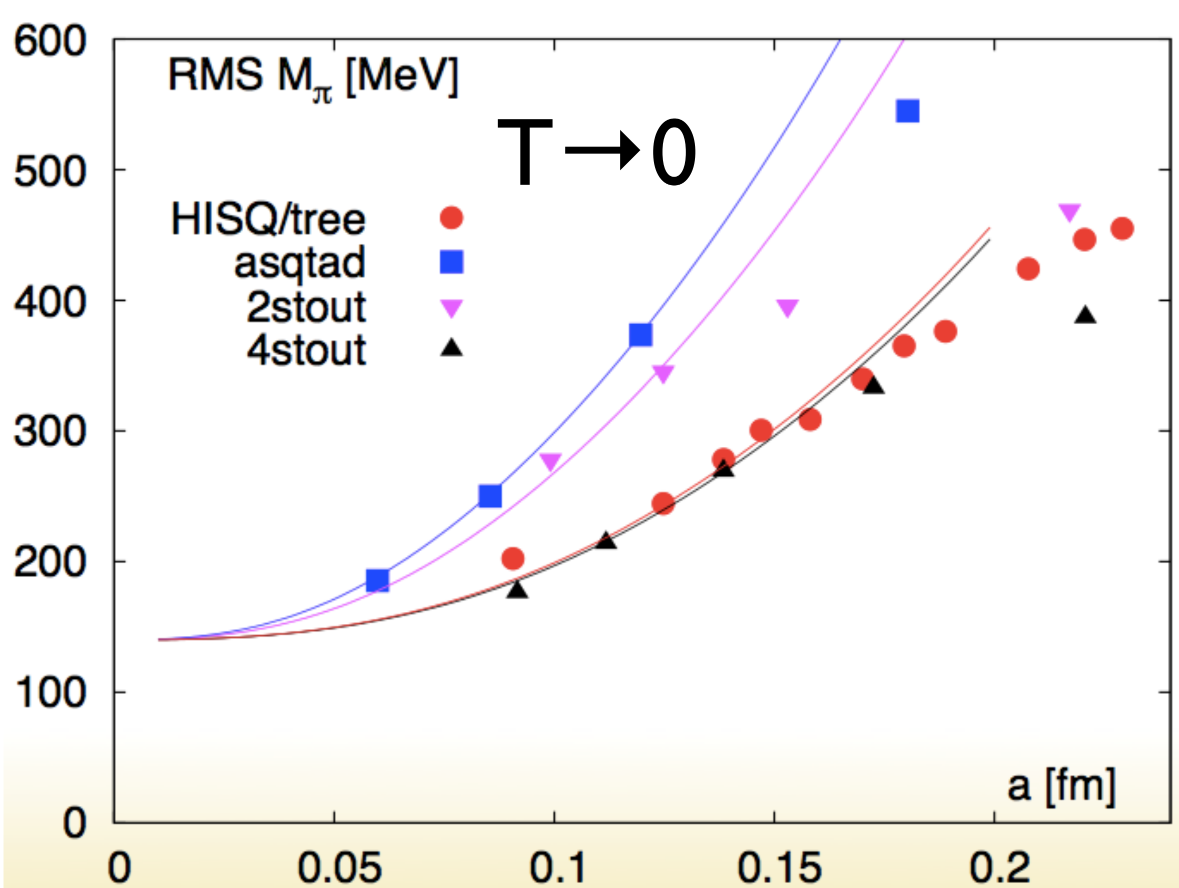
$\chi(n)$:Grassmann-valued fields with only color indices but without Dirac structure

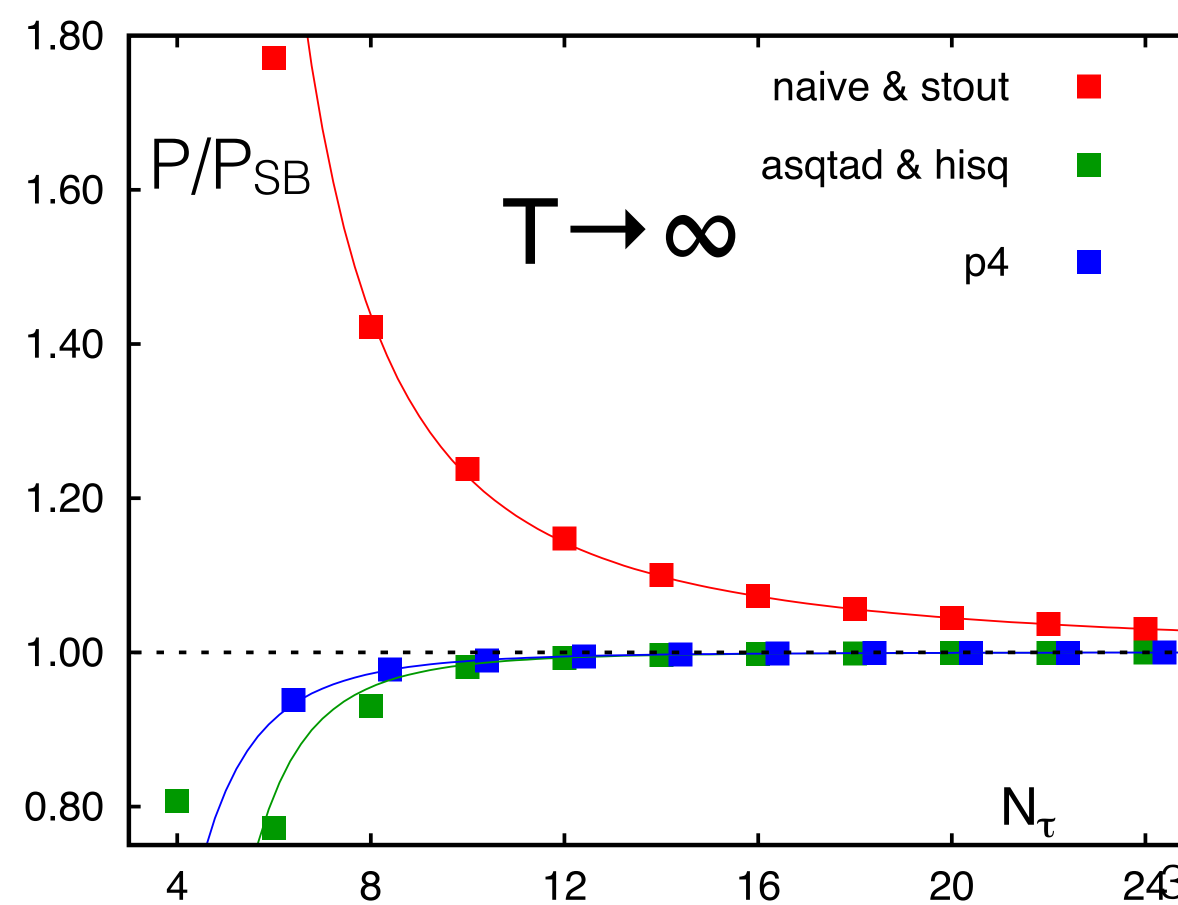
16 -> 4 tastes (doublers)

风(taste)自由度：中文翻译取自刘川《格点量子色动力学导论》

Taste symmetry breaking of staggered fermions

action(group)	improvements at T→0	improvements at T→∞
naïve (Mumbai)	none	none
p4(BNL-Bi)	poor	very good
asqtad(hotQCD)	ok	good
2stout(WB)	good	none
4stout(WB)	very good	none
HISQ(hotQCD)	very good	good





Chiral symmetry of QCD

$$S_F[\psi,\overline{\psi},A] = \int \mathrm{d}^4x\, L\left(\psi,\overline{\psi},A\right),\;\; L\left(\psi,\overline{\psi},A\right) = \overline{\psi}\,\gamma_\mu\left(\partial_\mu + \mathrm{i}\,A_\mu\right)\psi = \overline{\psi}\,D\psi$$

D: massless Dirac operator

Chiral rotation: $\psi \;\rightarrow\; \psi' = \mathrm{e}^{\mathrm{i}\alpha\gamma_5}\psi\;,\quad \overline{\psi} \;\rightarrow\; \overline{\psi}' = \overline{\psi}\,\mathrm{e}^{\mathrm{i}\alpha\gamma_5}$

- Lagrangian density is invariant under the chiral rotation:

$$L\left(\psi',\overline{\psi}',A\right) = \overline{\psi}'\,\gamma_\mu\left(\partial_\mu + \mathrm{i}\,A_\mu\right)\psi' = \overline{\psi}\,\mathrm{e}^{\mathrm{i}\alpha\gamma_5}\,\gamma_\mu\left(\partial_\mu + \mathrm{i}\,A_\mu\right)\mathrm{e}^{\mathrm{i}\alpha\gamma_5}\,\psi$$
$$= \overline{\psi}\,\mathrm{e}^{\mathrm{i}\alpha\gamma_5}\mathrm{e}^{-\mathrm{i}\alpha\gamma_5}\,\gamma_\mu\left(\partial_\mu + \mathrm{i}\,A_\mu\right)\psi = L\left(\psi,\overline{\psi},A\right)$$

- A mass term explicitly breaks the chiral symmetry: $m\,\overline{\psi}'\psi' = m\,\overline{\psi}\,\mathrm{e}^{i2\alpha\gamma_5}\,\psi$

$$P_R = \frac{\mathbb{1}+\gamma_5}{2}\,,\quad P_L = \frac{\mathbb{1}-\gamma_5}{2}$$
$$\psi_R = P_R\,\psi\,,\quad \psi_L = P_L\,\psi$$
$$\overline{\psi}_R = \overline{\psi}\,P_L\,,\quad \overline{\psi}_L = \overline{\psi}\,P_R$$

$\Rightarrow$

$$L\left(\psi,\overline{\psi},A\right) = \overline{\psi}_L\,D\,\psi_L + \overline{\psi}_R\,D\,\psi_R$$
$$m\,\overline{\psi}\,\psi = m\,\left(\overline{\psi}_R\,\psi_L + \overline{\psi}_L\,\psi_R\right)$$

- Essence of chiral symmetry: $D\,\gamma_5 + \gamma_5\,D = 0$

chiral symmetry on the lattice

- Massless Wilson Dirac operator breaks chiral symmetry

$$D^f(n|m)_{\alpha\beta,ab} = \frac{4}{a}\,\delta_{\alpha\beta}\delta_{ab}\delta_{n,m} - \frac{1}{2a}\sum_{\mu=\pm1}^{\pm4}(1-\gamma_\mu)_{\alpha\beta}\,U_\mu(n)_{ab}\,\delta_{n+\hat{\mu},m}$$

$$\gamma_5^\dagger = \gamma_5,\ \ \gamma_5^2 = 1\,,\ \{\gamma_5, \gamma_\mu\} = 0$$

- The Ginsparg-Wilson equation

$$D\,\gamma_5 + \gamma_5\,D = a\,D\,\gamma_5\,D \quad \xrightarrow{\text{lattice spacing } a \to 0} \quad D\,\gamma_5 + \gamma_5\,D = 0$$

- Lattice fermion satisfy the Ginsparg-Wilson equation preserve the chiral symmetry at nonzero lattice spacing

chiral rotation on the lattice

$$\psi' = \exp\left(\mathrm{i}\,\alpha\,\gamma_5\left(\mathbb{1} - \frac{a}{2}D\right)\right)\psi\,, \quad \overline{\psi}' = \overline{\psi}\exp\left(\mathrm{i}\,\alpha\left(\mathbb{1} - \frac{a}{2}D\right)\gamma_5\right)$$

Problem: Derive

$$\begin{aligned} L\left(\psi', \overline{\psi}'\right) = \overline{\psi}'\,D\,\psi' &= \overline{\psi}\,\exp\left(\mathrm{i}\,\alpha\left(\mathbb{1} - \frac{a}{2}D\right)\gamma_5\right)D\,\exp\left(\mathrm{i}\,\alpha\,\gamma_5\left(\mathbb{1} - \frac{a}{2}D\right)\right)\psi \\ &= \overline{\psi}\,\exp\left(\mathrm{i}\,\alpha\left(\mathbb{1} - \frac{a}{2}D\right)\gamma_5\right)\exp\left(-\mathrm{i}\,\alpha\left(\mathbb{1} - \frac{a}{2}D\right)\gamma_5\right)D\,\psi \\ &= \overline{\psi}\,D\,\psi = L\left(\psi, \overline{\psi}\right) \end{aligned}$$

chiral symmetry on the lattice

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Problem: Derive

$$\widehat{P}_R = \frac{\mathbb{1}+\widehat{\gamma}_5}{2}\,,\quad \widehat{P}_L = \frac{\mathbb{1}-\widehat{\gamma}_5}{2}\,,\quad \widehat{\gamma}_5 = \gamma_5\,(\mathbb{1}-a\,D)$$

$$\widehat{P}_R^2 = \widehat{P}_R\,,\quad \widehat{P}_L^2 = \widehat{P}_L\,,\quad \widehat{P}_R\,\widehat{P}_L = \widehat{P}_L\,\widehat{P}_R = 0\,,\quad \widehat{P}_R + \widehat{P}_L = \mathbb{1}$$

$$\psi_R = \widehat{P}_R\,\psi\,,\quad \psi_L = \widehat{P}_L\,\psi\,,\quad \overline{\psi}_R = \overline{\psi}\,P_L\,,\quad \overline{\psi}_L = \overline{\psi}\,P_R$$

$$\overline{\psi}D\,\psi = \overline{\psi}_L\,D\,\psi_L + \overline{\psi}_R\,D\,\psi_R$$

chiral fermions on the lattice

- Overlap fermion operator D_{ov} : only operator that satisfies the Ginsparg-Wilson equation

$$D_{\rm ov} = \frac{1}{a}\left(\mathbb{1} + \gamma_5\,{\rm sign}[H]\right)\,,\ {\rm sign}(H) = H|H|^{-1} = H(H^2)^{-\frac{1}{2}}\,,\ H = \gamma_5\,A$$

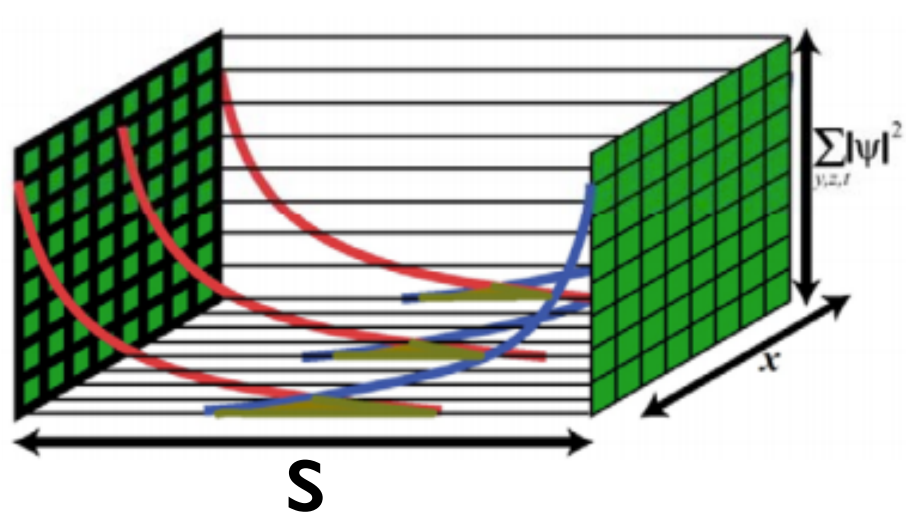
A denotes some suitable γ_5-hermitian "kernel" Dirac operator

large numerical cost due to the evaluation of $(HH^+)^{-1/2}$

costs ≳ 100 x costs of Wilson formulation

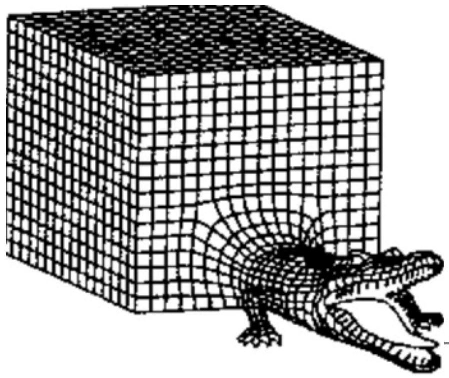
- Domain Wall fermions: introduce the fictitious 5th dimension of extent N_5

preserve exact chiral symmetry as $N_5 \to \infty$. Residual symmetry breaking is quantified by the additive renormalization factor m_{res} to the quark mass



costs ≳ N_5 x costs of Wilson formulation

N_5 = 16-64

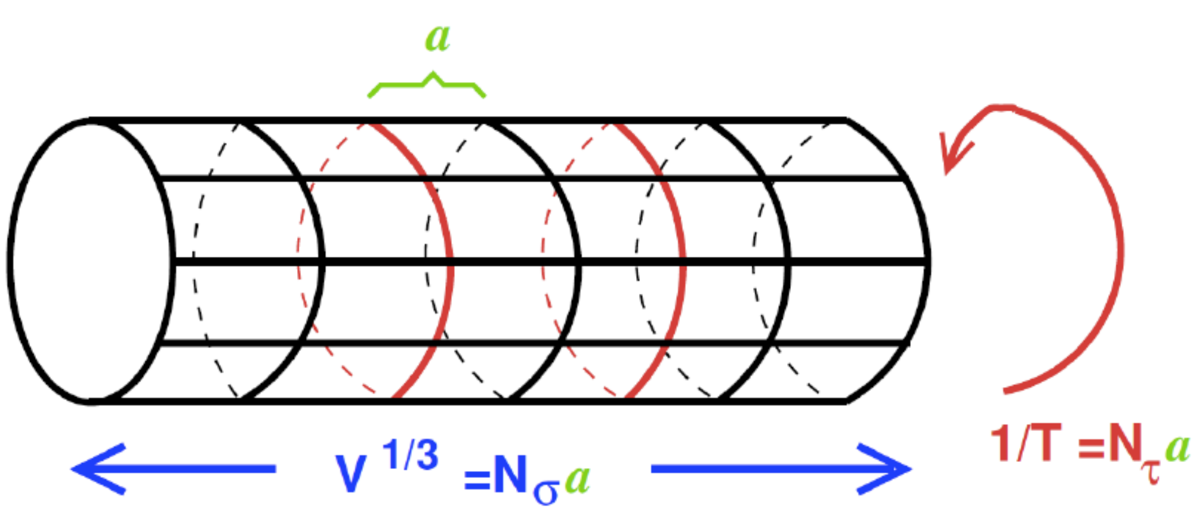


Recap: Discretization schemes

Discretization schemes	Chiral symmetry	Cost	Collaborations
Wilson fermions	Explicitly broken	OK	CLQCD, ETMC, HALQCD, FlowQCD, PACS,...
Improved Staggered fermions	Partially reserved	Cheap	MILC, HotQCD, CLQCD, NPQCD, BMW,...
Domain Wall fermions	Almost reserved	Expensive	JLQCD, RBRC, UKQCD, TWQCD,...
Overlap fermions	Exactly reserved	Very expensive	chiQCD, Bielefeld-Chenai,...

To recover QCD, thermodynamic and continuum limits are required!

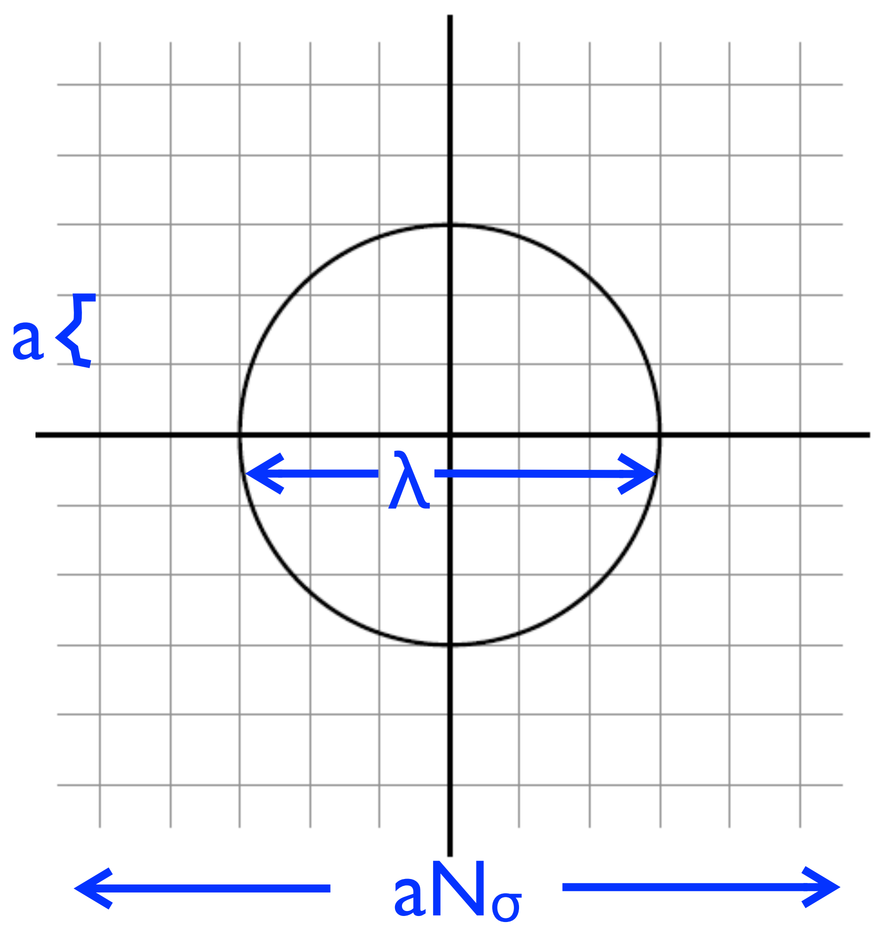
setup of Lattice QCD simulations



- Discretization schemes: Wilson, staggered…
- Four dim. Euclidean lattice: $N_\sigma^3 \times N_\tau$
- Temperature: $T = 1/(aN_\tau)$

UV cut: 1/a, IR cut: $1/(aN_\sigma)$

$$a \ll \lambda \ll aN_\sigma$$



Thermodynamic limit: $V \equiv (aN_\sigma)^3 \to \infty$
Continuum limit: $a \to 0$

Input parameters

- lattice gauge coupling: $\beta \equiv 6/g^2$
- quark masses: $am_u, am_d, am_s, am_c, \cdots$
- lattice size: N_τ, N_σ

No free parameters
input bare parameters of QCD Lagrangian
fixed by reproducing e.g. M_π, M_K etc

Current hot & dense lattice QCD simulations

Lattice QCD: discretized version of QCD on a Euclidean space-time lattice, reproduces QCD when lattice spacing a→0 (continuum limit)

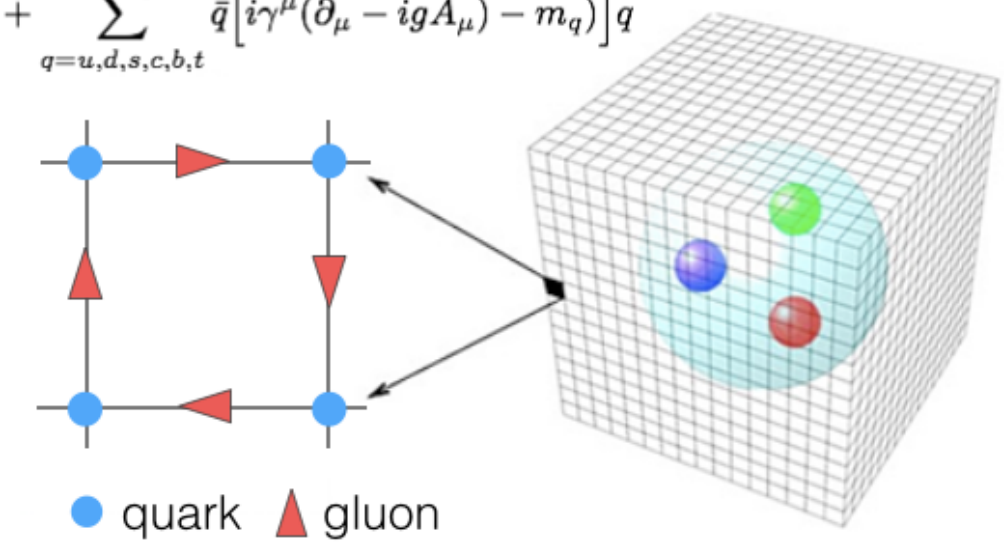
Mostly dynamical QCD with N_f=2+1 and physical pion mass

- Staggered actions at a≠0: taste symmetry breaking
  - 1 physical Goldstone pion +15 heavier unphysical pions
  - averaged pion mass, i.e. Root Mean Squared (RMS) pion mass
  - Smaller RMS pion mass → Better improved action: HISQ, stout
- Chiral fermions(Domain Wall/Overlap) at a≠0
  - preserves full flavor symmetry and chiral symmetries
  - computationally expensive to simulate, currently starts to produce interesting results on QCD thermodynamics

The lattice QCD Path integral

QCD Lagrangian

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q}\left[i\gamma^{\mu}(\partial_{\mu} - igA_{\mu}) - m_q\right]q$$



Discretization in
Euclidean space

quarks: lattice sites
gluons: lattice links

Supercomputing the QCD matter:

structural equivalence
between
statistical mechanics
& QFT on the lattice

$$< \mathcal{O} > = \frac{1}{Z} \int \mathcal{D}\mathcal{U}\ \mathcal{D}\psi\ \mathcal{D}\bar{\psi}\ \mathcal{O}\ e^{-S_{lat}}$$

$$S_{lat} = S_g + S_f$$

$$Z = \int \mathcal{D}\mathcal{U}\ \mathcal{D}\psi\ \mathcal{D}\bar{\psi}\ e^{-S_{lat}} = \int \mathcal{D}\mathcal{U}\ e^{-S_g}\ \det M_f$$

$N_c \otimes N_f \otimes N_{spin} \otimes N_d \otimes N_\sigma \otimes N_\tau^3 \gtrsim 10^6$

det M_f = 1: Quenched approximation

det M_f =/= 1: dynamic/full QCD simulation

格点量子色动力学模拟

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\mathcal{U} \ \mathrm{det M_f} \ \mathcal{O} \ \exp(-S_G) \ , \quad Z = \int \mathcal{D}\mathcal{U} \ \mathrm{det M_f} \ \exp(-S_G)$$

重要抽样： $$\mathrm{d}P(U) = \frac{\det \mathrm{M_f} \ e^{-S_G[U]} \mathcal{D}[U]}{\int \mathcal{D}[U] \ \det \mathrm{M_f} \ e^{-S_G[U]}}$$

$$\langle \mathcal{O} \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}[U_n]$$

U

U_n: 组态

格点计算步骤：

1. 产生组态(gauge configurations)
2. 基于组态计算特定观测量
3. 抽取物理

类比实验研究中的
加速器
探测器
数据分析

格点量子色动力学：求解大型稀疏矩阵(M)的逆

- 手征凝聚 (chiral condensate)

$$\langle \bar{q}q \rangle = \frac{\partial \ln Z}{\partial m_q} = \frac{n_f}{4} \langle \mathrm{Tr} M^{-1} \rangle$$

Conjugate Gradient

$M \, \mathrm{x} = y$

$\mathrm{x} = M^{-1} y$

矩阵大小 10^9！

- lnZ对化学势μ的偏导 (general susceptibility)

$$\frac{\partial^2 \ln Z}{\partial \mu^2} = \left\langle \frac{n_f}{4} \frac{\partial^2 (\ln \det \mathrm{M})}{\partial \mu^2} \right\rangle + \left\langle \left(\frac{n_f}{4} \frac{\partial (\ln \det \mathrm{M})}{\partial \mu} \right)^2 \right\rangle$$

$$\mathrm{Tr}\left(M^{-1} \frac{\partial^2 M}{\partial \mu^2} \right) - \mathrm{Tr}\left(M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} \right) \qquad \mathrm{Tr}\left(M^{-1} \frac{\partial M}{\partial \mu} \right)$$

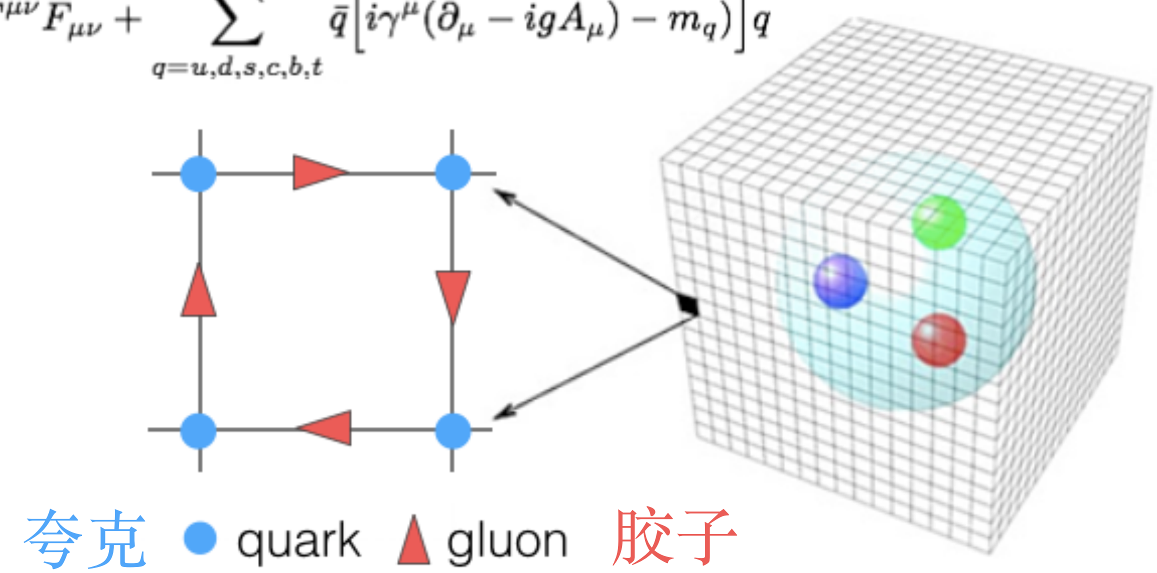
一般需要10^7次求逆

回顾：格点量子色动力学

第一性原理出发的(从头开始算)、系统地研究QCD非微扰性质的理论方法

QCD Lagrangian 量子色动力学拉格朗日量

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q}\left[i\gamma^{\mu}(\partial_{\mu} - igA_{\mu}) - m_q\right]q$$



- 将欧氏时空离散化为有一定间距的格子
- 夸克放在点上，胶子作为点与点之间的连线
- 将作用量离散化(Wilson, staggered etc)，定义路径积分的量度
- 定义可观测的物理量

连续极限+热力学极限回到QCD

计算资源主要用在：计算大型稀疏矩阵的逆

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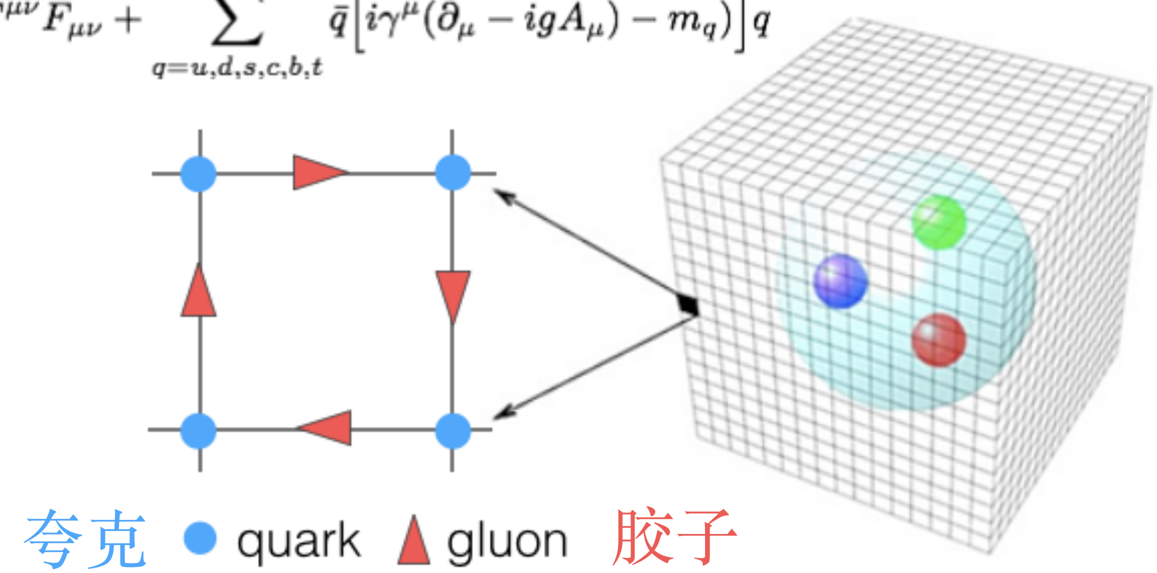

格点计算步骤：

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2. 基于组态计算特定观测量
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类比实验研究中的

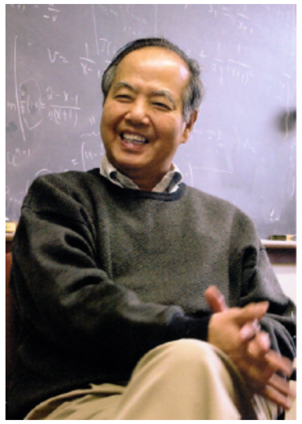
加速器

探测器

数据分析

课程目标

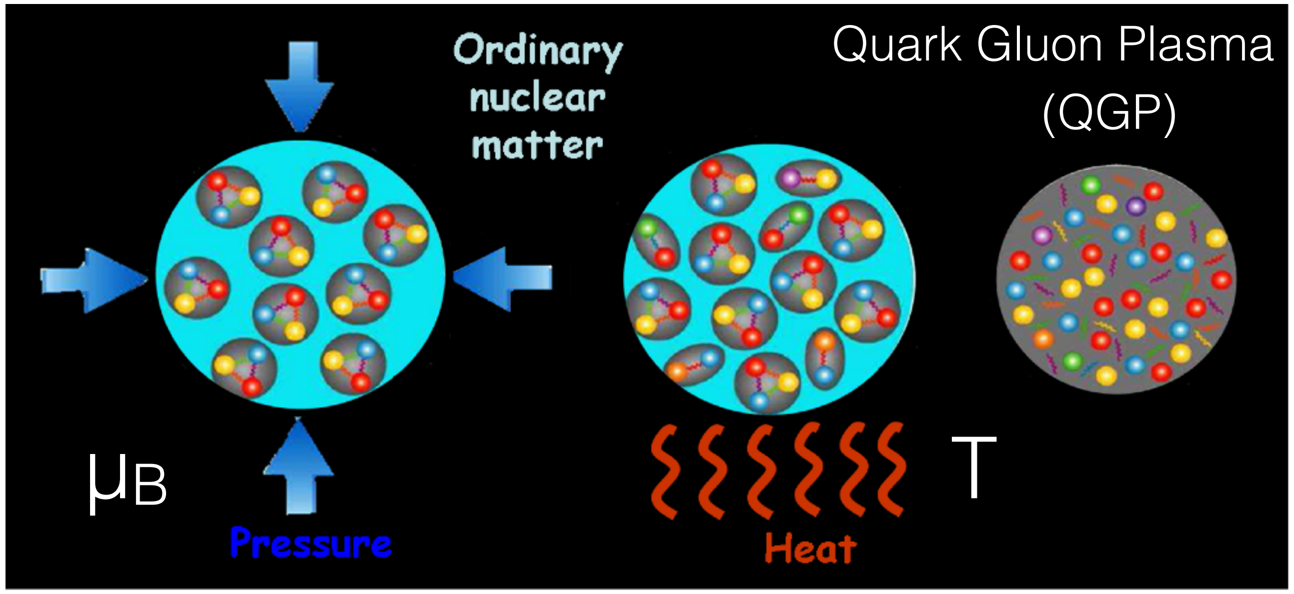
- 介绍格点QCD基础，了解其非微扰定义
  - ✤ “Quantum Chromodynamics on the Lattice”, C. Gattringer & C. B. Lang, Springer 2010
  - ✤ “Lattice QCD for Novices”, G. Peter Lepage, arXiv:hep-lat/0506036
  - ✤ 格点量子色动力学导论，刘川，北京大学出版社, 2017
- 看懂有限温度密度格点QCD相关文献： famous plots
  - ✤ “Thermodynamics of strong-interaction matter from Lattice QCD”, 丁亨通, F. Karsch, S. Mukherjee, arXiv:1504.05274
  - ✤ Conference proceedings in the annual “lattice conference”
    - Lattice 2018, Michigan, USA
    - Lattice 2019, CCNU, Wuhan, China
    - Lattice 2021, MIT, USA
    - Lattice 2022, Bonn, Germany
    - …



真空激发——实验室中产生新的物质形态?!

找到丢失的对称性?

夸克胶子等离子体



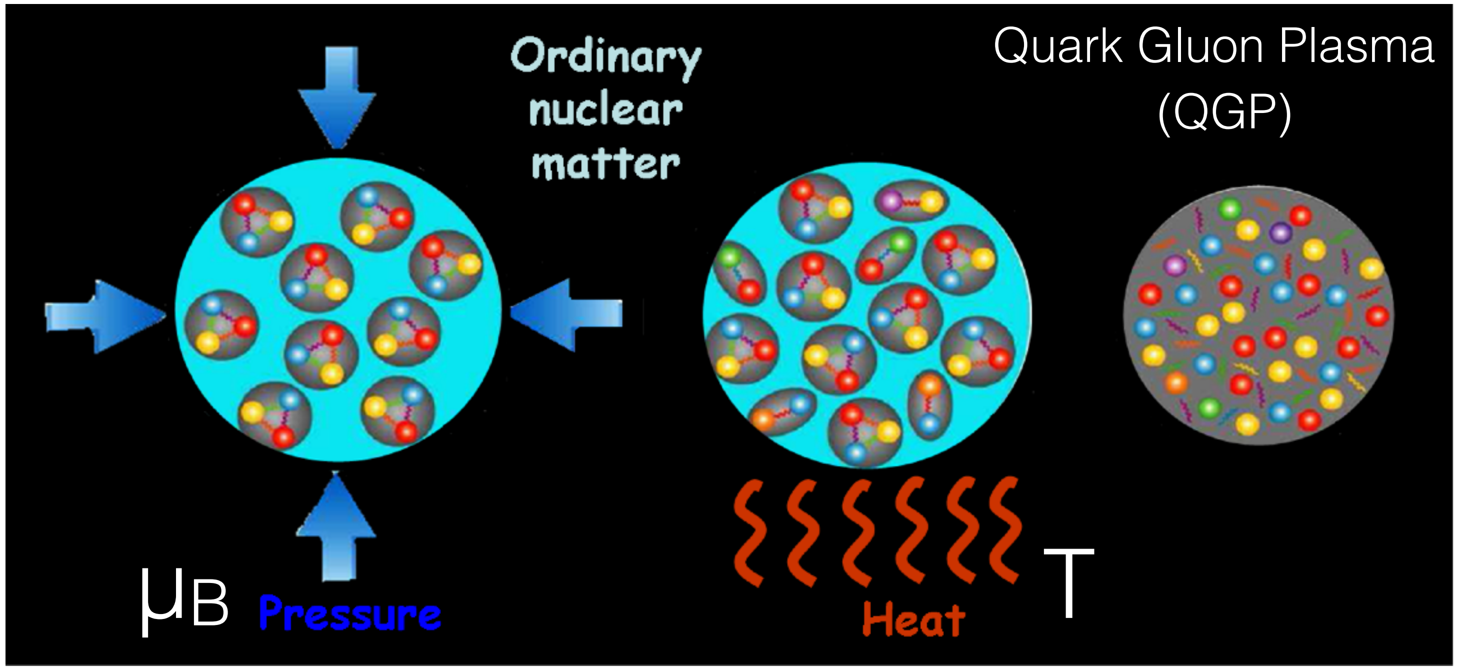
“The whole is more than sum of its parts.”
Aristotle, Metaphysica 10f-1045a

从还原论到整体论

“核子重如牛，对撞生新态。”

Ink painting masterpiece 1986:
"Nuclei as Heavy as Bulls, Through Collision
Generate New States of Matter”,
by Li Keran,
reproduced from open source works of T.D.Lee.

Symmetry restoration in extreme conditions: QCD phase transitions



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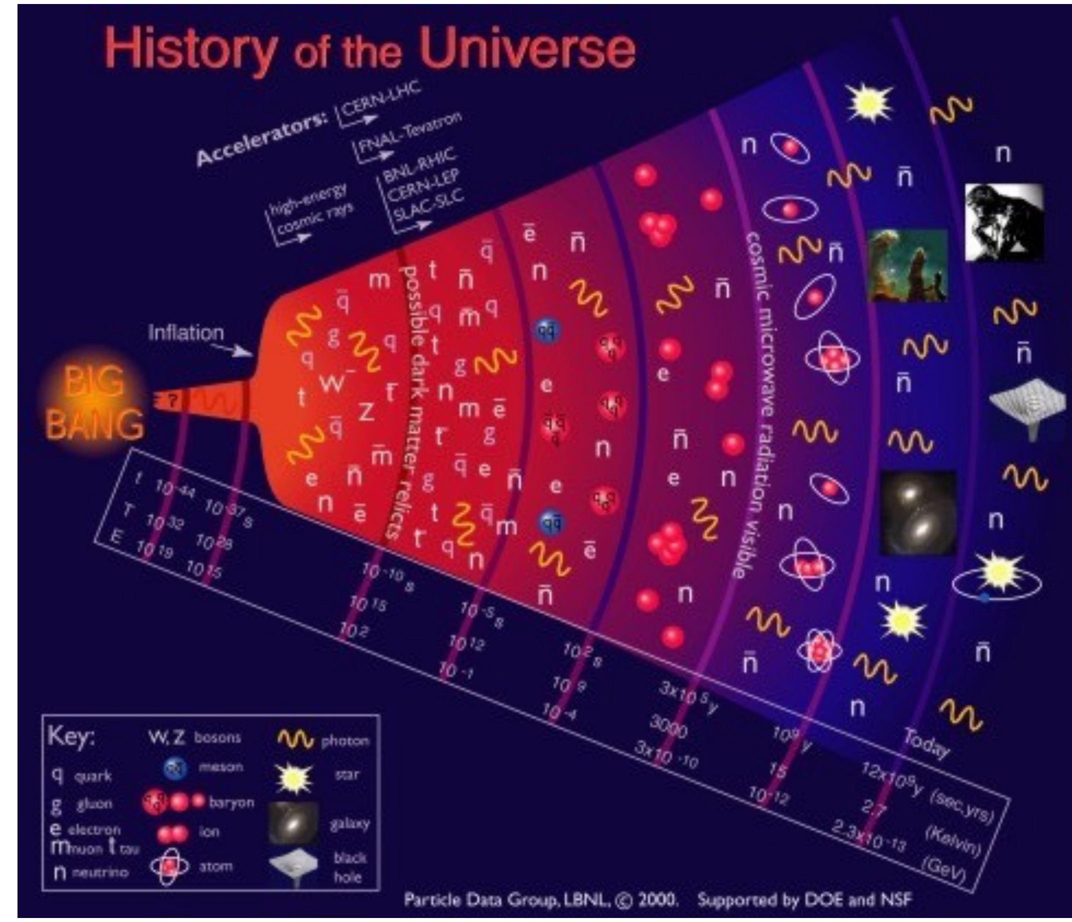
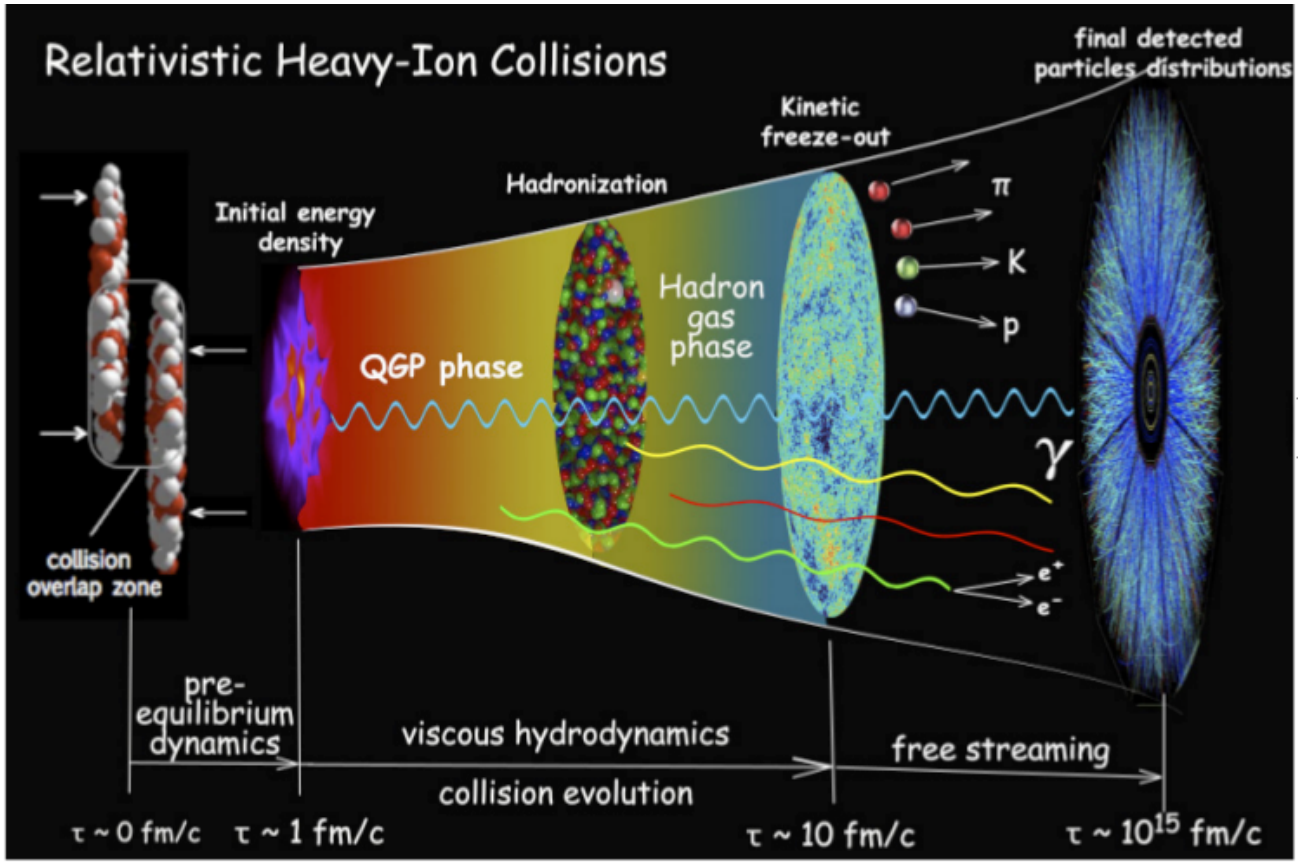


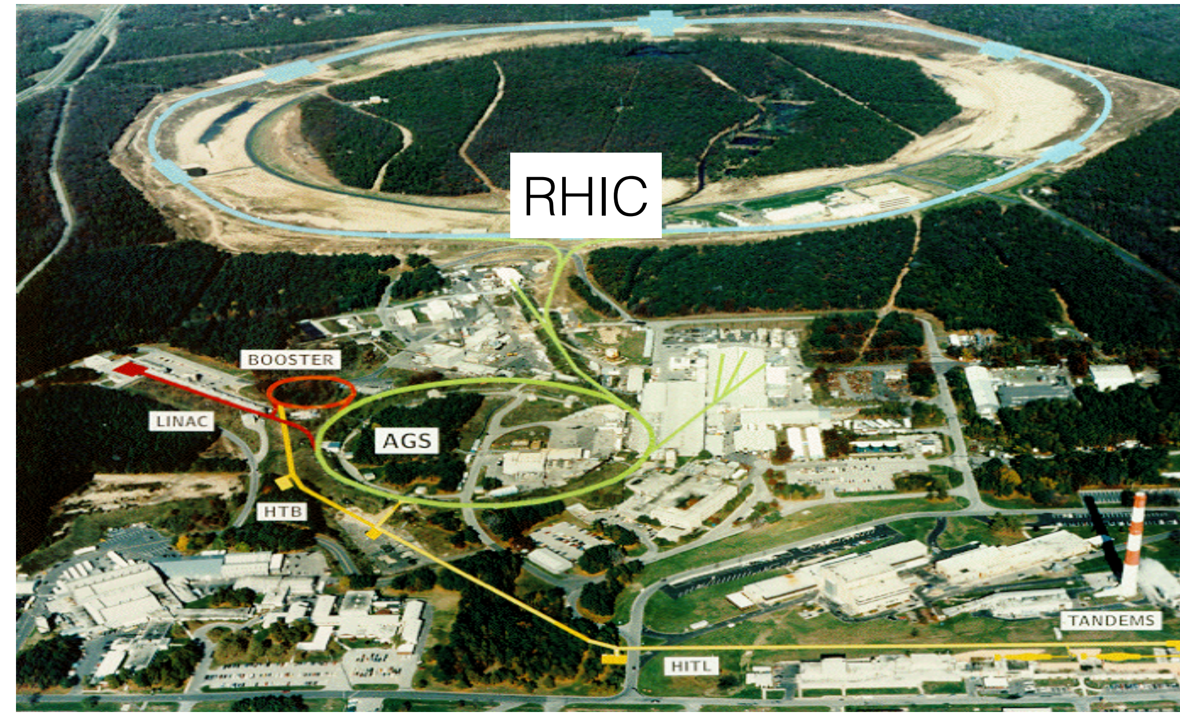
What are the phases of strong-interaction matter and what roles do they play in cosmos?

What are the T_c, orders and universality classes of (chiral & deconfinement) phase transitions?

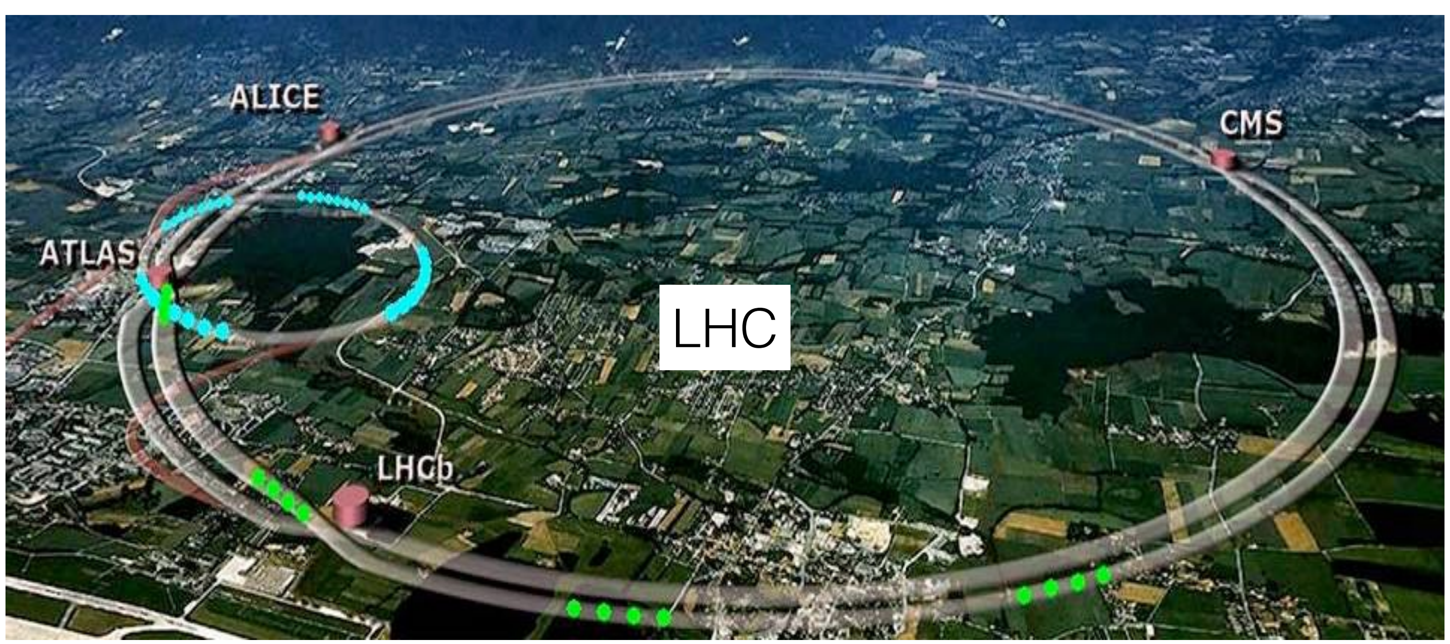
What does QCD predict for the properties of the strong-interaction matter in extreme conditions?

实验室中的“小爆炸”: 重新产生夸克胶子等离子体

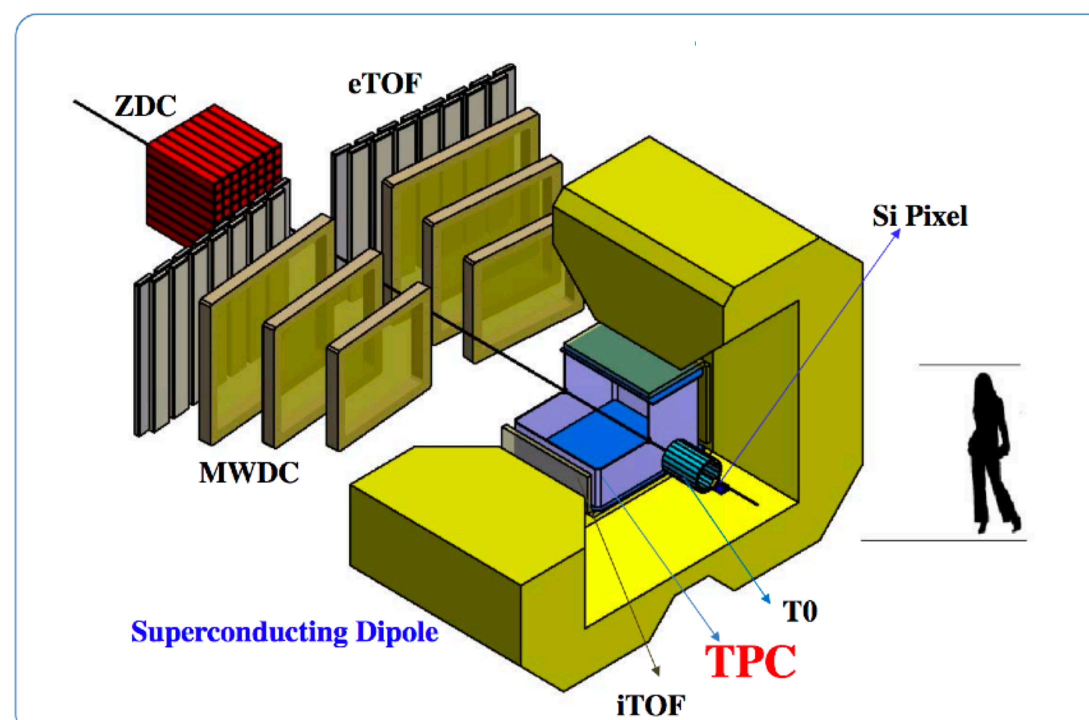




相对论重离子对撞机 (Relativistic Heavy Ion Collider)
@美国布鲁克海文国家实验室



大型强子对撞机(Large Hadron Collider)@欧洲核子研究中心



冷密核物质测量谱仪(CEE)@中科院近代物理研究所

华中师范大学核科学计算中心

Nuclear Science Computing Center at CCNU

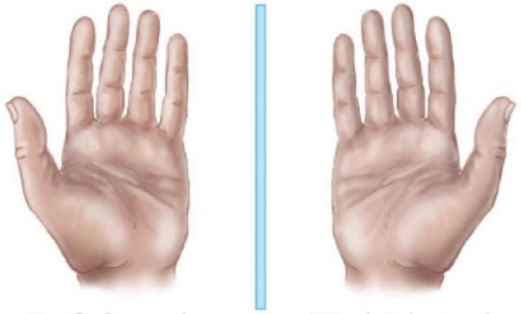
- 简称： **NSC³**

N: Nuclear， **S**: Science， **C³**: Color 3 -> QCD

强相互作用理论(QCD)中夸克带有红绿蓝三种颜色

“道生一，一生二，二生三，三生万物” —- 《道德经》老子 600 BC

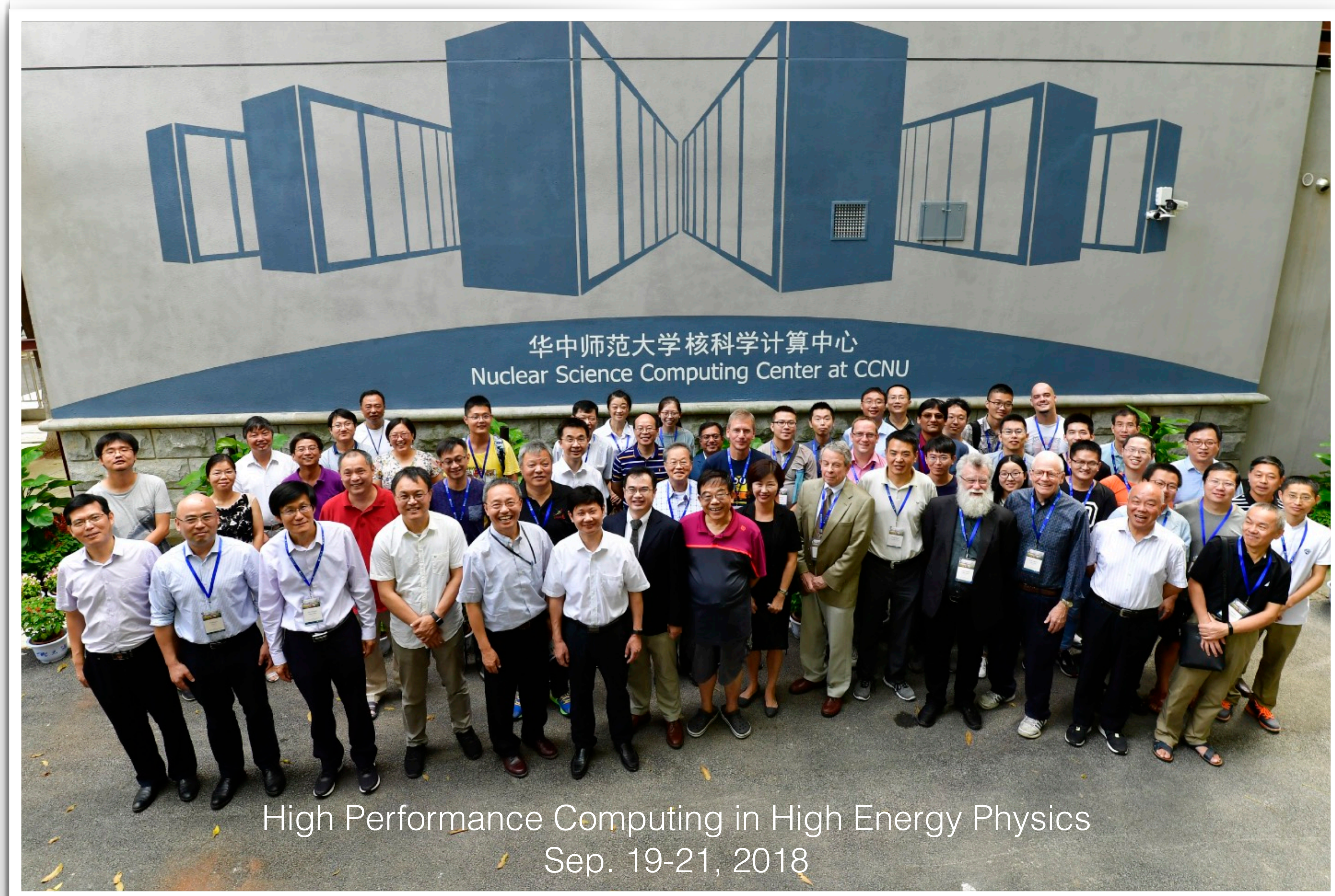
Confinement	**C**hirality	**C**riticality
禁闭	手征	临界行为



华中师范大学核科学计算中心
Nuclear Science Computing Center at CCNU

计算决定未来

国内首个有限温度格点QCD专用超算平台，2018年成立



43 computing nodes
(304 V100 +40 A100 GPUs)

Peak performance:
3 PFlops/s
(每秒3千万亿次浮点运算)

Storage:
6PB

June, 2021 TOP 500 The List. The GREEN 500

华中师范大学核科学计算中心
Nuclear Science Computing Center at CCNU

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综述文章

THERMODYNAMICS OF STRONG-INTERACTION MATTER FROM LATTICE QCD

利用格点QCD研究强相互作用物质的热力学性质

Heng-Tong Ding

Key Laboratory of Quark & Lepton Physics (MOE), Institute of Particle Physics, Central China Normal University, Wuhan, 430079, China

Frithjof Karsch

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We review results from lattice QCD calculations on the thermodynamics of strong-interaction matter with emphasis on input these calculations can provide to the exploration of the phase diagram and properties of hot and dense matter created in heavy ion experiments. This review is organized as follows:

1) Introduction
2) QCD thermodynamics on the lattice
3) QCD phase diagram at high temperature
4) Bulk thermodynamics
5) Fluctuations of conserved charges
6) Transport properties
7) Open heavy flavors and heavy quarkonia
8) QCD in external magnetic fields
9) Summary

夸克胶子等离子体

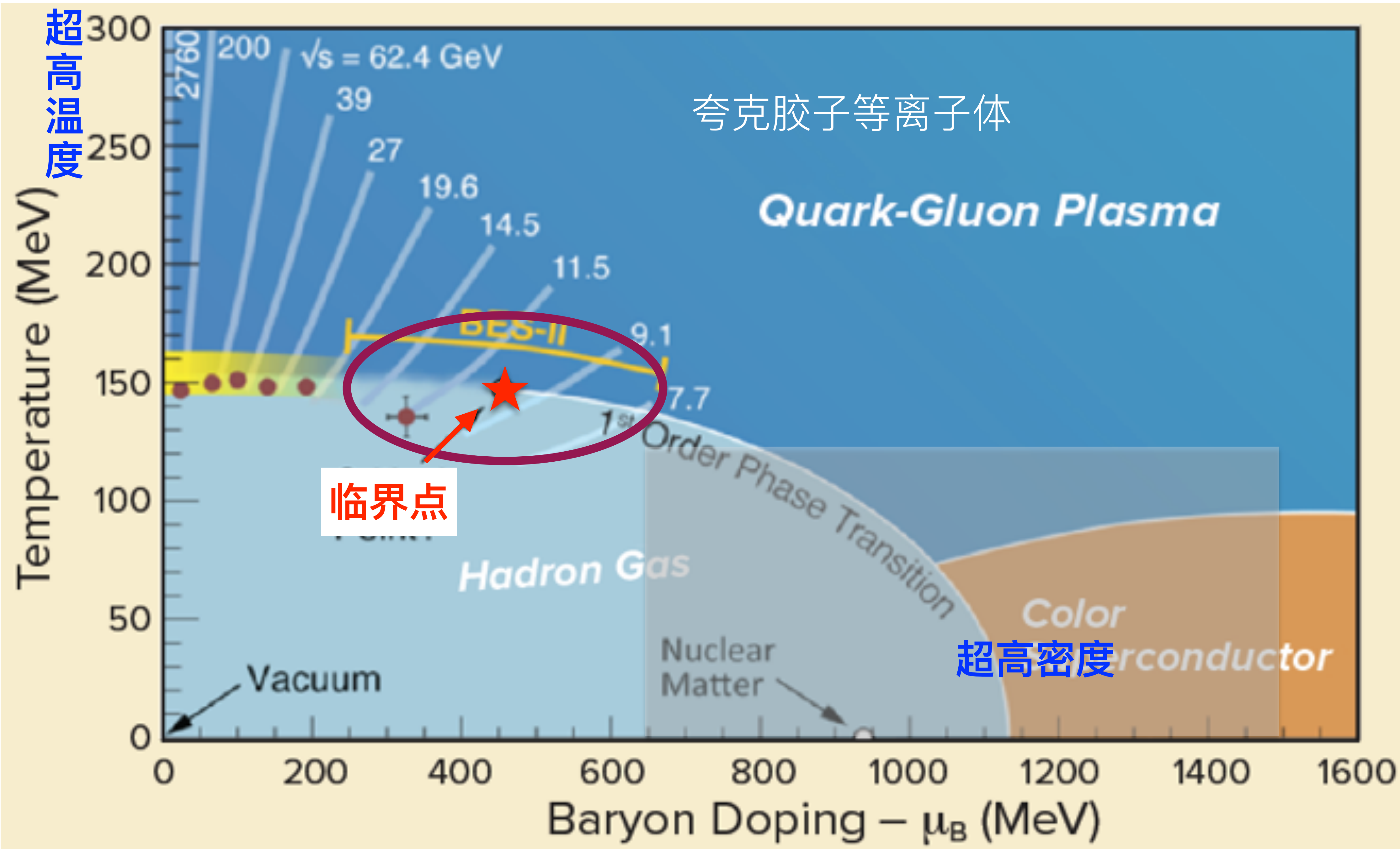
平衡态
&
近平衡态

丁亨通, F. Karsch, S. Mukherjee, https://arxiv.org/pdf/1504.05274

ESI(前1%)高被引文章,总被引308次

热密核物质：探索QCD相结构, 寻找QCD 临界点

QCD相结构图



Famous plots

#1: What is the QCD Equation of State (EoS) ?

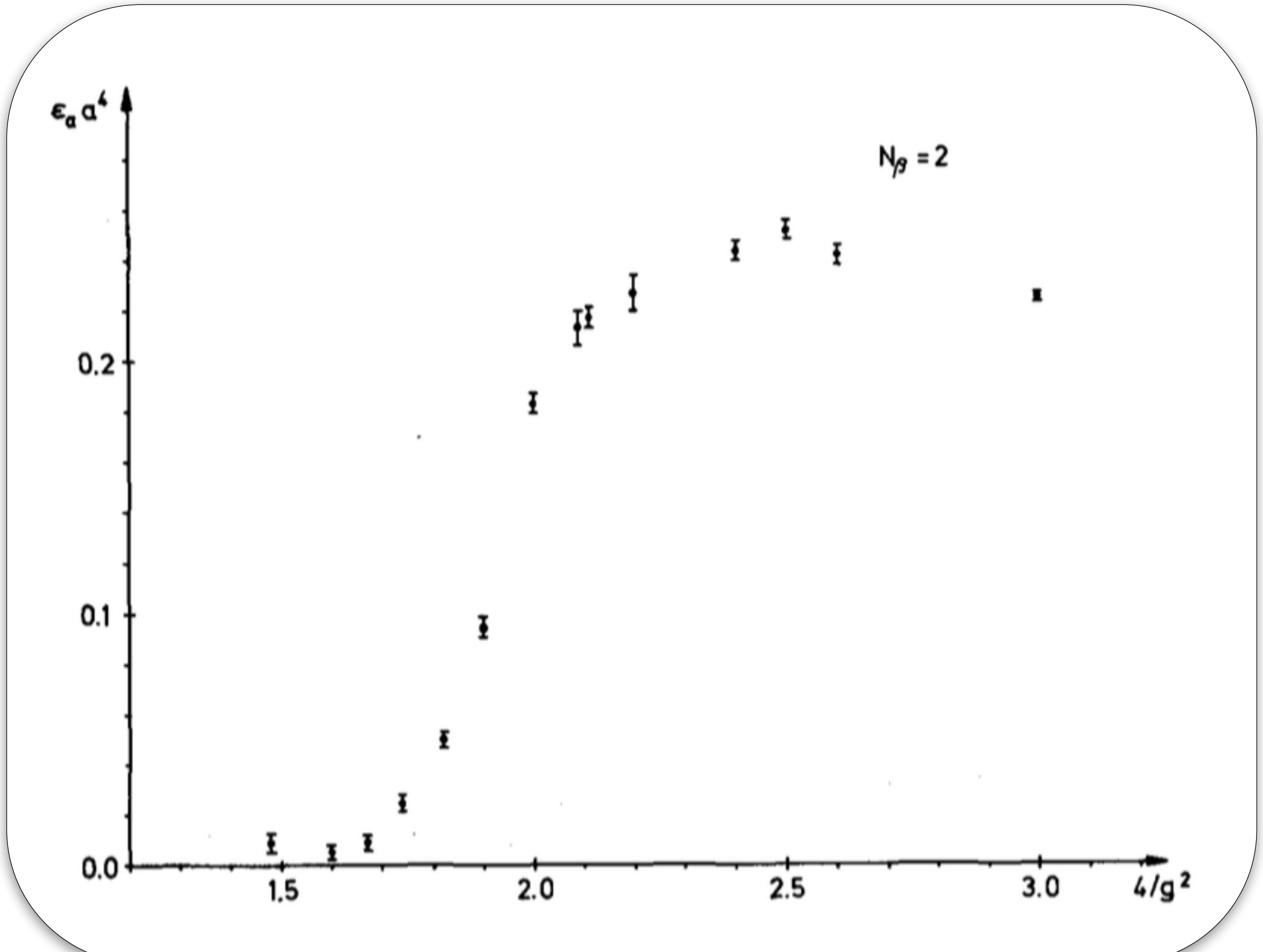
#2: At what temperature a QGP can be formed ?

#3: What happens if # of baryons is more than that of anti-baryons ?

Famous plots #1:

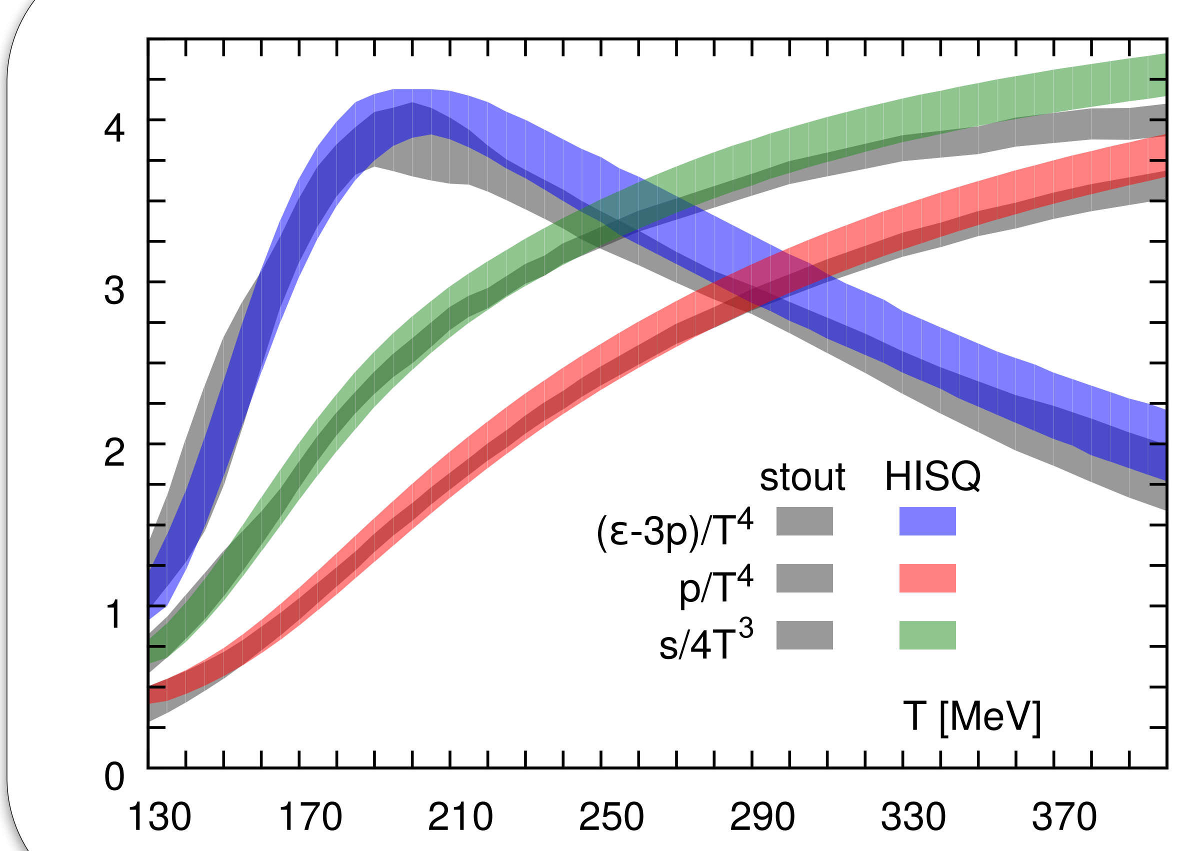
Lattice QCD calculation of EoS at $\mu_B = 0$

SU(2) pure gauge; Quenched QCD at a finite lattice cutoff of Nt=2



J. Engels, F. Karsch, H. Satz, I. Montvay, [Bielefeld]
Phys. Lett. B 101 (1981) 89-94

N_f=2+1, physical point continuum extrapolated



HotQCD, PRD 90 (2014) 094503
Cited by 1074 records

Quenched QCD v.s. dynamical QCD

$$Z = \int \mathcal{D}U \prod_{f=u,d,s,\cdots} \mathcal{D}\psi^{(f)}\,\mathcal{D}\bar{\psi}^{(f)}\, e^{-S_G - S_F} = \int \mathcal{D}U e^{-S_G} \prod_{f=u,d,s,\cdots} \det M_f$$

Integrate out the Grassmann variables

$$< \mathcal{O} >= \frac{1}{Z} \int \mathcal{D}U\, \mathcal{O}\, e^{-S_G} \prod_{f=u,d,s,\cdots} \det M_f$$

- **Quenched QCD:** $\det M_f$=constant, computationally cheap, no sea quarks
- **Dynamical (full) QCD:** $\det M_f(U)$, more computing resources needed
- **N_f = #+# QCD:** N_f=2+1 QCD: $m_u=m_d\neq m_s$, N_f=3 QCD: $m_u=m_d=m_s$, N_f=1+1+1 QCD: $m_u\neq m_d\neq m_s$, N_f=2+1+1 QCD: $m_u=m_d\neq m_s\neq m_c$
- **Physical mass point:** u, d, s quark masses are tuned to reproduce the pion, kaon, and $\eta_{s\bar{s}}$ masses
- **Stout & HISQ:** two different improved staggered discretization schemes (see slide 34)

QCD thermodynamics

- Free energy(F), pressure(P), entropy (S), energy density (ϵ)

$$F(T,V) = -T\ln Z(T,V) - F_0, \quad F_0 = -\lim_{T\to 0} \ln Z(T,V)$$

$$\mathrm{d}F = -p\mathrm{d}V - S\mathrm{d}T \quad \Rightarrow \quad p = -\frac{\partial F}{\partial V}\Big|_T = -\frac{F}{V} = \frac{TlnZ}{V}$$

$$\epsilon = \frac{U}{V} = \frac{F+TS}{V} = \frac{T^2}{V}\frac{\ln Z}{\partial T}\Big|_V = T^2\frac{\partial(p/T)}{\partial T}\Big|_V, \quad s = \frac{S}{V} = \frac{\epsilon + p}{T}$$

- Trace anomaly: $\frac{\Theta^{\mu\mu}}{T^4} \equiv \frac{\epsilon - 3p}{T^4} = T\frac{\partial}{\partial T}(p/T^4)$

- Integration method: $\frac{p}{T^4} = \frac{p_0}{T_0^4} + \int_{T_0}^{T} dT' \frac{\Theta^{\mu\mu}(T')}{T'^5}$

$$\epsilon = \Theta^{\mu\mu} + 3p$$

$$s = (\Theta^{\mu\mu} + 4p)/T$$

$$\frac{\Theta^{\mu\mu}}{T^4} \equiv \frac{\epsilon - 3p}{T^4} = T\frac{\partial}{\partial T}(p/T^4)$$

$$p = -\frac{\partial F}{\partial V}\Big|_T = -\frac{F}{V} = \frac{T ln Z}{V}$$

$$Z_{LCP}(\beta, N_\sigma, N_\tau) = \int \prod_{x,\mu} \mathrm{d}U_{x,\mu}\, e^{-S_E(U)}$$

$V = (aN_\sigma)^3$

$T = \frac{1}{aN_\tau}$

T varies from a with N_τ fixed

$\beta \equiv \beta(a)$: Lattice gauge coupling

$\hat{m}_l(\beta)$: Line of constant physics

$$\frac{\Theta^{\mu\mu}(T)}{T^4} = -R_\beta(\beta)\frac{N_\tau^4}{N_\sigma^3}\left(\frac{1}{N_\tau}\left\langle\frac{\mathrm{d}S_E}{\mathrm{d}\beta}\right\rangle_\tau - \frac{1}{N_0}\left\langle\frac{\mathrm{d}S_E}{\mathrm{d}\beta}\right\rangle_0\right) \equiv \frac{\Theta_G^{\mu\mu}(T)}{T^4} + \frac{\Theta_F^{\mu\mu}(T)}{T^4}$$

$$R_\beta(\beta) \equiv T\frac{\mathrm{d}\beta}{\mathrm{d}T} = -a\frac{\mathrm{d}\beta}{\mathrm{d}a}$$

$$S_E(U) = \beta S_G(U) - S_F(U,\beta)$$

$$S_F(U,\beta) = \frac{1}{2}\,\mathrm{Tr}\ln D(\hat{m}_l(\beta)) + \frac{1}{4}\,\mathrm{Tr}\ln D(\hat{m}_s(\beta))$$

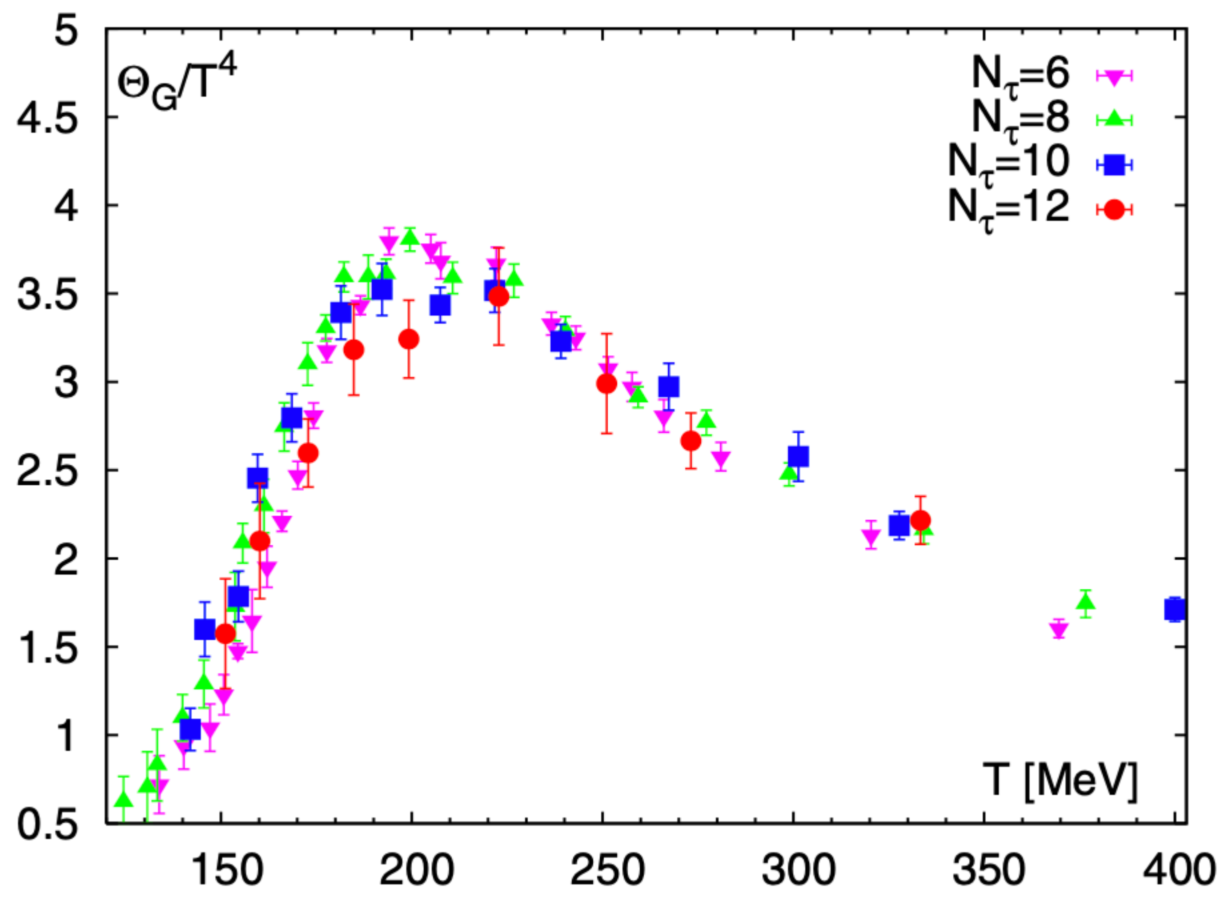
$$\langle\bar{\psi}\psi\rangle_{q,x} \equiv \frac{1}{4}\frac{1}{N_\sigma^3 N_x}\langle \mathrm{Tr} D^{-1}(\hat{m}_q)\rangle_x, \qquad q = l, s, \qquad x = 0, \tau, \qquad \langle s_G\rangle_x \equiv \frac{1}{N_\sigma^3 N_x}\langle S_G\rangle_x.$$

$$R_m(\beta) = \frac{1}{\hat{m}_l(\beta)}\frac{\mathrm{d}\hat{m}_l(\beta)}{\mathrm{d}\beta}$$

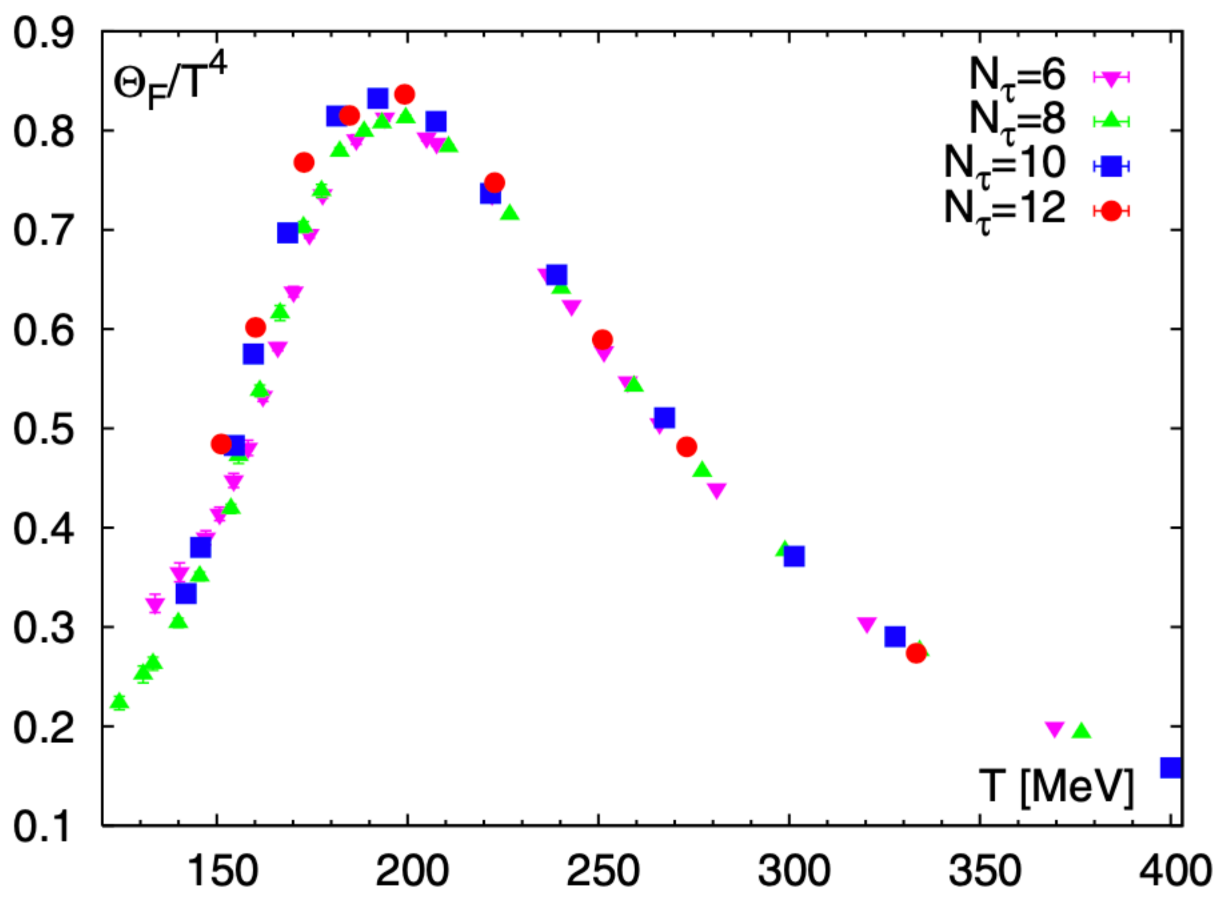
$$\frac{\Theta_G^{\mu\mu}(T)}{T^4} = R_\beta[\langle s_G\rangle_0 - \langle s_G\rangle_\tau]N_\tau^4$$

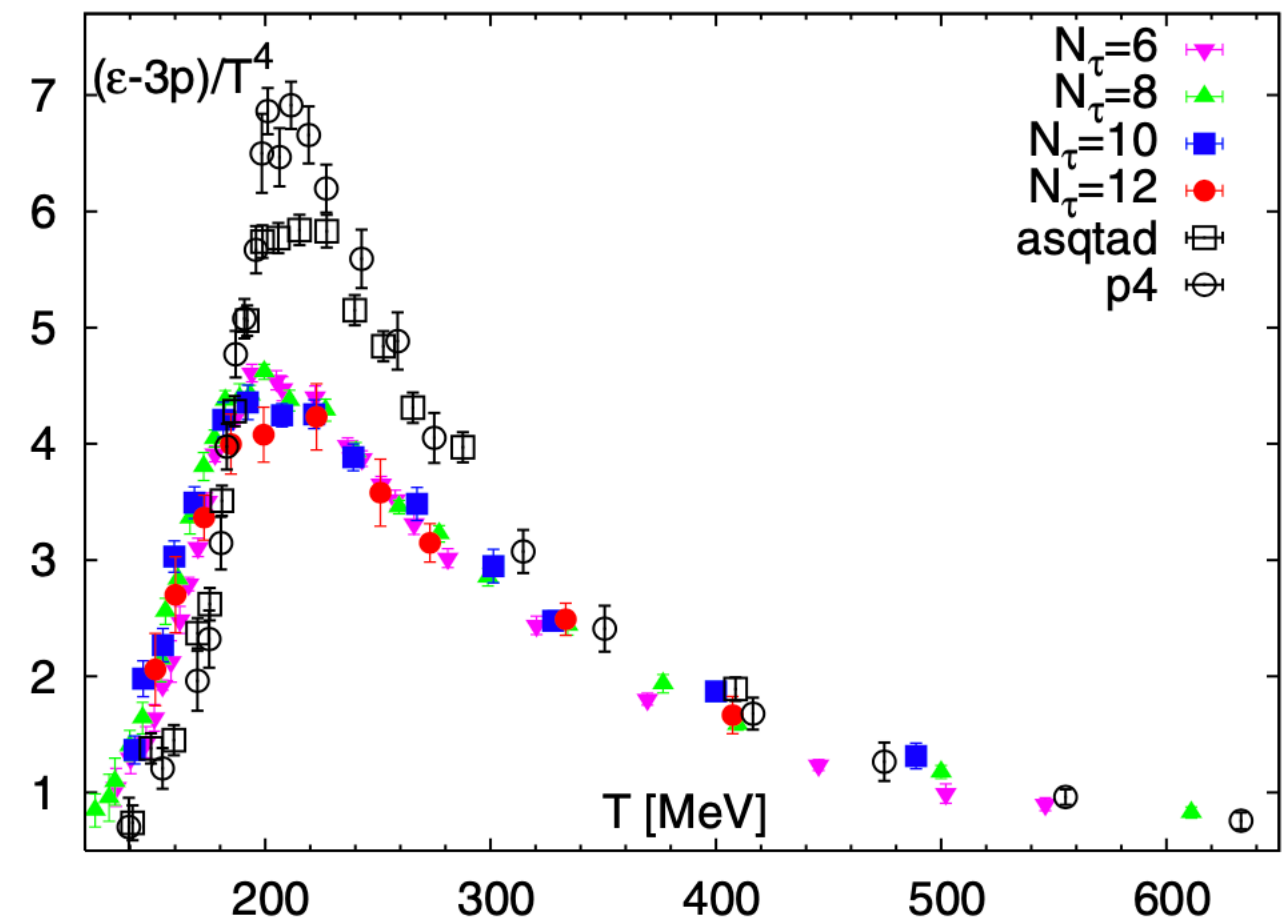
Problem: Derive these formulae

$$\frac{\Theta_F^{\mu\mu}(T)}{T^4} = -R_\beta R_m[2m_l(\langle\bar{\psi}\psi\rangle_{l,0} - \langle\bar{\psi}\psi\rangle_{l,\tau}) + m_s(\langle\bar{\psi}\psi\rangle_{s,0} - \langle\bar{\psi}\psi\rangle_{s,\tau})]N_\tau^4$$



QCD trace anomaly

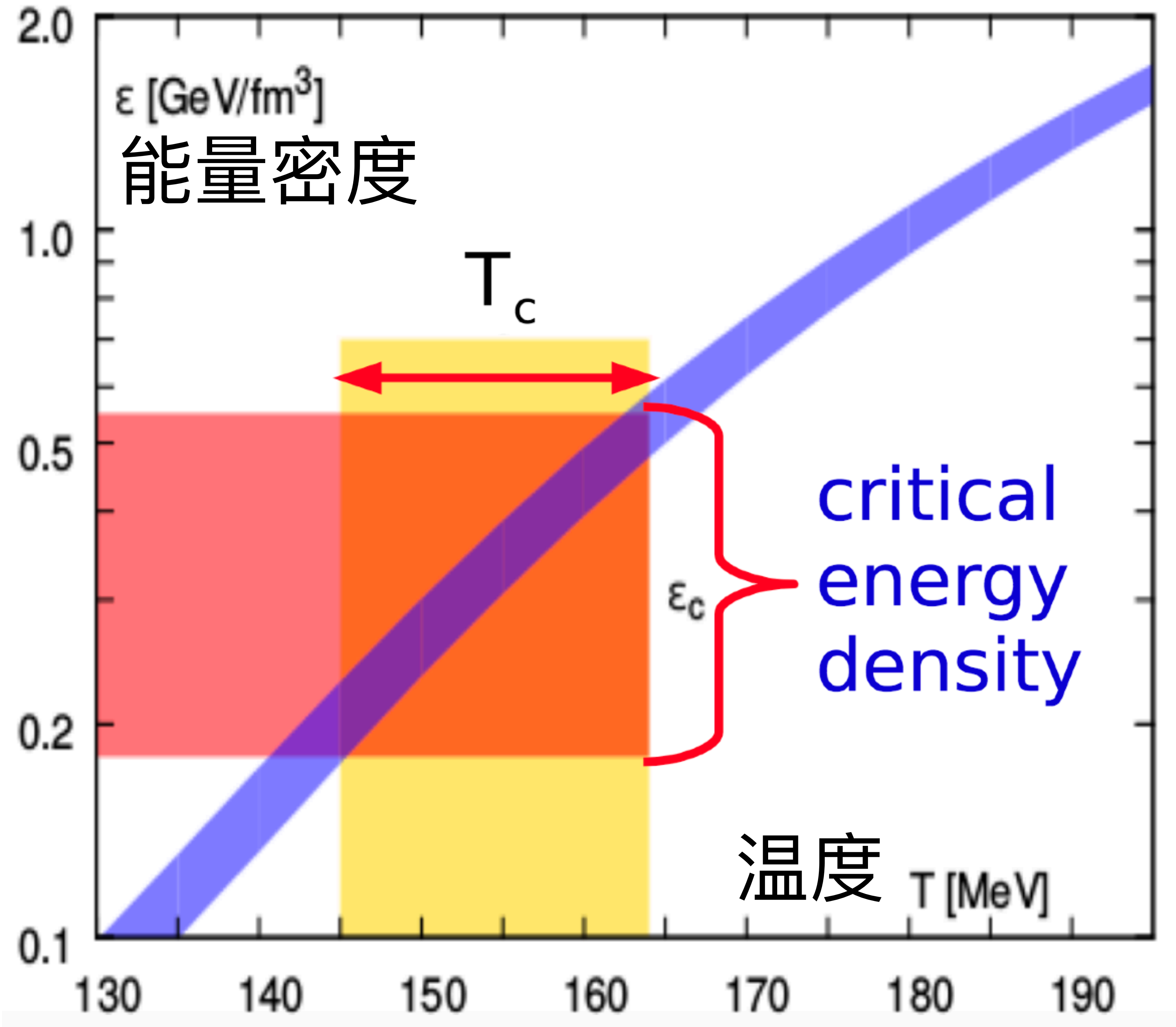




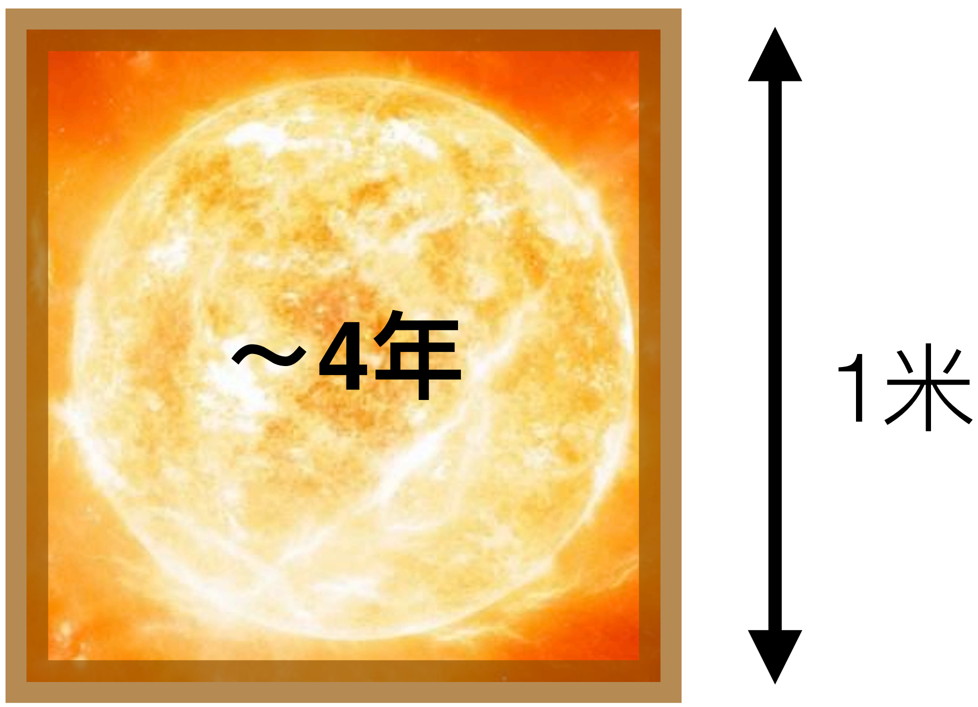
HotQCD, PRD 90 (2014) 094503
Cited by 1074 records

夸克胶子等离子体的能量密度

Nf=2+1 QCD at physical point



$\varepsilon_c \simeq 5 \times 10^{34}$ J/m^3

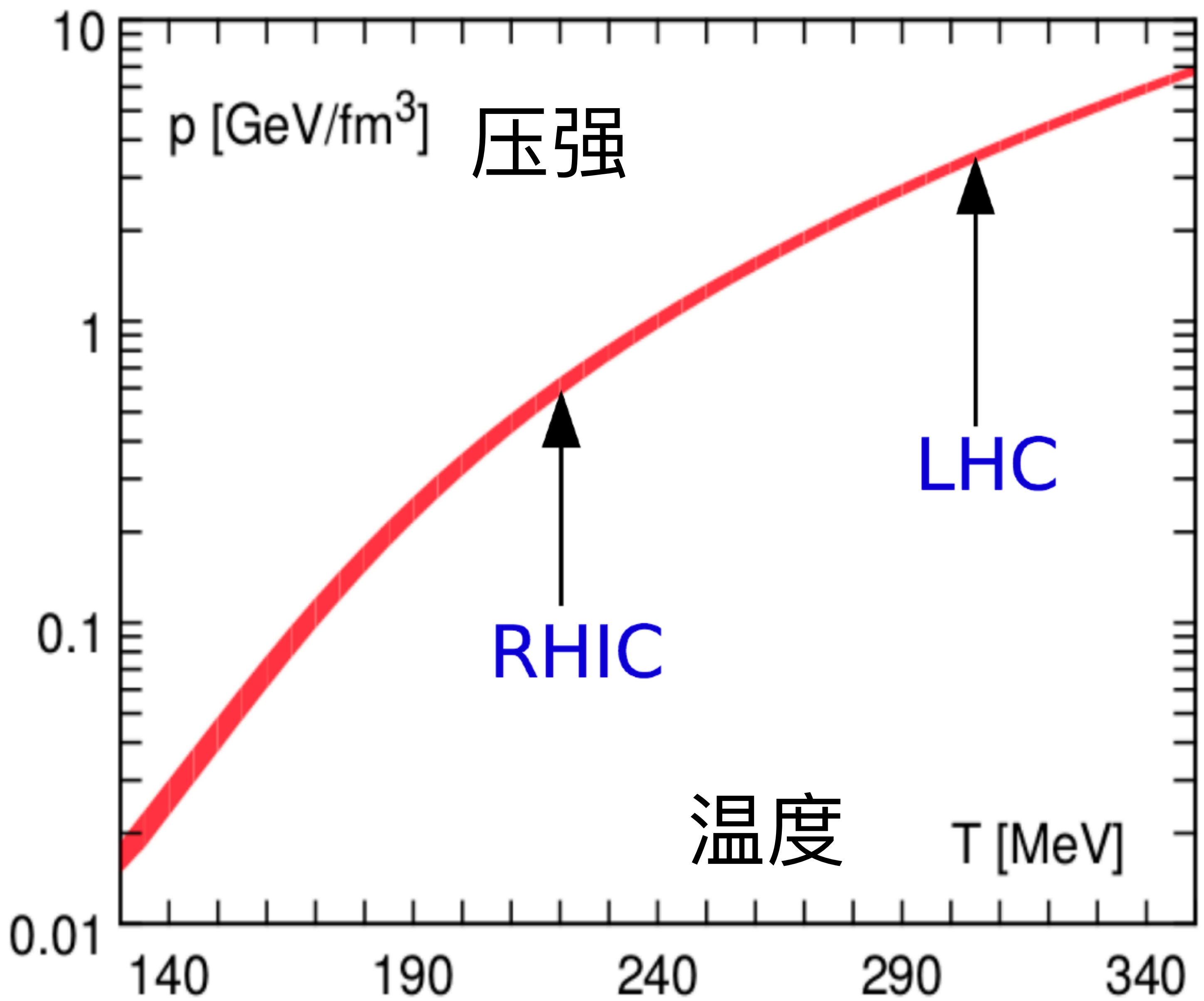


A.Bazavov,…**丁亨通** et al.[HotQCD], Phys.Rev. D90 (2014) 094503

总被引1074次

夸克胶子等离子体内的压强

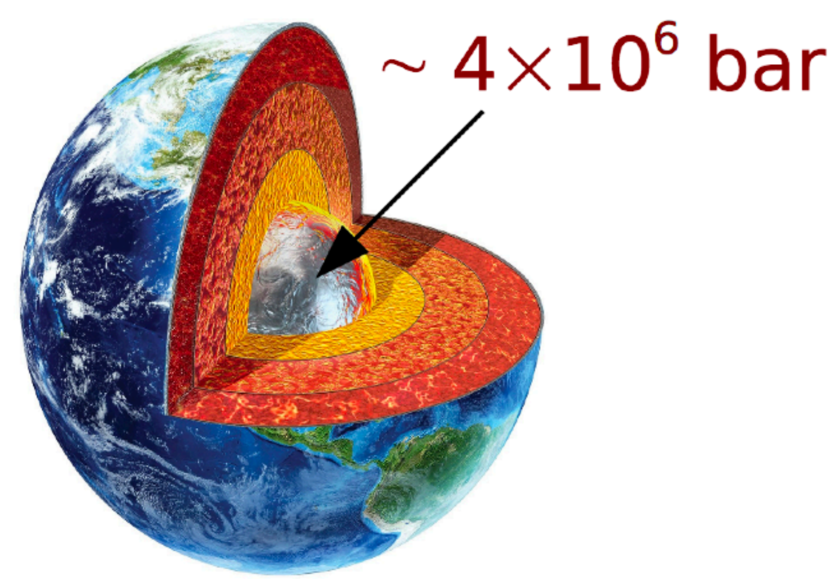
N_f=2+1 QCD at physical point



A.Bazavov,…**丁亨通** et al.[HotQCD], Phys.Rev. D90 (2014) 094503

总被引1074次

RHIC: p ≃10^{30} bar



Famous plots

#1: What is the QCD Equation of State (EoS) ?

#2: At what temperature a QGP can be formed ?

#3: What happens if # of baryons is more than that of anti-baryons ?

Landau functional of QCD

Pisarski & Wilczek (84')

Symmetry: $SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A$

Chiral field: $\Phi_{ij} \sim \frac{1}{2}\bar{q}^j(1-\gamma_5)q^i = \bar{q}^j_R q^i_L$

Chiral transformation: $\Phi \to e^{-2i\alpha_A} V_L \, \Phi \, V_R^\dagger$

$$\mathcal{L}_{eff} = \frac{1}{2}\operatorname{tr}\partial\Phi^\dagger\partial\Phi + \frac{a}{2}\operatorname{tr}\Phi^\dagger\Phi + \frac{b_1}{4!}\left(\operatorname{tr}\Phi^\dagger\Phi\right)^2 + \frac{b_2}{4!}\operatorname{tr}\left(\Phi^\dagger\Phi\right)^2$$

→ SU(Nf)LxSU(Nf)RxU(1)A

$$- \frac{c}{2}\left(\det\Phi + \det\Phi^\dagger\right)$$

→ SU(Nf)LxSU(Nf)R

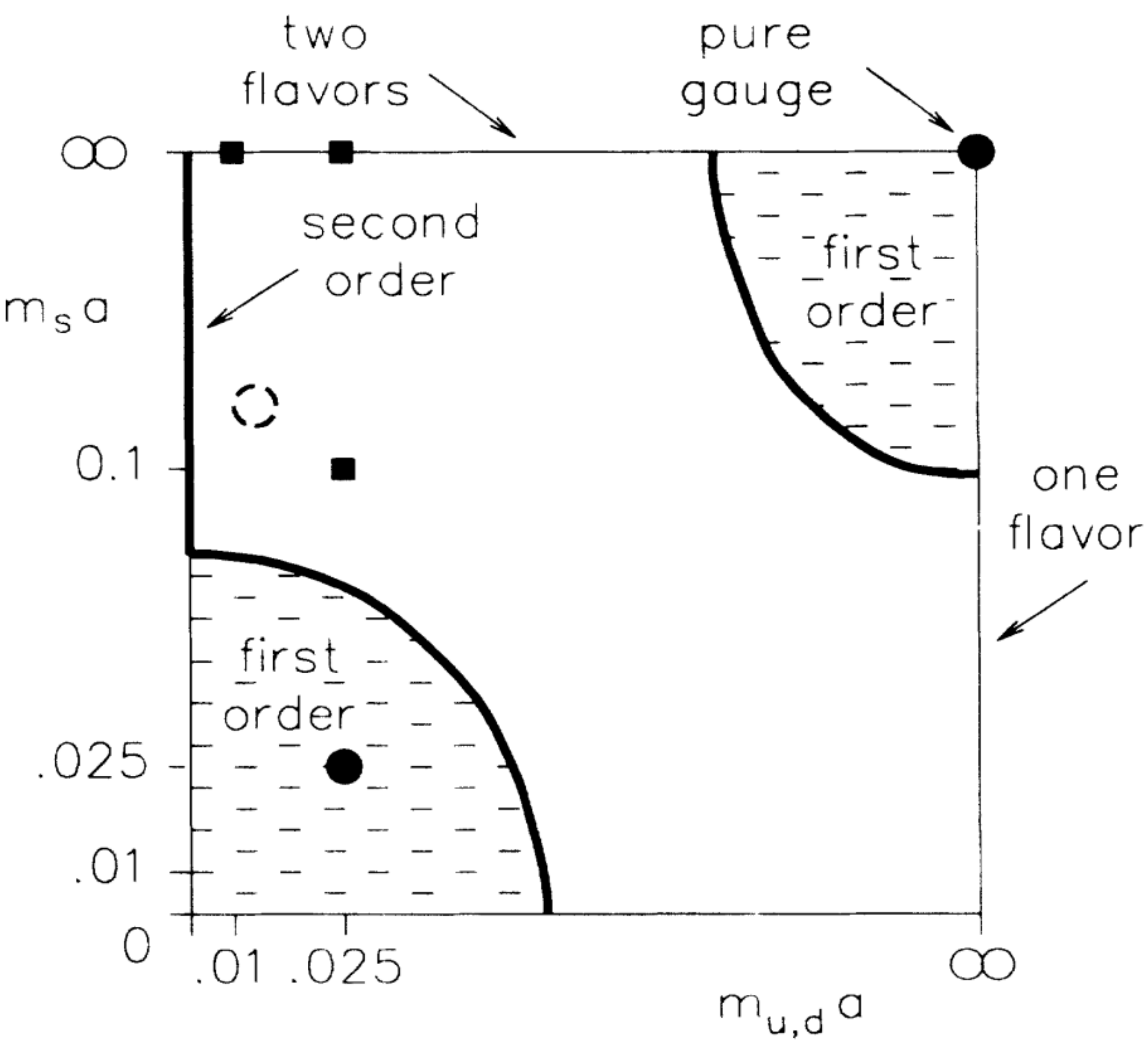
$$- \frac{d}{2}\operatorname{tr} h\left(\Phi + \Phi^\dagger\right).$$

→ Quark mass term

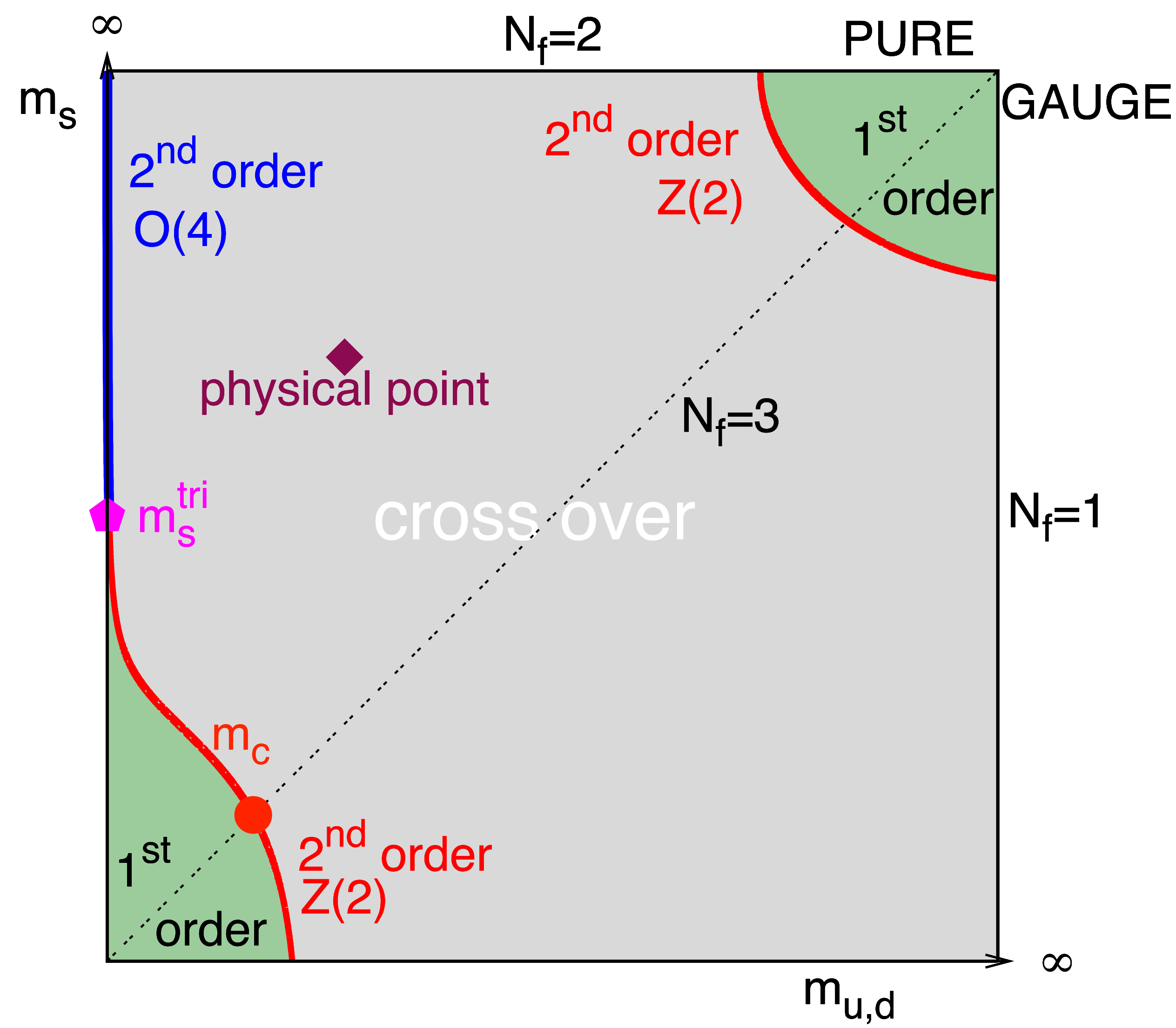
Results on phase transitions should be eventually checked by Lattice QCD

Famous plots #2: 哥伦比亚相图(Columbia plot)

夸克质量平面中的QCD相图



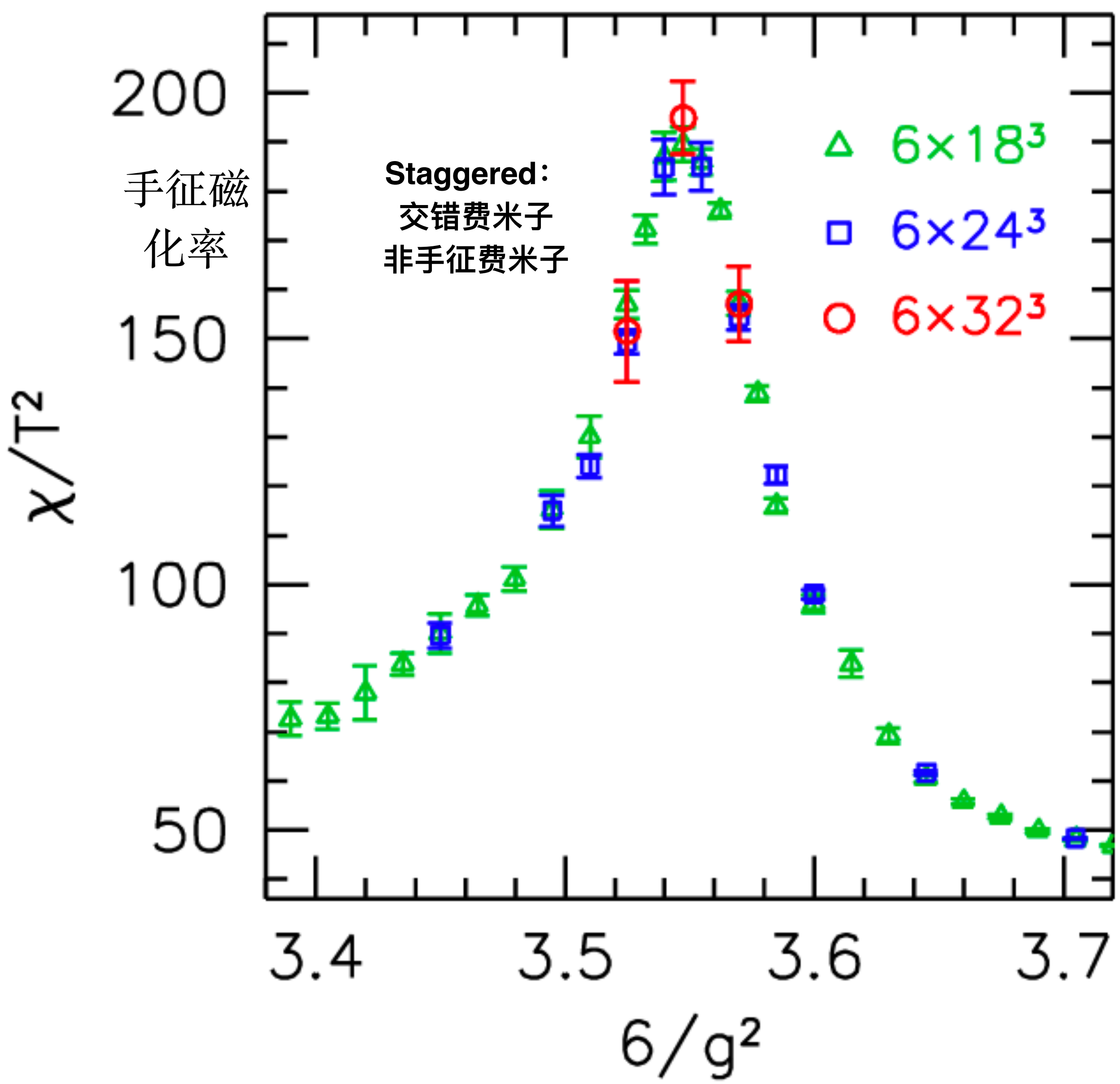
F. Brown, F. Butler, H. Chen, N. Christ, et al., [Columbia] Phys.Rev.Lett. 65 (1990) 2491-2494



丁亨通, F. Karsch, S. Mukherjee, arXiv:1504.05274

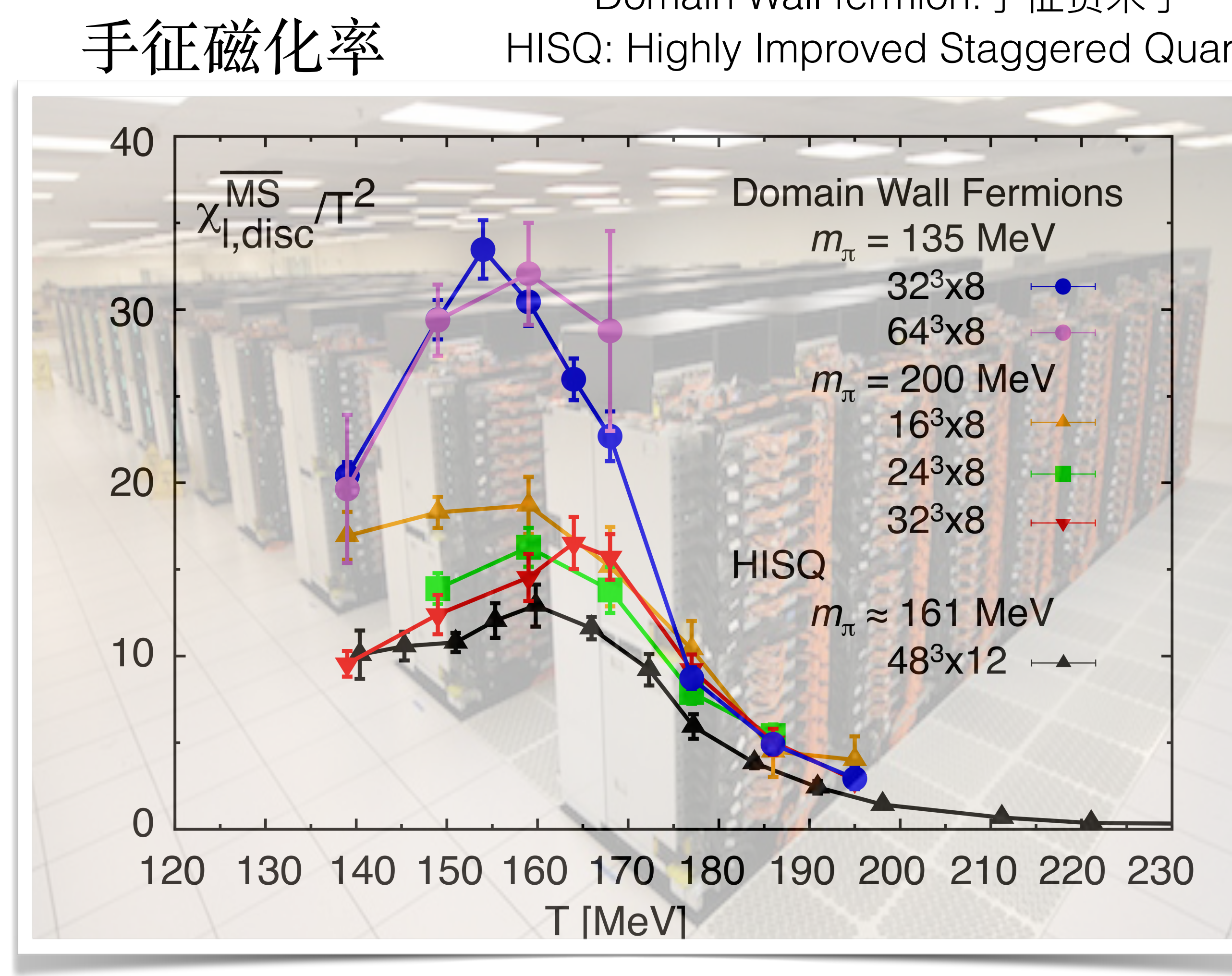
Order of the N_f=2+1 QCD transition at the physical point

crossover transition



Y. Aoki et al., Nature 443 (2006) 675-678
Cited by 1516 records

Domain Wall fermion:手征费米子
HISQ: Highly Improved Staggered Quarks



背景为IBM BGQ超级计算机

《物理评论快报》编辑推荐阅读、美国物理学会《观点》杂志报道

T. Bhattacharya,…**丁亨通**,…et al.[HotQCD],
PRL,113(2014)082001

Cited by 355 records

Ginzburg-Landau-Wilson approach

Partition function: $$Z = \int [\mathrm{d}\sigma] \exp\left(- \int \mathrm{dx}\, \mathcal{L}_{eff}\left(\sigma(\mathrm{x}); K\right)\right)$$

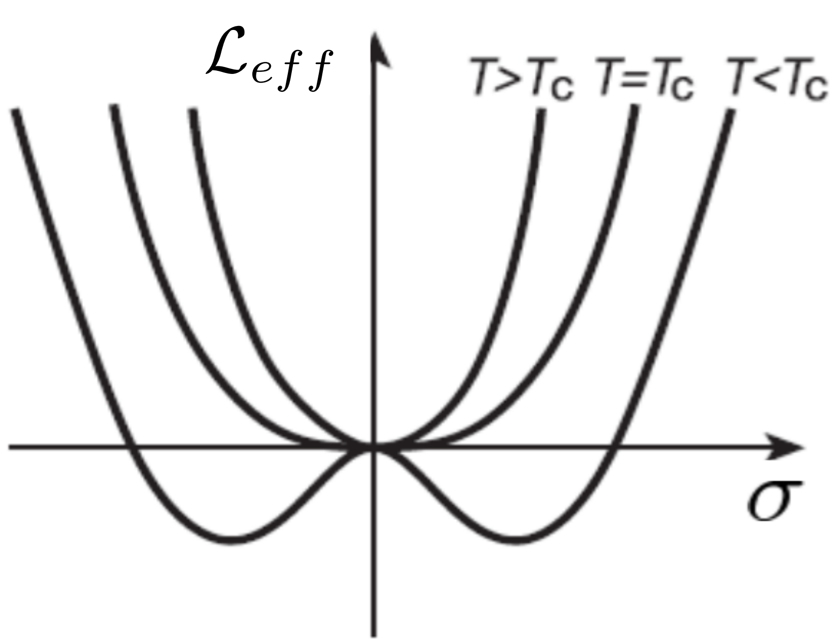
Landau function: $$\mathcal{L}_{eff} = \frac{1}{2}(\nabla\sigma)^2 + \sum_n a_n(K)\sigma^n$$ Same symmetry with the underlying theory

σ(x): order parameter field; K={m,μ}: external parameters

2nd order phase transition

Z(2) Ising model, N_f=2 QCD

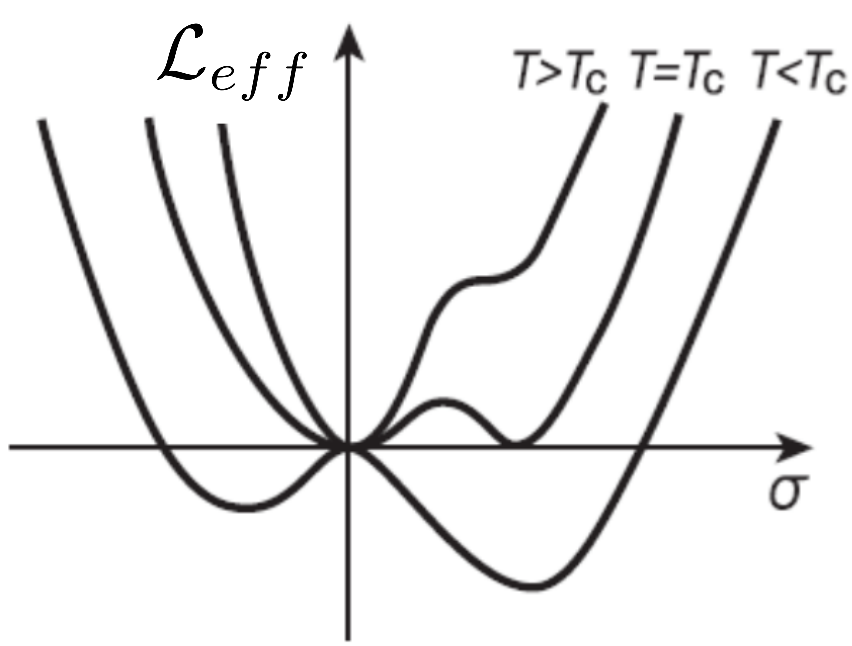
$$\mathcal{L}_{eff} = \frac{1}{2}a\sigma^2 + \frac{1}{4}b\sigma^4$$



1st order phase transition

Z(3) Potts model, N_f=3 QCD

$$\mathcal{L}_{eff} = \frac{1}{2}a\sigma^2 - \frac{1}{3}c\sigma^3 + \frac{1}{4}b\sigma^4$$



Ginzburg-Landau-Wilson approach

Partition function: $$Z = \int [\mathrm{d}\sigma] \exp\left(- \int \mathrm{dx}\, \mathcal{L}_{eff}\left(\sigma(\mathrm{x}); K\right)\right)$$

Landau function: $$\mathcal{L}_{eff} = \frac{1}{2}\left(\nabla\sigma\right)^2 + \sum_n a_n(K)\sigma^n$$ Same symmetry with the underlying theory

σ(x): order parameter field; K={m,μ}: external parameters

2nd order phase transition

order parameter M:
continuous in T

fluctuations of M:

$$\chi(T) = \frac{T}{V}(\langle M^2\rangle - \langle M\rangle^2)$$

$$\chi(T_c) \sim V^{(2-\eta)/3}$$

1st order phase transition

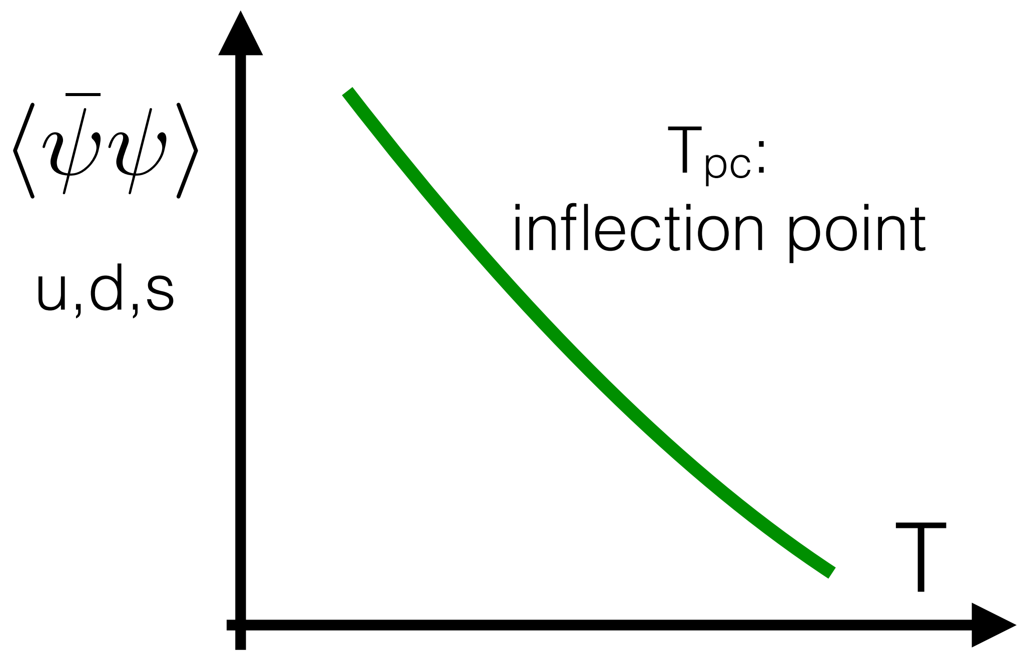
M:
discontinuous in T

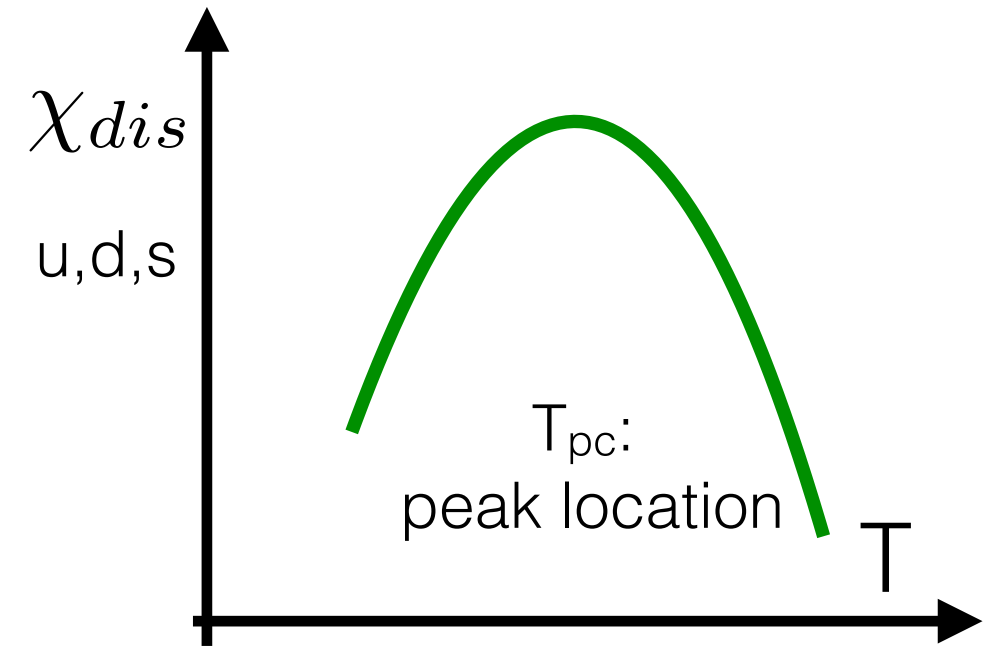
fluctuations of M:

$$\chi(T_c) \sim V$$

Crossover transition temperature T_{pc} in the real world

- Crossover nature of the transition





- Chiral phase transition: most likely 2nd order, 3d O(4)

Ejiri et al., PRD 80(2009)094505,
HotQCD, arXiv:1903.04801
…

- A well-defined **chiral crossover transition temperature**: based on scaling properties of QCD

HTD, P. Hegde, O. Kaczmarek et al.
[HotQCD], arXiv:1903.04801

连续相变

- 埃伦费斯特(Paul Ehrenfest)的相变分类： 相变时两相化学势的n-1阶偏微商相等，n阶偏微商不相等，则这个相变就叫n级相变

- 连续相变：$n \geq 2$

序参量关联长度在临界点附近趋于无穷

标度变换不变性

标度律

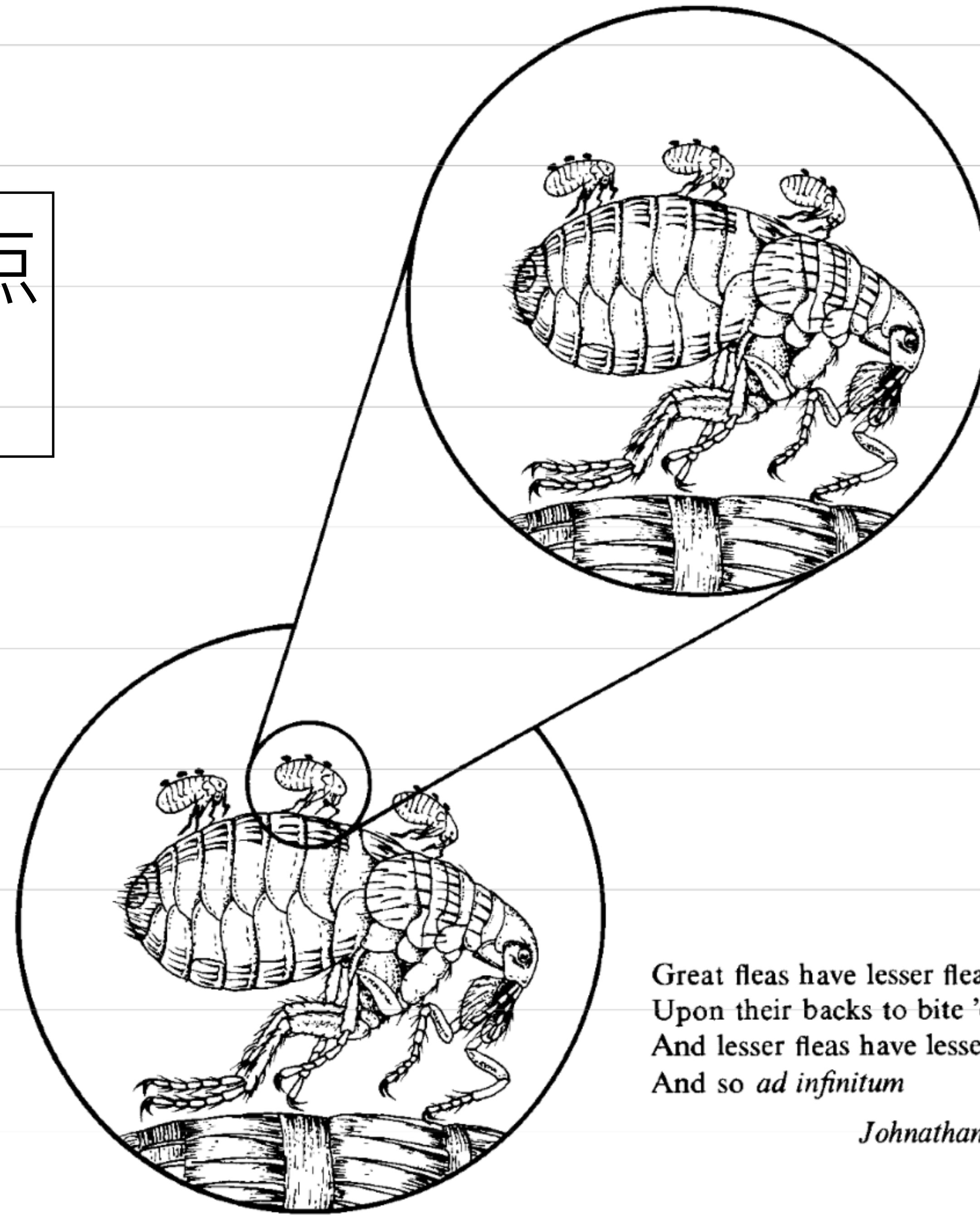


Fig. 16.3 Scale invariance.

Kerson Huang, Statistical Mechanics, ISBN-0-471-81518-7

Universal behavior of chiral phase transition in N_f=2+1 QCD at μ_B=0

Behavior of the free energy close to critical lines

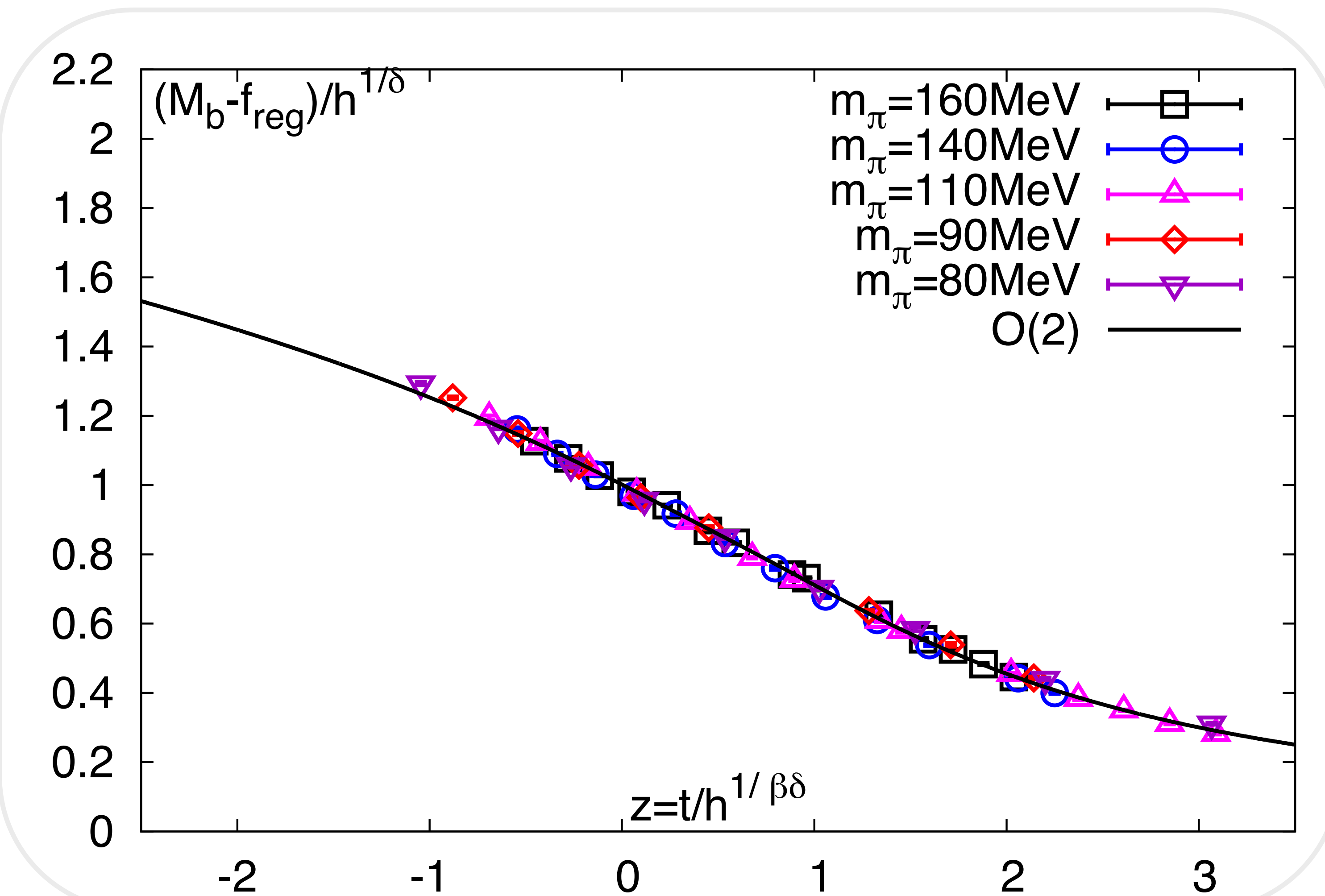
$$f(m,T)=h^{1+1/\delta} f_s(z) + f_{reg}(m,T), \qquad z=t/h^{1/\beta\delta}$$

h: external field, t: reduced temperature, β,δ: universal critical exponents

$$M = -\partial f(t,h)/\partial h = h^{1/\delta} f_G(z) + f_{reg}(t,h)$$

h ~ m; t ~ T-T_c

fG(z): (O(2))scaling functions



Good evidence of O(N) scaling for chiral phase transition

Sheng-Tai Li, Lattice 2016

Scaling behavior of chiral observables

chiral condensate: $\Sigma(T,\mu_B) \sim m^{1/\delta} f_G$

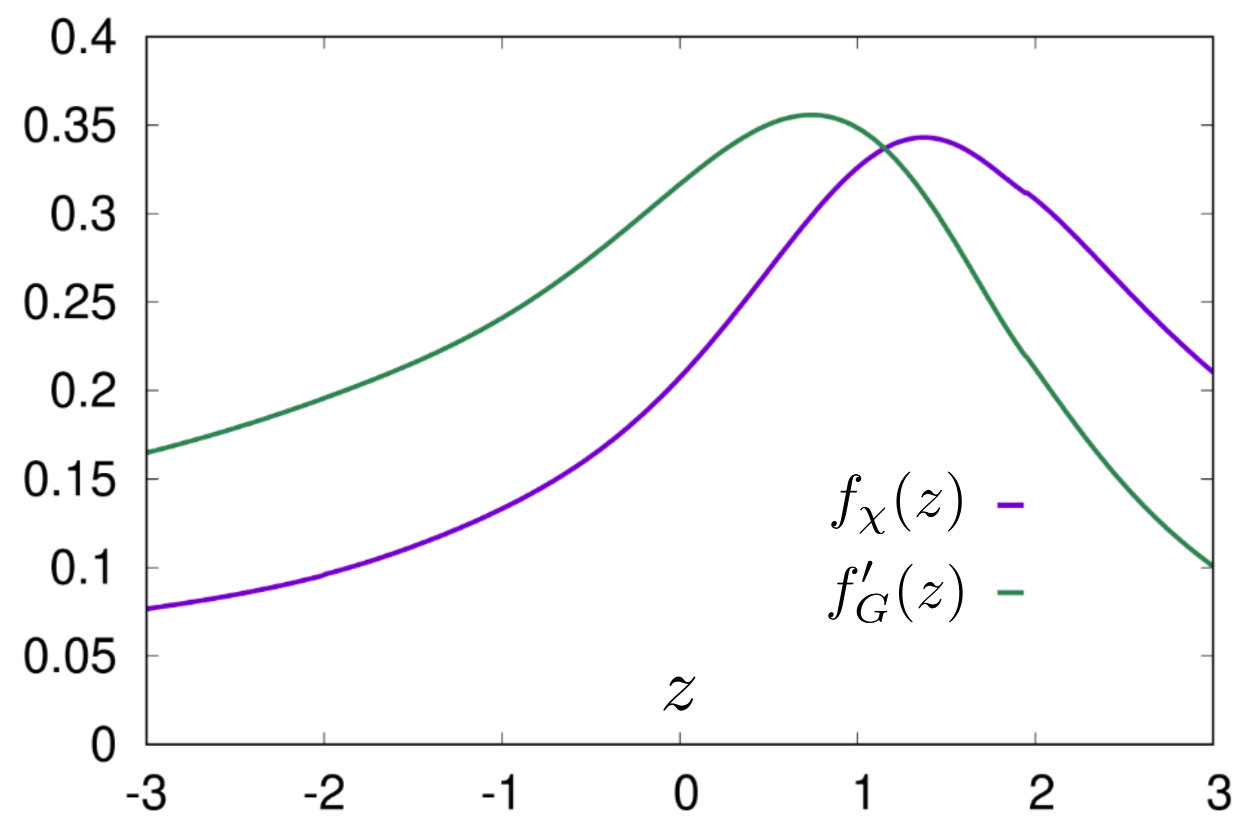
chiral susceptibility: $\chi^\Sigma(T,\mu_B) \sim m^{1/\delta-1} f_\chi$

Taylor expansions:

$$\Sigma(T,\mu_X) = \sum_{n=0}^{\infty} \frac{C_{2n}^{\Sigma}(T)}{(2n)!}\left(\frac{\mu_X}{T}\right)^{2n} \qquad \chi(T,\mu_X) = \sum_{n=0}^{\infty} \frac{C_{2n}^{\chi}(T)}{(2n)!}\left(\frac{\mu_X}{T}\right)^{2n}$$

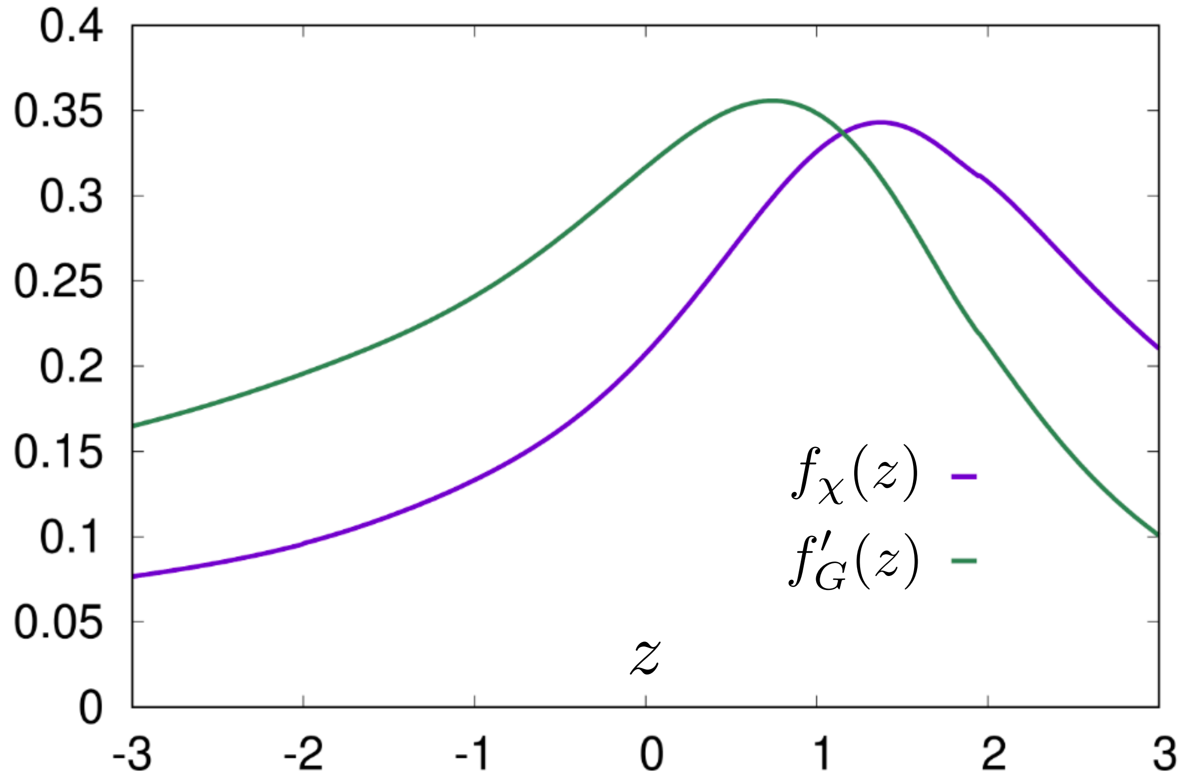
$\partial_T \chi^\Sigma(T)$, $\partial_T C_0^\chi(T)$, $C_2^\chi(T)$ $\sim \quad m^{1/\delta-1-1/\beta\delta} f'_\chi(z)$

$\partial_T^2 C_0^\Sigma(T)$, $\partial_T C_2^\Sigma(T)$ $\sim \quad m^{1/\delta-2/\beta\delta} f''_G(z)$



$z \sim \left((T-T_c^0)/T_c^0 + K(\mu_B/T)^2\right)/m^{\frac{1}{\beta\delta}}$

Well-defined notation of chiral crossover transition temperature



$z \sim \left((T - T_c^0)/T_c^0 + K(\mu_B/T)^2\right)/m^{\frac{1}{\beta\delta}}$

$$\left.\begin{array}{l}\partial_T \chi^\Sigma(T) \\ \partial_T C_0^\chi(T) \\ C_2^\chi(T)\end{array}\right\} \sim m^{1/\delta - 1 - 1/\beta\delta} f'_\chi(z)$$

$$\left.\begin{array}{l}\partial_T^2 C_0^\Sigma(T) \\ \partial_T C_2^\Sigma(T)\end{array}\right\} \sim m^{1/\delta - 2/\beta\delta} f''_G(z)$$

- 5 conditions to extract Tc: maxima of f_χ and f'_G

$\partial_T \chi^\Sigma(T) = 0$ $\partial_T C_0^\chi(T) = 0$ $C_2^\chi(T) = 0$ $\partial_T^2 C_0^\Sigma(T) = 0$ $\partial_T C_2^\Sigma(T) = 0$

- m=0: all these susceptibilities diverge at a unique T
- m=/=0: non-unique temperatures, crossover

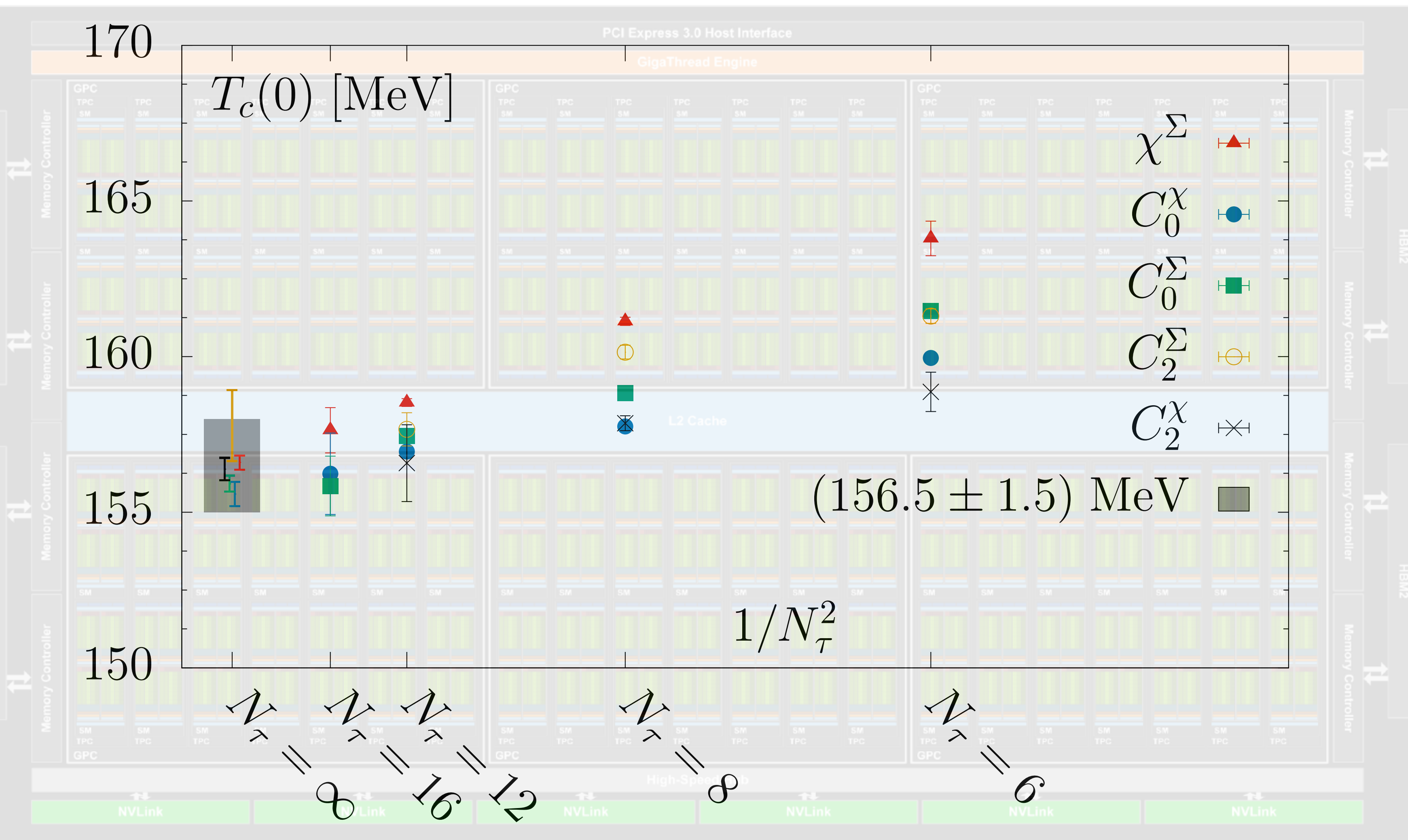
华中师范大学核科学计算中心

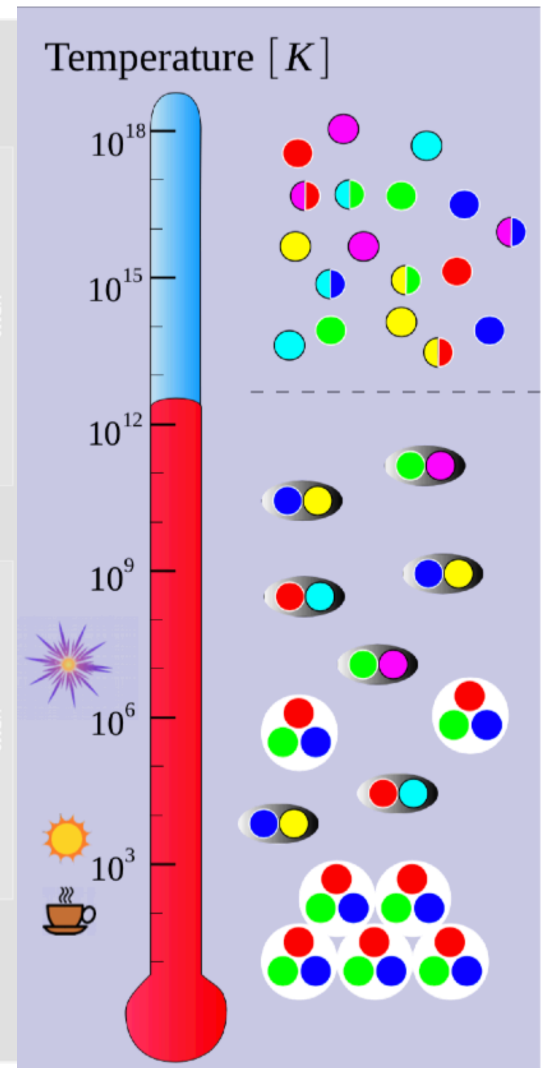
强子相到夸克胶子等离子体相的转变温度

$T_c(0)$=156.5(1.5)MeV ～1.8×10^{12} K

精准结果

连续外推





室温：
293.15 K

太阳表面温度：
～5.8×10^3 K

太阳中心温度：
～1.57×10^7 K

0 ← a

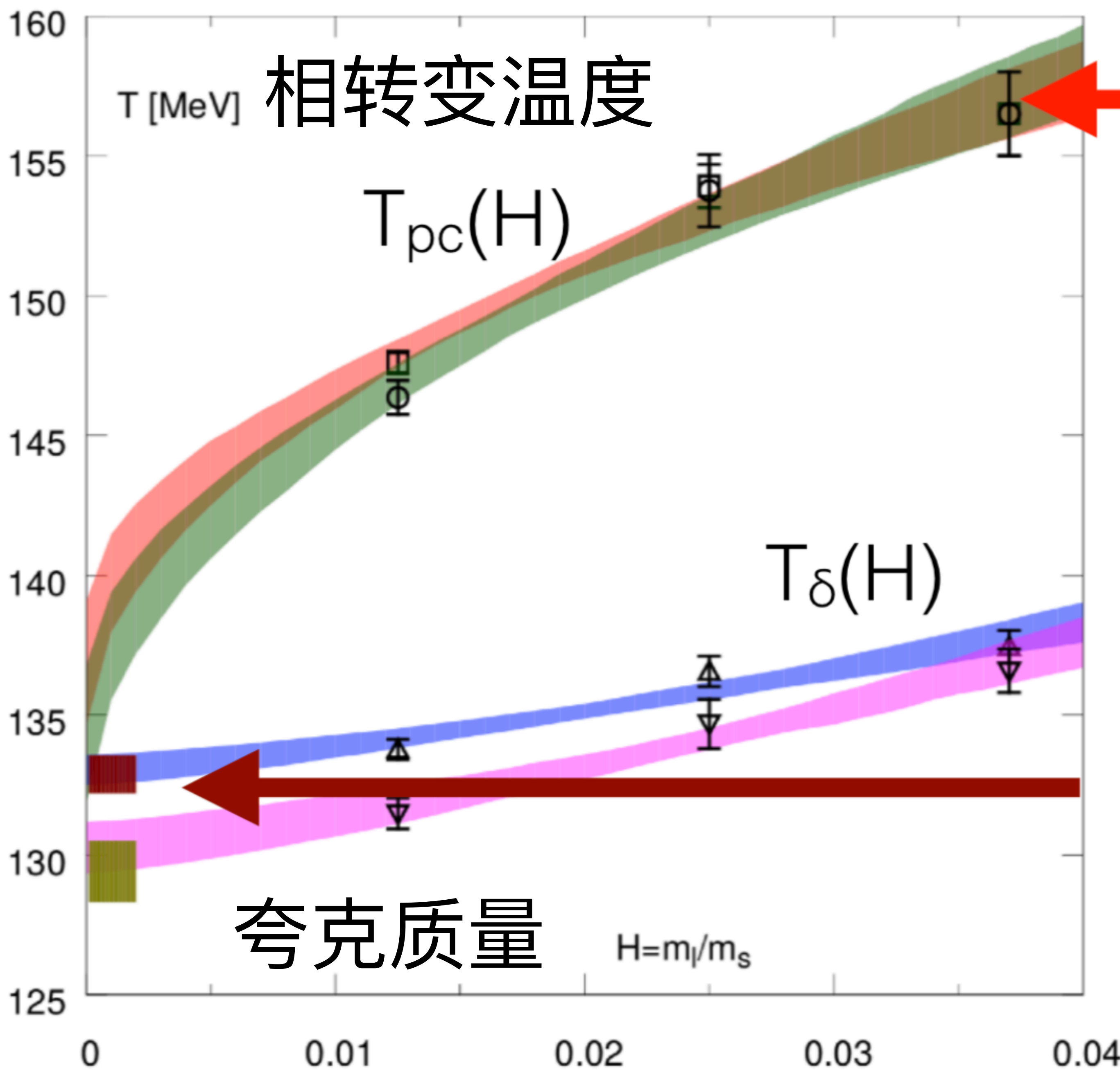
背景为V100
图形处理器(GPU)

A. Bazavov, **丁亨通**, P. Hegde et al. [HotQCD],
Phys. Lett. B795 (2019) 15, 总被引386次

华中师范大学核科学计算中心

量子色动力学手征相变温度

QCD临界点的温度上限



真实物理世界中的
相转变温度
T_{pc}^{phy} = 156.5(1.5) MeV

$$T_{pc}(H) = T_c^0 \left(1 + \frac{z_p}{z_0} H^{\frac{1}{\beta\delta}} \right)$$

二阶相变,O(4)群普适类

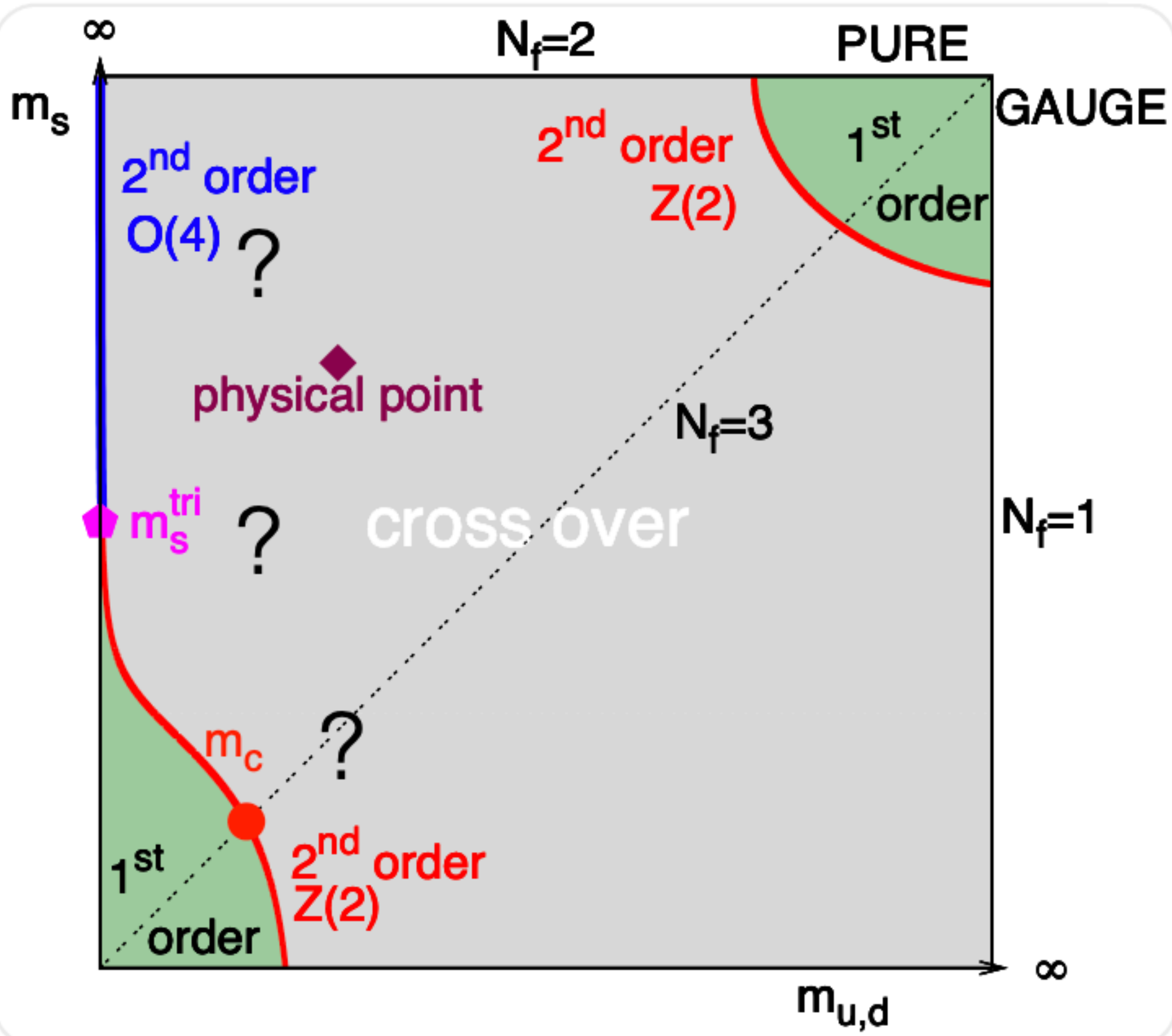
手征极限下的相变温度

$$T_c^0 = 132^{+3}_{-6}\ \mathrm{MeV}$$

丁亨通，P. Hegde et al.，Phys. Rev. Lett. 123(2019) 062002，总被引150次

Nature of chiral phase transition

Columbia plot:
QCD phase diagram in quark mass plane



- At physical point $T_{pc} \approx 156$ MeV

HotQCD, PLB 795 (2019) 15
WB, PRL125 (2020) 052001

- Chiral phase transition T_c =132(+3)(-6)MeV

HotQCD, PRL 123 (2019) 062002

$U_A(1)$ symmetry:

- Broken, 2nd order (O(4)) phase transition

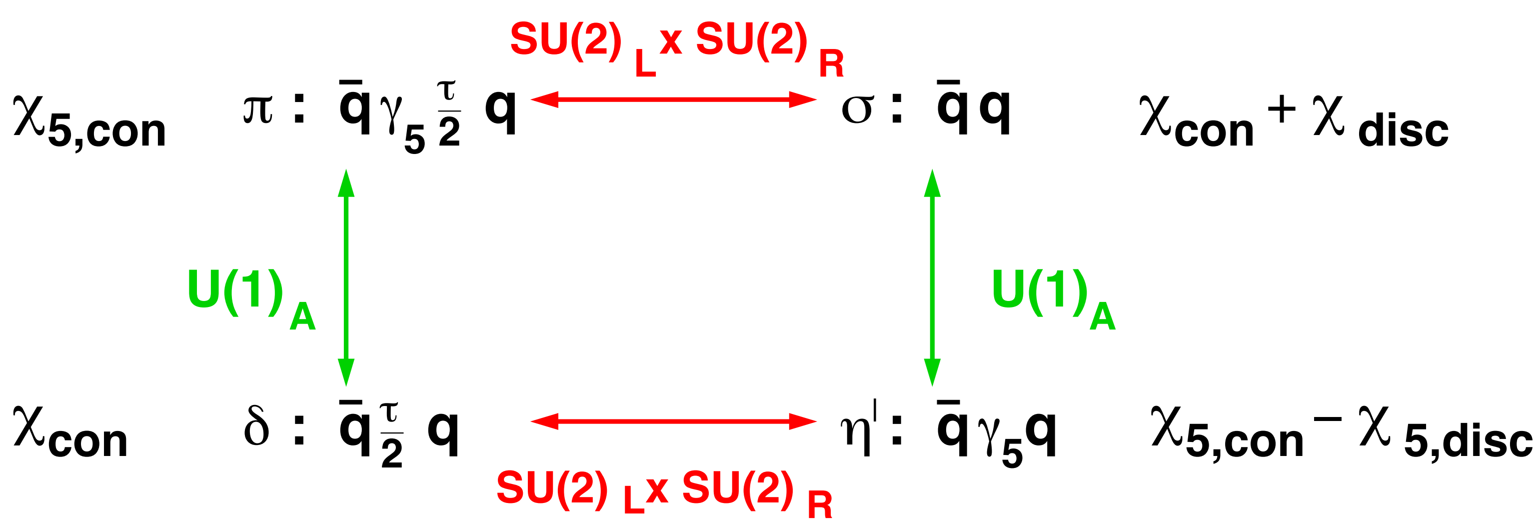
Pisarski and Wilczek, PRD 29 (1984) 338

- Effectively restored, 1st or 2nd order ($U(2)_L \otimes U(2)_R / U(2)_V$)

Butti, Pelissetto and Vicari, JHEP 08 (2003) 029
Pelissetto & Vicari, PRD 88 (2013) 105018
Grahl, PRD 90 (2014) 117904

Signature of symmetry restorations

- Susceptibilities defined as integrated two point correlation functions of the local operators, e.g. $\chi_\pi = \int d^4x \langle \pi^i(x)\pi^i(0)\rangle$ with $\pi^i(x) = i\bar{\psi}_l(x)\gamma_5\tau^i\psi_l(x)$



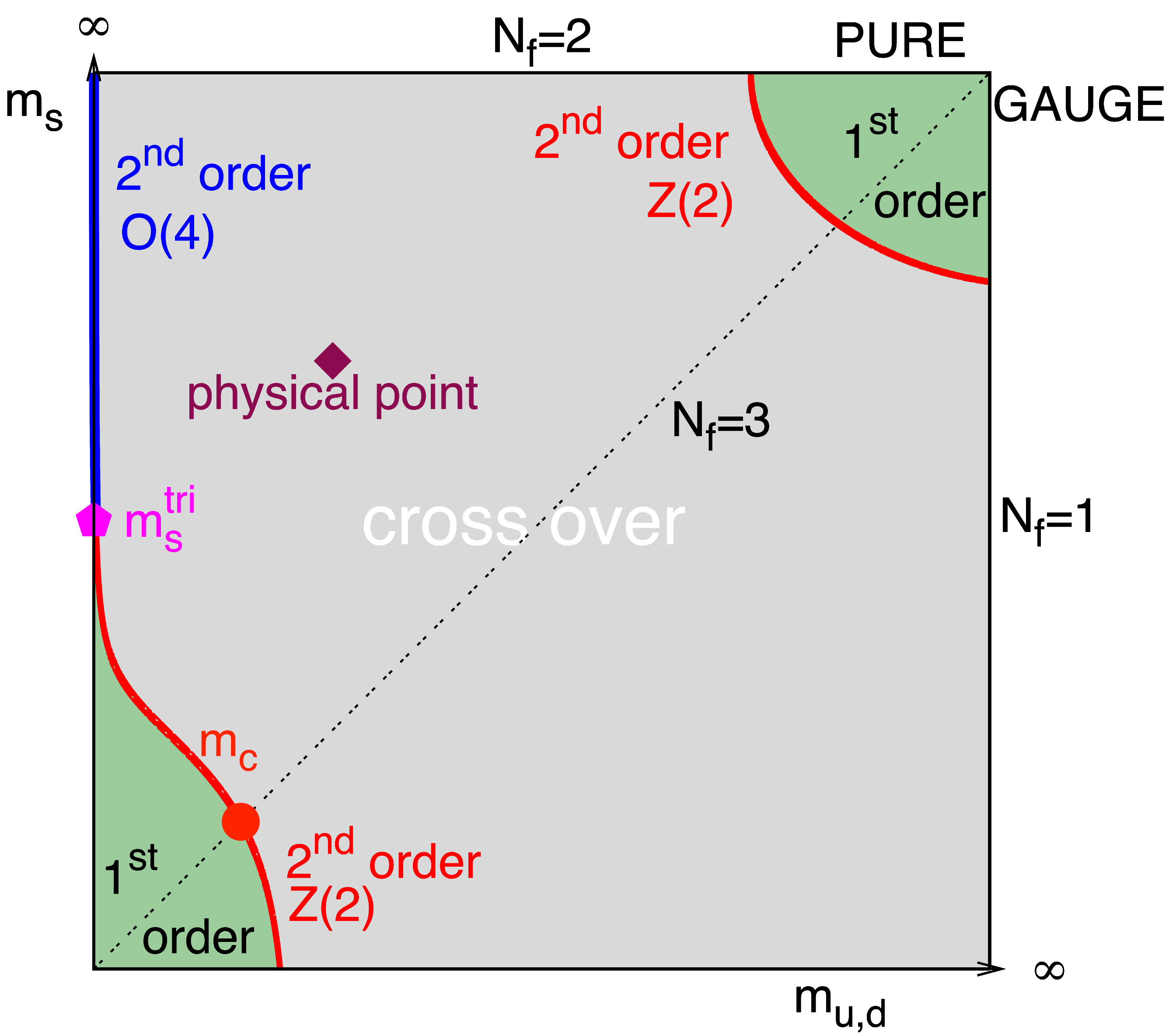
Restoration of $SU(2)_L x SU(2)_R$: $\chi_\pi - \chi_\sigma = 0$, $\chi_\delta - \chi_\eta = 0$ ⇒ $\chi_\pi - \chi_\delta = \chi_{disc} = \chi_{5,disc}$

Effective restoration of $U(1)_A$: $\chi_\pi - \chi_\delta = 0$, $\chi_\sigma - \chi_\eta = 0$ ⇒ $\chi_\pi - \chi_\delta = \chi_{disc} = \chi_{5,disc} = 0$

$$\chi_{\rm disc} = \frac{T}{V}\int d^4x \left\langle \left[\bar{\psi}(x)\psi(x) - \langle\bar{\psi}(x)\psi(x)\rangle\right]^2\right\rangle$$

Lattice setup

local GPU computers @CCNU

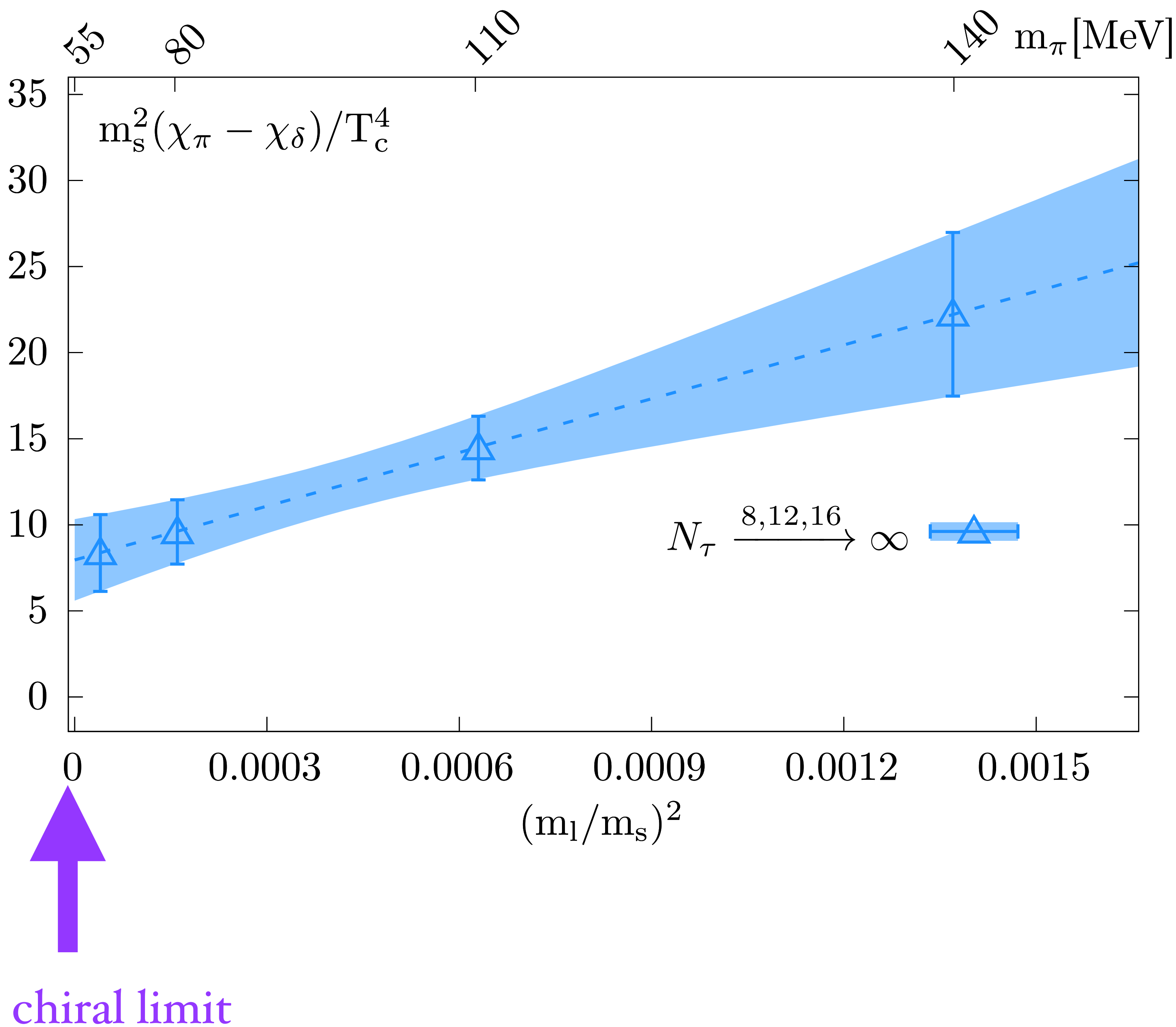


HTD, S.-T. Li, A. Tomiya, S. Mukherjee, X.-D. Wang, 张瑜
arXiv: 2011.04870

- At a single T=205 MeV
- HISQ/tree action
- N_f=2+1:
  - ☑ Nt=8,12,16 (a=0.12,0.08,0.06 fm)
  - ☑ $m_s^{phy}/\mathbf{m_l}$ = 20, 27, 40, 80, 160

    m_π ≈160,140,110, 80, 55 MeV
  - ☑ $9 \geq N_s/N_t \geq 4$

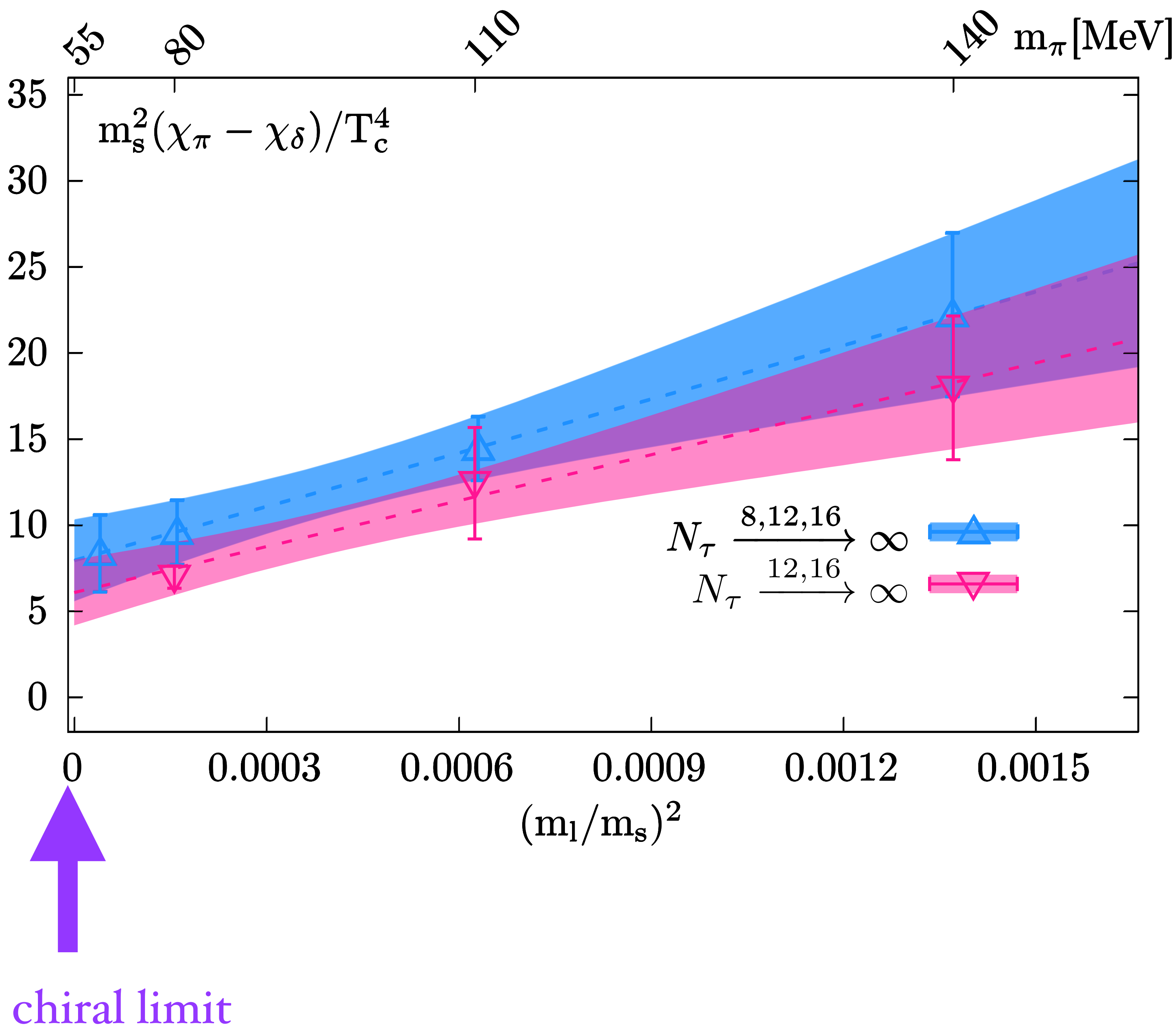
Continuum and chiral extrapolations with $m_\pi \leq 140$ MeV data at T≈ 205 MeV



- **Joint fit**: simultaneous fits
  Continuum: quadratic in $1/N_\tau$
  Chiral: quadratic in quark mass

Value at $N_\tau \to \infty$ and $m \to 0$:
8.0 ± 2.4

Continuum and chiral extrapolations with $m_\pi \leq 140$ MeV data at T≈ 205 MeV



- **Joint fit**: simultaneous fits

  Continuum: quadratic in $1/N_\tau$

  Chiral: quadratic in quark mass

  Value at $N_\tau \to \infty$ and $m \to 0$:
  8.0 ± 2.4

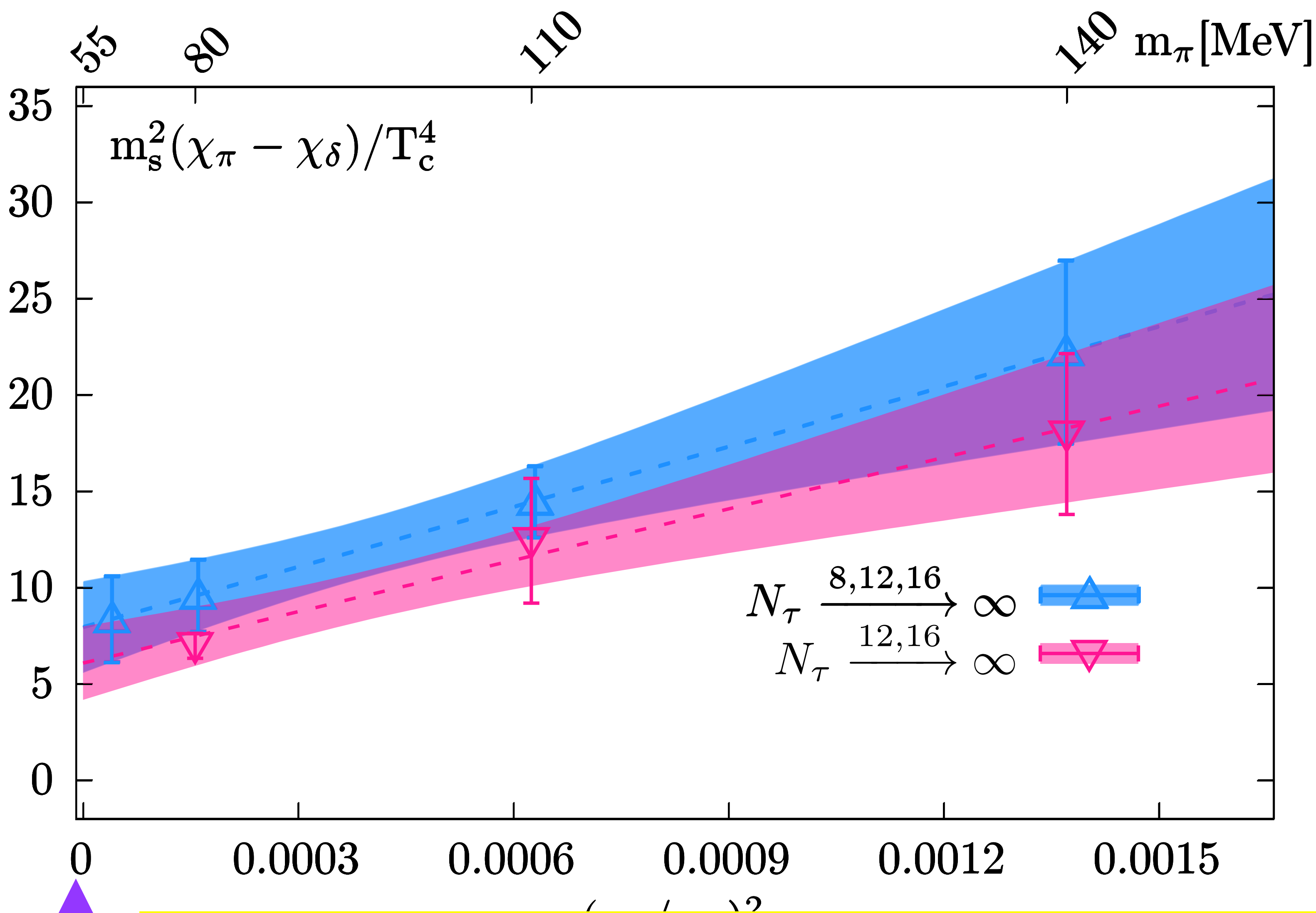
- **Sequential fit:** first continuum and then chiral extrapo.

  Continuum: quadratic in $1/N_\tau$ with N_τ=12 & 16 data

  Chiral: quadratic in quark mass

  Value at $N_\tau \to \infty$ and $m \to 0$:
  6.1 ± 1.9

Continuum and chiral extrapolations with $m_\pi \leq 140$ MeV data at T≈ 205 MeV



- **Joint fit**: simultaneous fits

  Continuum: quadratic in $1/N_\tau$

  Chiral: quadratic in quark mass

Value at $N_\tau \to \infty$ and $m \to 0$:
8.0 ± 2.4

- **Sequential fit:** first continuum and then chiral extrapo.

  Continuum: quadratic in $1/N_\tau$ with N_τ=12 & 16 data

  ...mass

  ...→0 :

Axial anomaly remains manifested in the $U(1)_A$ measure at a 2-3 sigma level

Indication: Chiral phase transition is 2nd order O(4)

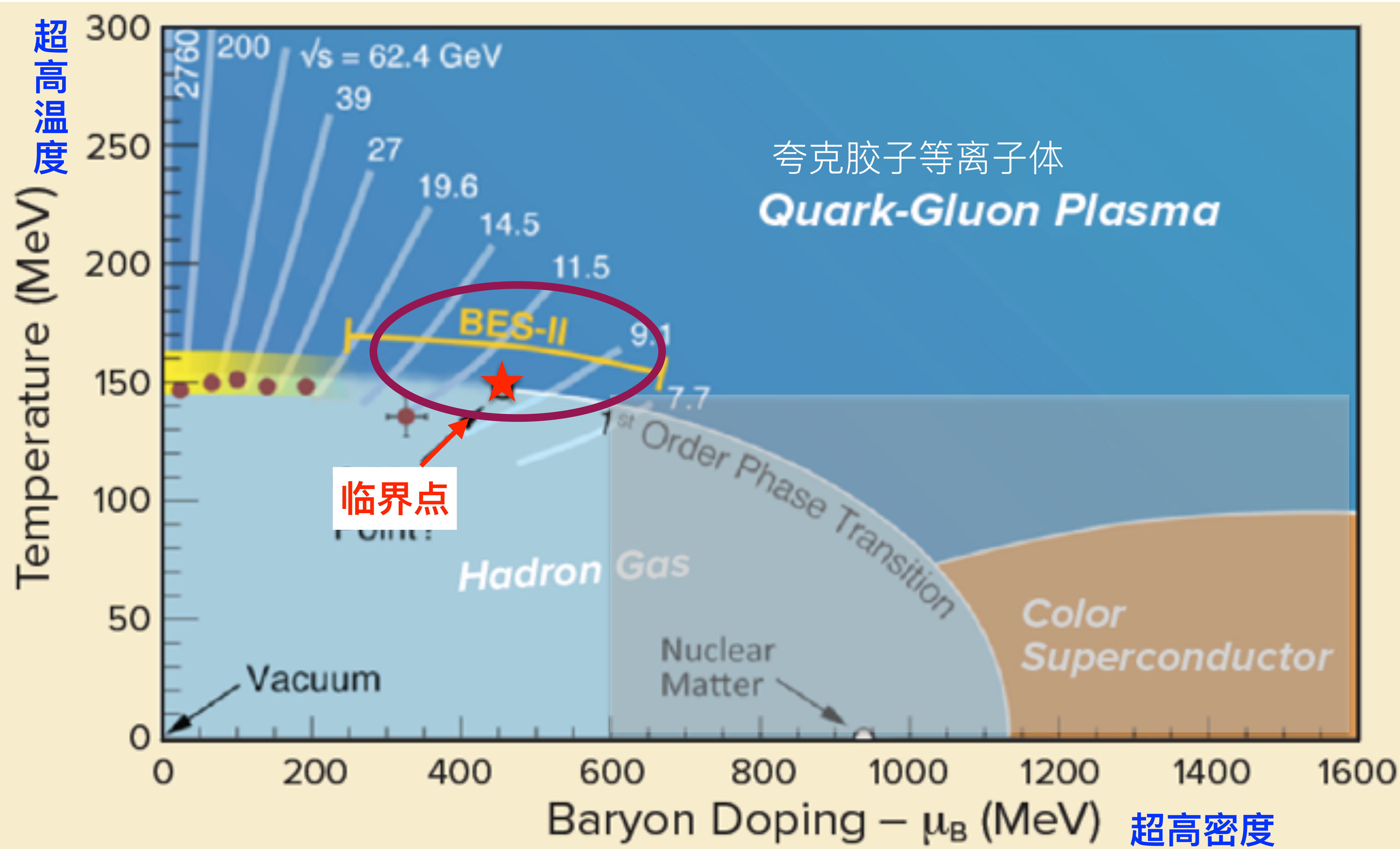
Famous plots

#1: What is the QCD Equation of State (EoS) ?

#2: At what temperature a QGP can be formed ?

#3: What happens if # of baryons is more than that of anti-baryons ?

净重子数目不为零时的QCD 相结构



格点量子色动力学模拟

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\mathcal{U} \ \mathrm{det M_f} \ \mathcal{O} \ \exp(-S_G) \ , \quad Z = \int \mathcal{D}\mathcal{U} \ \mathrm{det M_f} \ \exp(-S_G)$$

重要抽样：$\mathrm{d}P(U) = \dfrac{\det \mathrm{M_f} \ e^{-S_G[U]} \mathcal{D}[U]}{\int \mathcal{D}[U] \ \det \mathrm{M_f} \ e^{-S_G[U]}}$

$\det M_f$ 正定

- γ5-hermiticity: $(\gamma_5 M)^\dagger = \gamma_5 M$ or $M^\dagger = \gamma_5 M \gamma_5$

$$\det[M]^* = \det[M^\dagger] = \det[\gamma_5 M \gamma_5] = \det[M] \Rightarrow \det M \in \mathbb{R}$$

$$0 \le \det[M] \det[M] = \det[M] \det[M^\dagger] = \det[M M^\dagger]$$

Wilson fermion matrix (slide 31) satisfies γ5-hermiticity

非零重子化学势能下的格点QCD模拟

符号问题

$$\mathrm{d}P(U) = \frac{\det \mathrm{M_f}(\mu)\ e^{-S_G[U]}\mathcal{D}[U]}{\int \mathcal{D}[U]\ \det \mathrm{M_f}(\mu)\ e^{-S_G[U]}}$$

为复数　　不正定

γ5-hermiticity 不再成立

$$M^{\dagger}(-\mu) = \gamma_5 M(\mu)\gamma_5$$

- 重要抽样不再适用
- 数值有正又有负，结果非常小，误差基本不能控制：NP-hard Problem (Non-deterministic Polynomial time Problem)
- 凝聚态物理中存在类似问题：Hubbard模型等
- 在传统意义上的计算机一般算法解决不了这个问题
    - 量子计算机?
    - 将NP问题转化成P问题?

CMI

Millennium Prize Problems

Demonstration of the sign problem using a toy model

$$Z = \sum_{\{\phi(x)=\pm 1\}} \mathrm{sign}(\phi)\, e^{-S(\phi)} \;; \quad Z_0 = \sum_{\{\phi(x)=\pm 1\}} e^{-S(\phi)}$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{\{\phi(x)=\pm 1\}} \mathcal{O}(\phi)\mathrm{sign}(\phi)\, e^{-S(\phi)} = \frac{\langle \mathcal{O}(\phi)\, \mathrm{sign}(\phi) \rangle_0}{\langle \mathrm{sign}(\phi) \rangle_0}$$

$$\langle \mathrm{sign}(\phi) \rangle_0 = \frac{Z}{Z_0} = e^{-(f-f_0)V/T} \ll 1$$

$f(f_0)$: free energy density corresponding to $Z(Z_0)$

$$\frac{\Delta \mathrm{sign}(\phi)}{\langle \mathrm{sign}(\phi) \rangle_0} = \frac{\sqrt{\langle \mathrm{sign}^2 \rangle_0 - \langle \mathrm{sign} \rangle_0^2}}{\sqrt{N} \langle \mathrm{sign} \rangle_0} \simeq \frac{e^{(f-f_0)V/T}}{\sqrt{N}} \ll 1 \quad \Rightarrow \quad N \gg e^{2(f-f_0)V/T}$$

Solve the Problem 5.7

in Yagi, Hatsuda & Miake
Quark-Gluon plasma, from big bang to little bang
中文版：王群，马余刚 & 庄鹏飞

Lattice simulations at nonzero μ_B

- Taylor Expansion method, Imaginary chemical potential, Complex Langevin...

- Taylor expansion of the QCD pressure:

Allton et al., Phys.Rev. D66 (2002) 074507
Gavai & Gupta et al., Phys.Rev. D68 (2003) 034506

$$\frac{p}{T^4} = \frac{1}{VT^3} \ln \mathcal{Z}(T, V, \hat{\mu}_u, \hat{\mu}_d, \hat{\mu}_s) = \sum_{i,j,k=0}^{\infty} \frac{\chi_{ijk}^{BQS}}{i!j!k!} \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

☑ Taylor expansion coefficients at μ=0 are computable in LQCD

$$\chi_{ijk}^{BQS} \equiv \chi_{ijk}^{BQS}(T) = \frac{1}{VT^3} \frac{\partial P(T,\hat{\mu})/T^4}{\partial \hat{\mu}_B^i \partial \hat{\mu}_Q^j \partial \hat{\mu}_S^k}\Big|_{\hat{\mu}=0}$$

☑ Thermodynamic quantities can be obtained using relations, e.g.

$$\frac{\epsilon - 3p}{T^4} = T \frac{\partial P/T^4}{\partial T} = \sum_{i,j,k=0}^{\infty} \frac{T\, \mathrm{d}\chi_{ijk}^{BQS}/\mathrm{d}T}{i!j!k!} \left(\frac{\mu_B}{T}\right)^i \left(\frac{\mu_Q}{T}\right)^j \left(\frac{\mu_S}{T}\right)^k$$

lnZ对化学势能μ的偏导 (general susceptibility)

$$\chi_{ijk}^{BQS} \equiv \chi_{ijk}^{BQS}(T) = \frac{1}{VT^3} \frac{\partial P(T,\hat{\mu})/T^4}{\partial \hat{\mu}_B^i \partial \hat{\mu}_Q^j \partial \hat{\mu}_S^k}\Big|_{\hat{\mu}=0} \quad , \quad \frac{p}{T^4} = \frac{1}{VT^3} \ln \mathcal{Z}(T,V,\hat{\mu}_u,\hat{\mu}_d,\hat{\mu}_s)$$

$$Z = \int \mathcal{D}U e^{-S_G} \det M_u^{1/4} \det M_d^{1/4} \det M_s^{1/4}$$

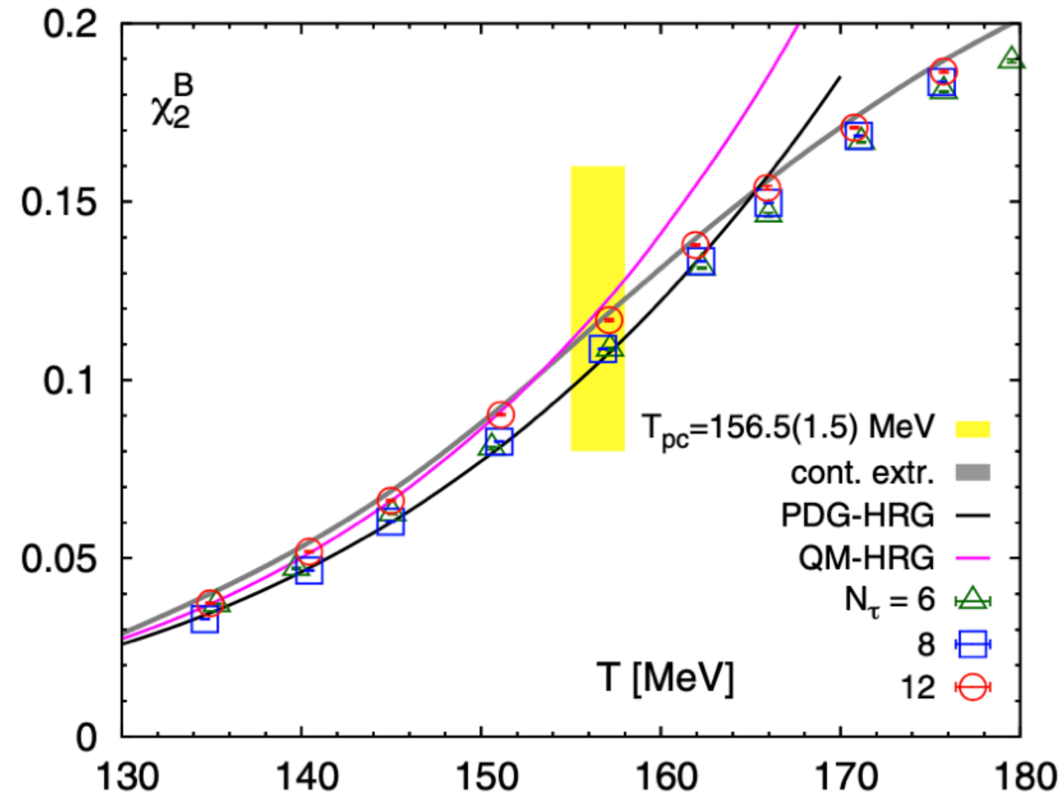
$$\boxed{\frac{\partial \ln \det M}{\partial \mu} = \mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial \mu}\right)}$$

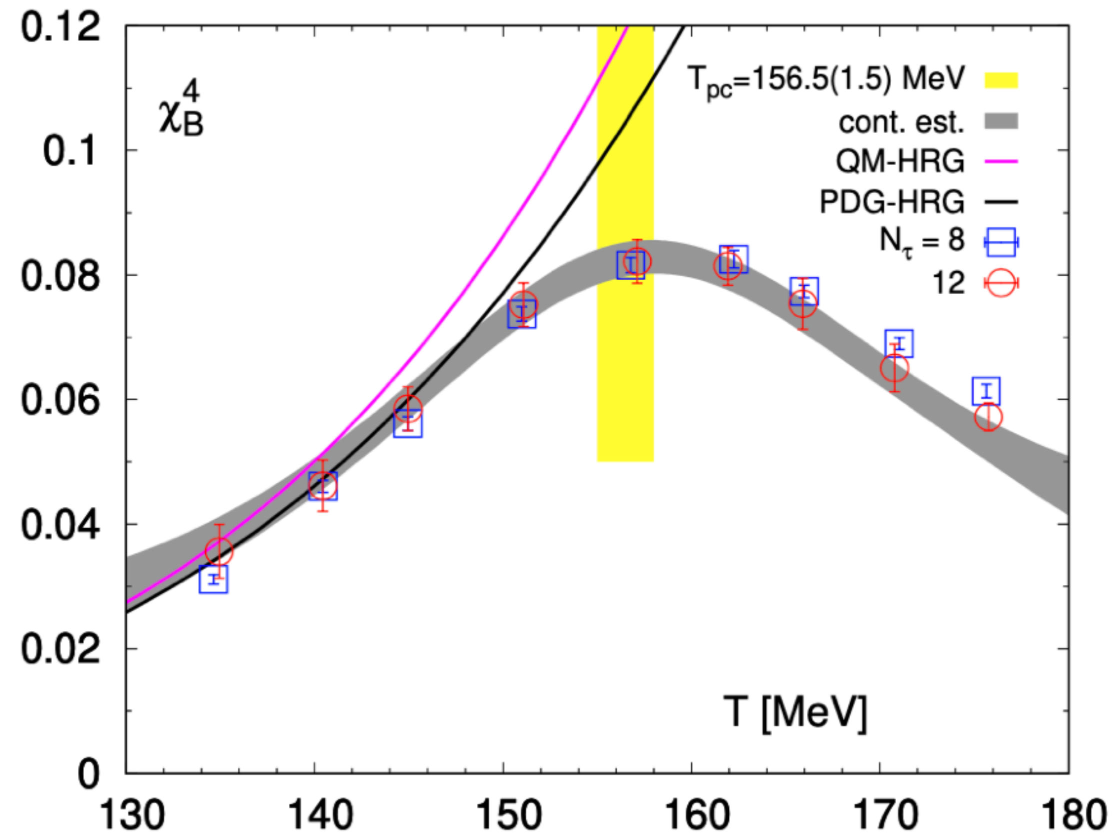
Problem:
Derive

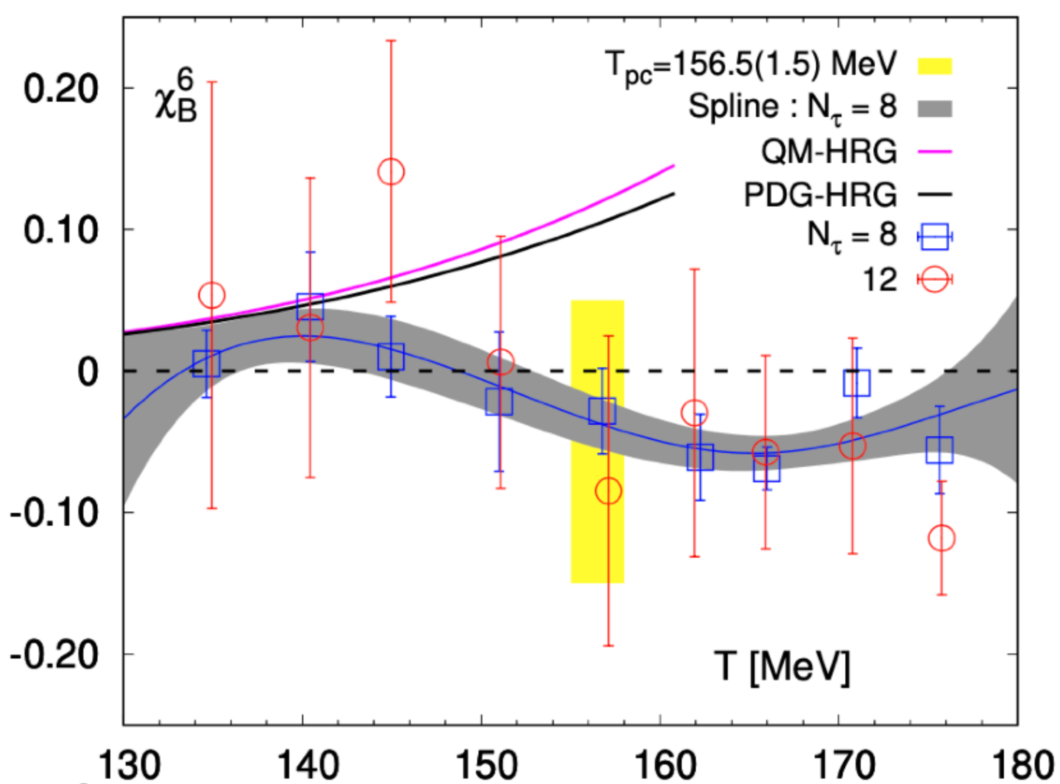
$$\frac{\partial^2 \ln Z}{\partial \mu^2} = \left\langle \frac{n_f}{4} \frac{\partial^2 (\ln\ \det\ \mathrm{M})}{\partial \mu^2} \right\rangle + \left\langle \left(\frac{n_f}{4} \frac{\partial (\ln\ \det\ \mathrm{M})}{\partial \mu} \right)^2 \right\rangle$$

$$\mathrm{Tr}\left(M^{-1}\frac{\partial^2 M}{\partial \mu^2}\right) - \mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial \mu} M^{-1}\frac{\partial M}{\partial \mu}\right) \qquad \mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial \mu}\right)$$

Taylor expansion coefficients at μ_B=0



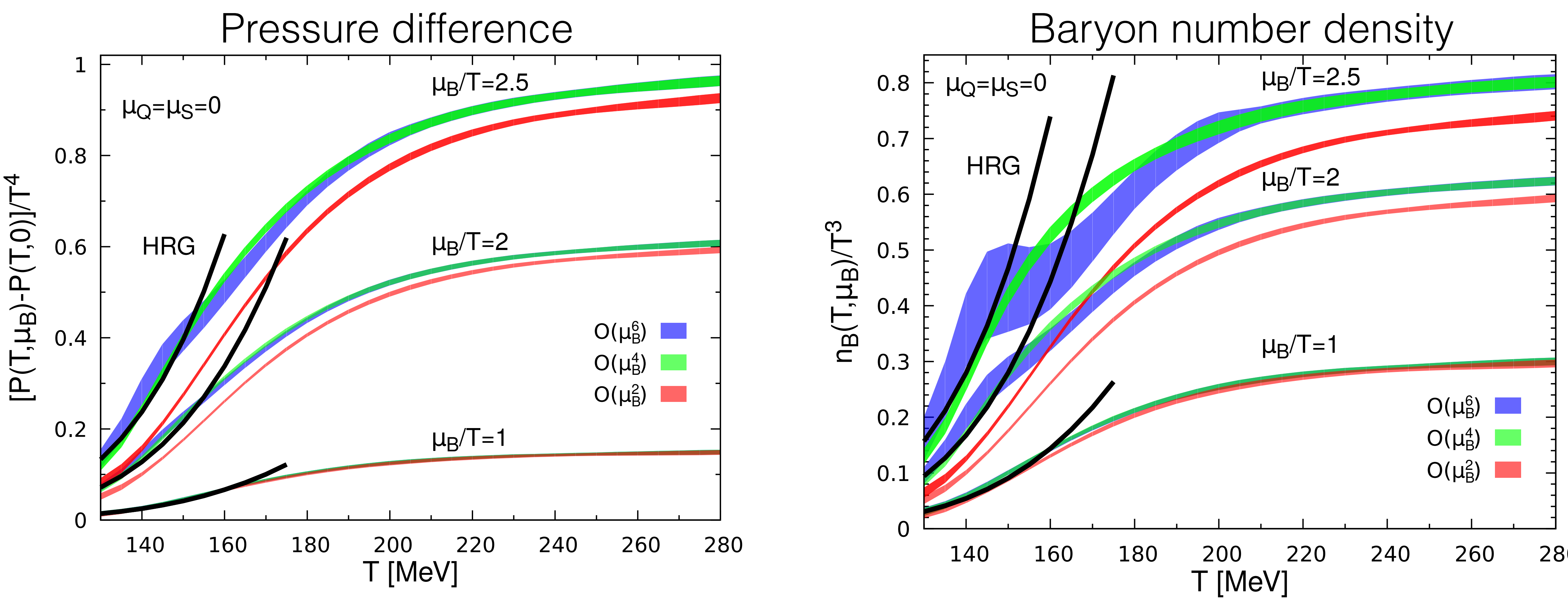




$$\chi_n^B(T) = \frac{\partial^n P(T,\mu_B)/T^4}{\partial \hat{\mu}_B^n}\Big|_{\hat{\mu}_B=0}$$

Famous plots #3:

QCD Equation of State at small baryon density



A. Bazavov, HTD. P. Hegde et al.,[HotQCD], Phys.Rev.D 95 (2017) 5, 054504
Cited by 370 records

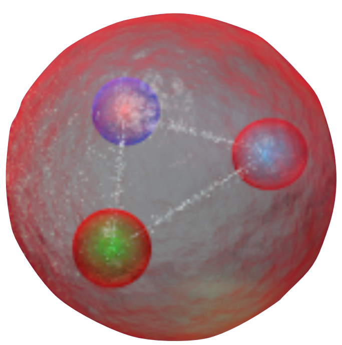
$$\frac{P(T,\mu_B)-P(T,0)}{T^4}=\sum_{n=1}^{\infty}\frac{\chi_{2n}^B(T)}{(2n)!}\left(\frac{\mu_B}{T}\right)^{2n}=\frac{1}{2}\chi_2^B(T)\hat{\mu}_B^2\left(1+\frac{1}{12}\frac{\chi_4^B(T)}{\chi_2^B(T)}\hat{\mu}_B^2+\frac{1}{360}\frac{\chi_6^B(T)}{\chi_2^B(T)}\hat{\mu}_B^4+\cdots\right)$$

The EoS is well under control at $\mu_B/T \lesssim 2$ or $\sqrt{s_{NN}} \gtrsim 12$ GeV

Changes of degree of freedom in thermal QCD

Baryon number —> B

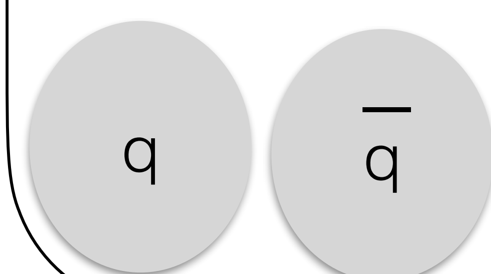
Baryon number fluctuation —> B^2



Bound state of quarks

B=1, -1

B^2=1

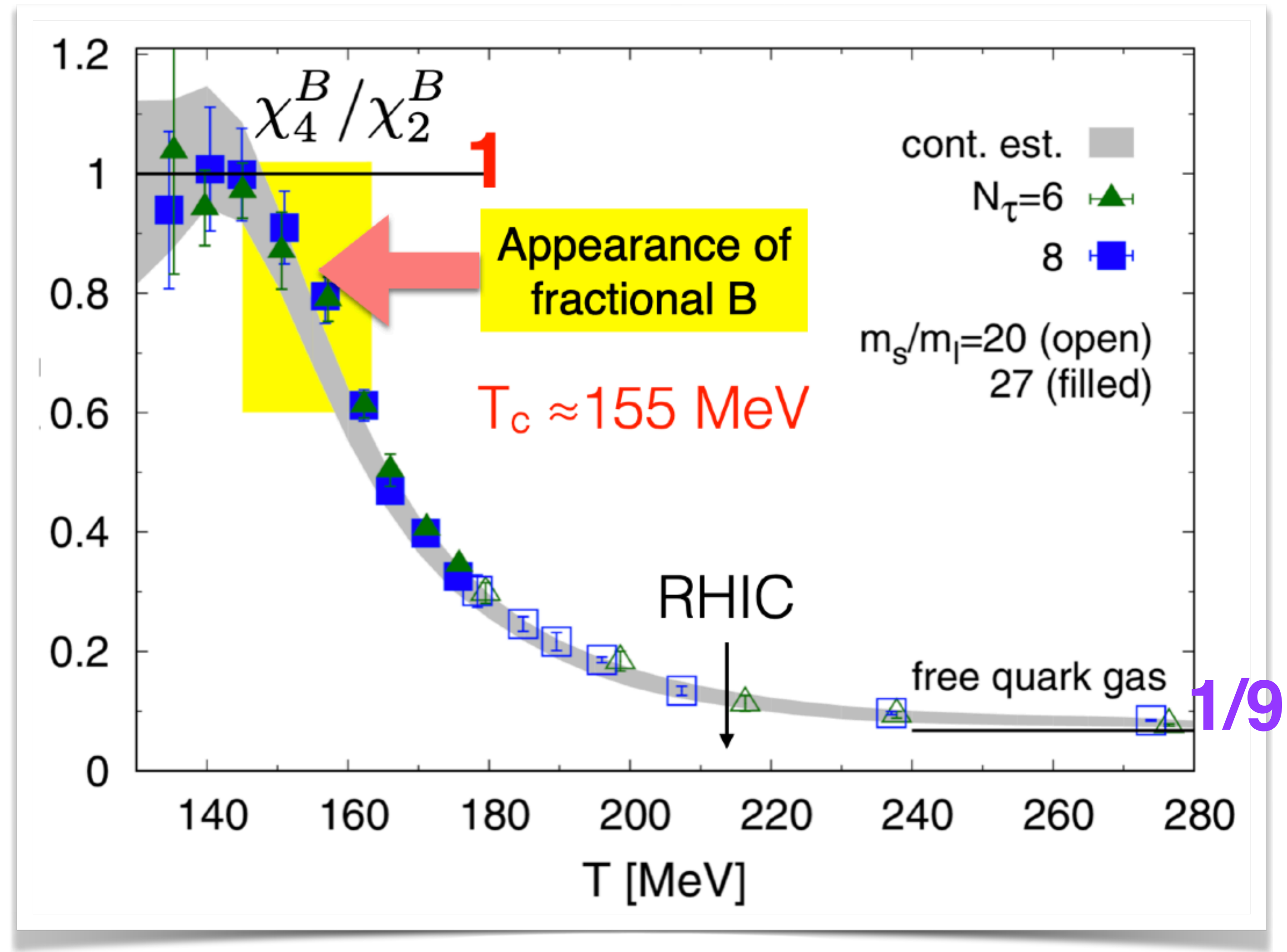


Unbounded quarks

B=1/3, -1/3

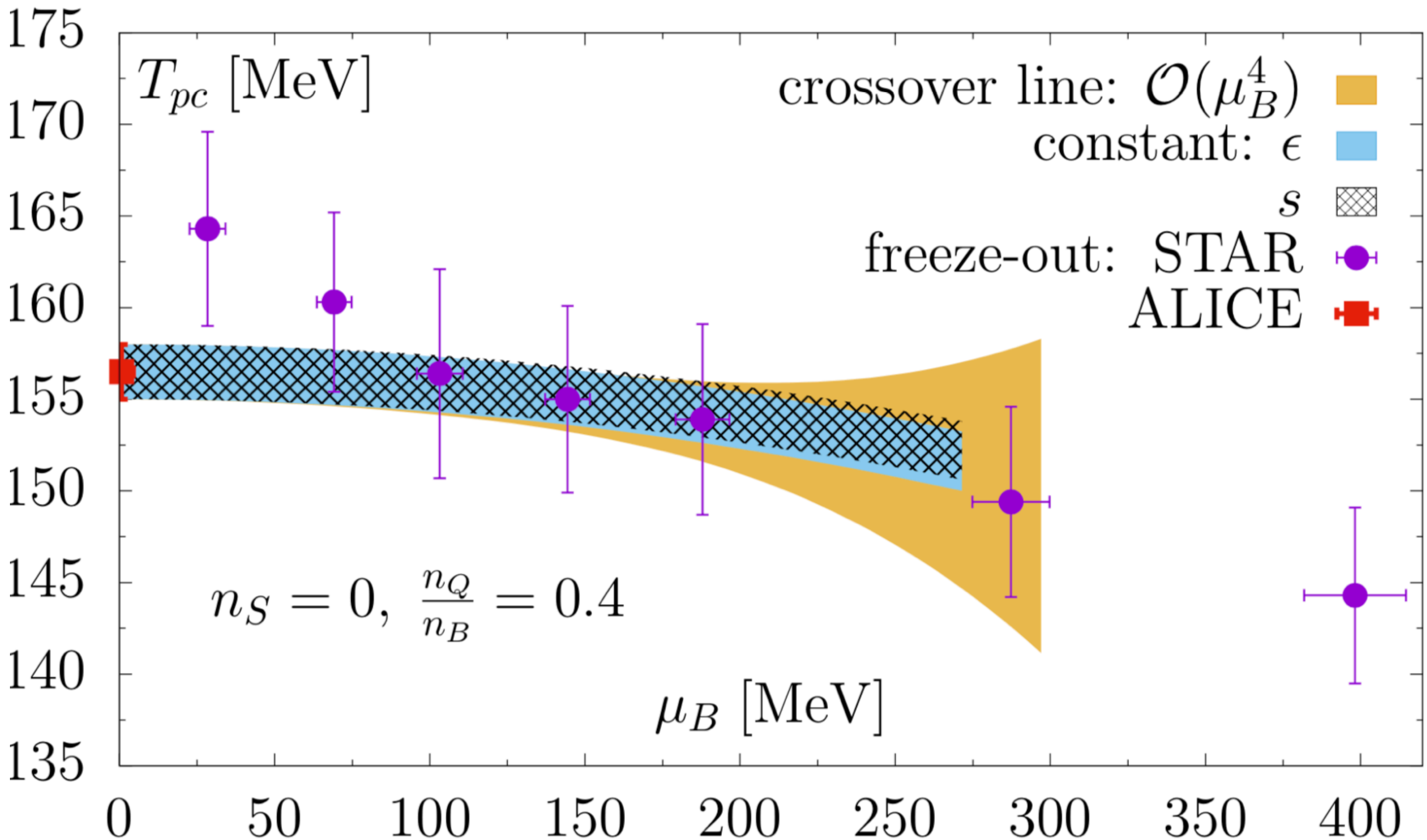
B^2=1/9

measure of fluctuations of B



Bielefeld-BNL-CCNU: PRL 111(2013) 082301, PLB 737(2014) 210

Chiral crossover line: $T_{pc}(\mu_B) = T_{pc}(0)\left(1 - \kappa_2\left(\frac{\mu_B}{T}\right)^2 - \kappa_4\left(\frac{\mu_B}{T}\right)^4\right)$



A. Bazavov, **丁亨通**, P. Hegde et al. [HotQCD],
Phys. Lett. B795 (2019) 15, 总被引386次

hot & dense lattice QCD

Other contents/frontiers not covered but very important

electrical conductivity & baryon diffusion

energy loss of heavy quark in hot & dense medium

thermal dilepton & photon emission from QGP

shear & bulk viscosities

fate of heavy quarkonia

QCD in the external magnetic field

…

See recent reviews:

HTD, F. Karsch, S. Mukherjee, Int. J. Mod. Phys. E 24 (2015) no.10, 1530007

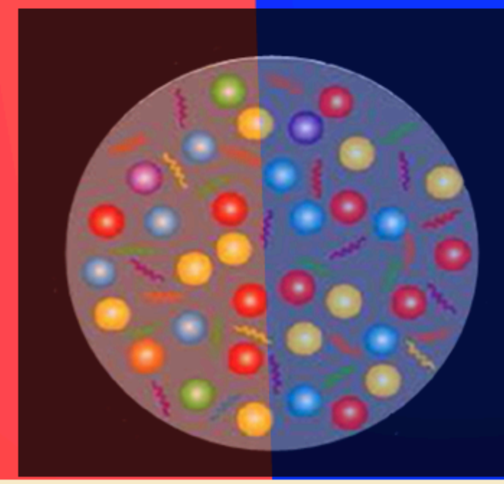
plenary talks@lattice conference: HTD, arXiv:1702.00151, S. Kim, arXiv:1702.02297

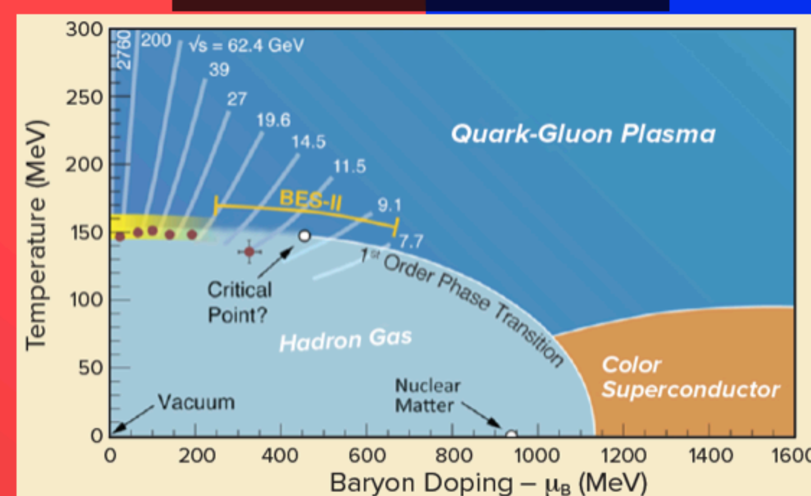
C. Schmidt & S. Sharma, arXiv:1701.04707

G. Endrodi, PoS CPOD2014 (2015) 038

实验

唯象





理论

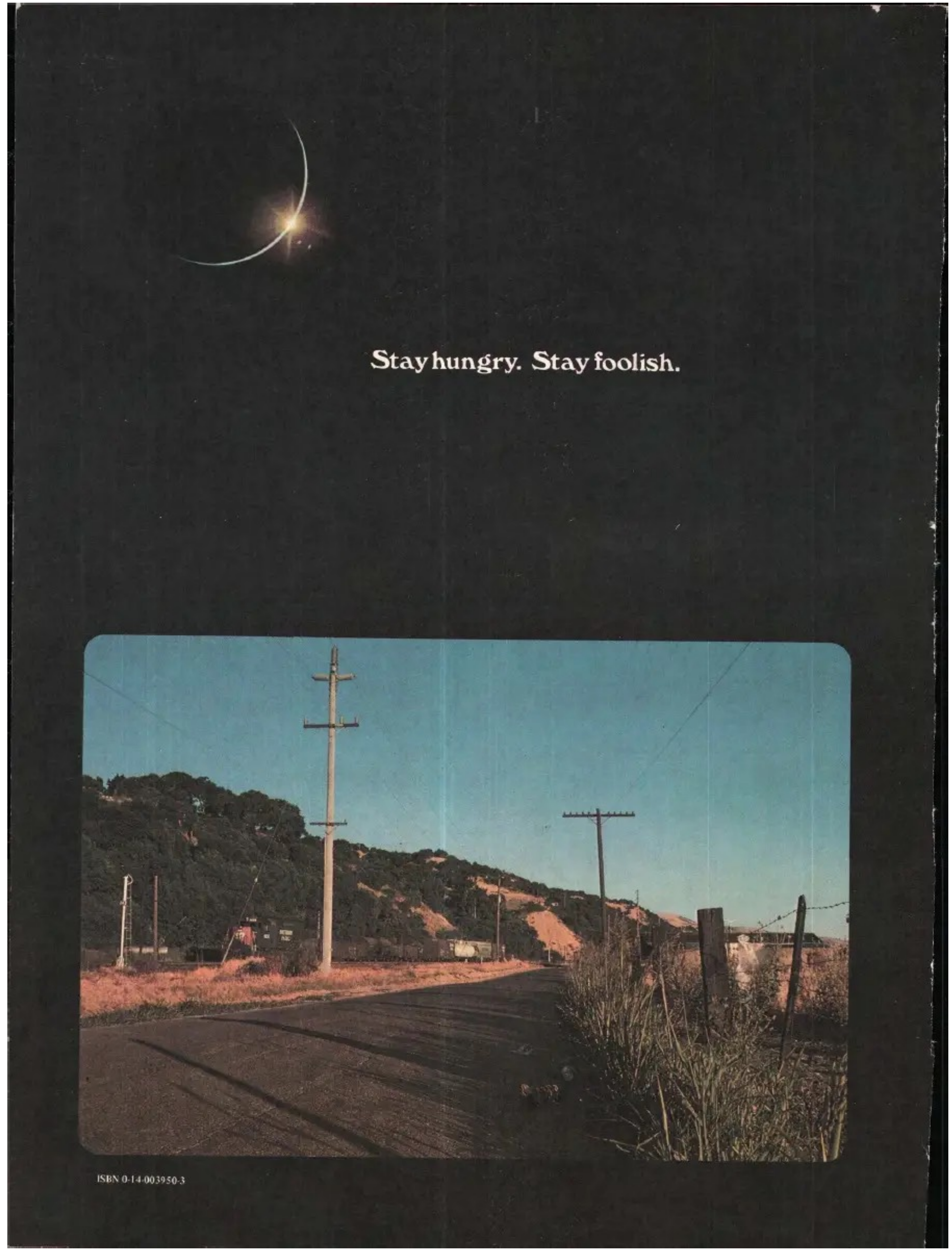
格点量子色动力学(第一性原理超算)

微扰量子色动力学

有效理论

...

结束语



#1180 October 1974 titled *Whole Earth Epilog*