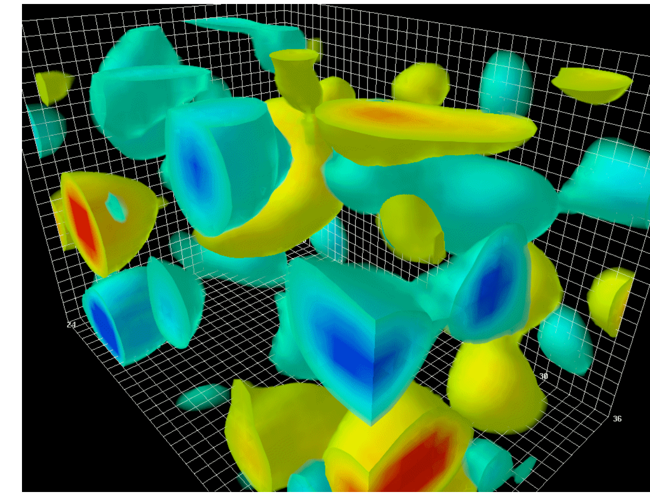
Nuclear Science Computing Center at CCNU



Brief Introduction to Lattice Quantum ChromoDynamics

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原子核结构与中高能重离子碰撞交叉学科理论讲习班
湖州师范学院，2021.7.17

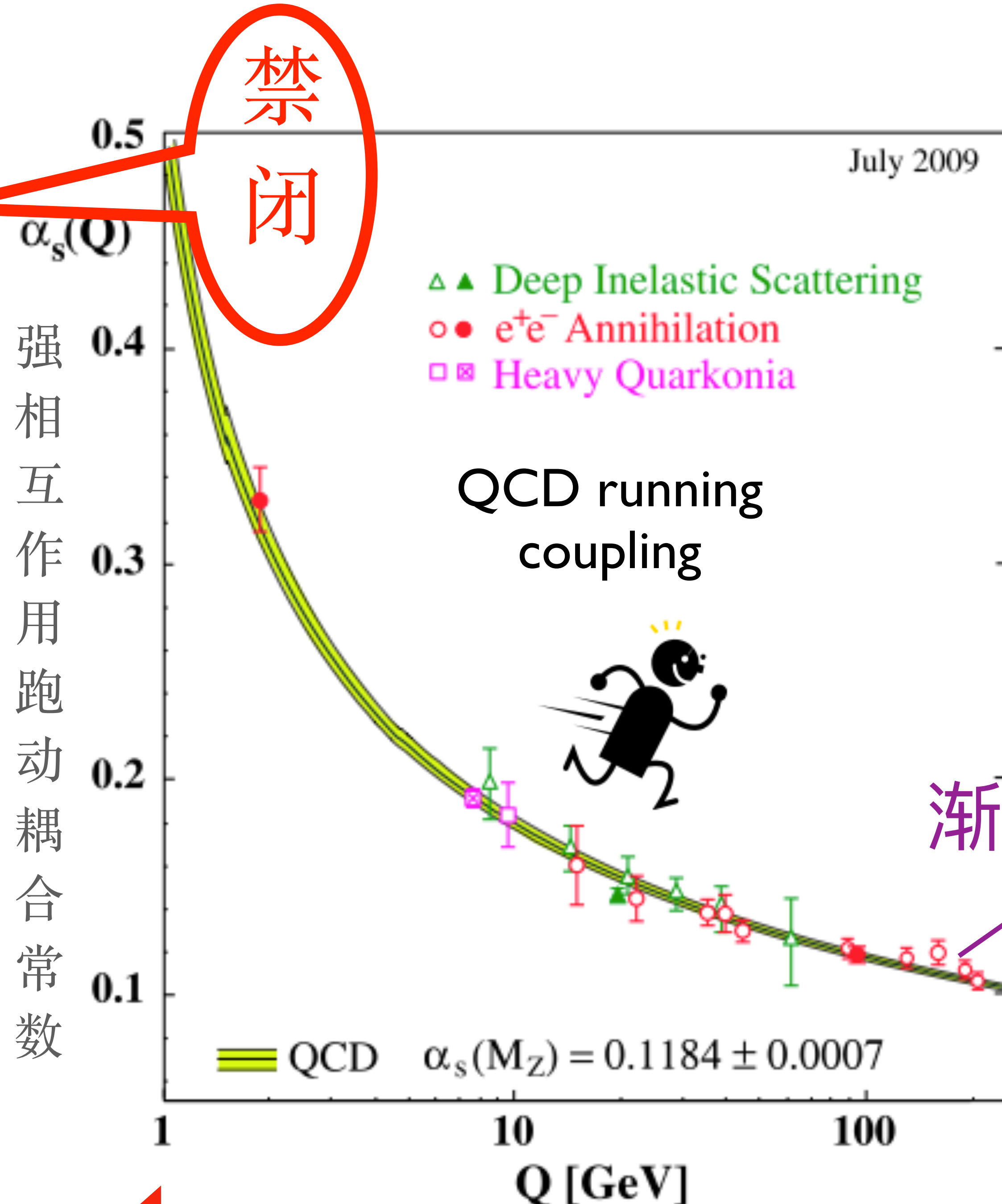
Outline

- What is Lattice QCD (LQCD) ? — 10 min
- LQCD simulations — 25 min
- Famous plots — 40 min
- Questions — 15 min

强相互作用特性：渐近自由与禁闭

Millennium Prize Problems

非微扰



渐近自由

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

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

Confinement of quarks*

Kenneth G. Wilson

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

(Received 12 June 1974)

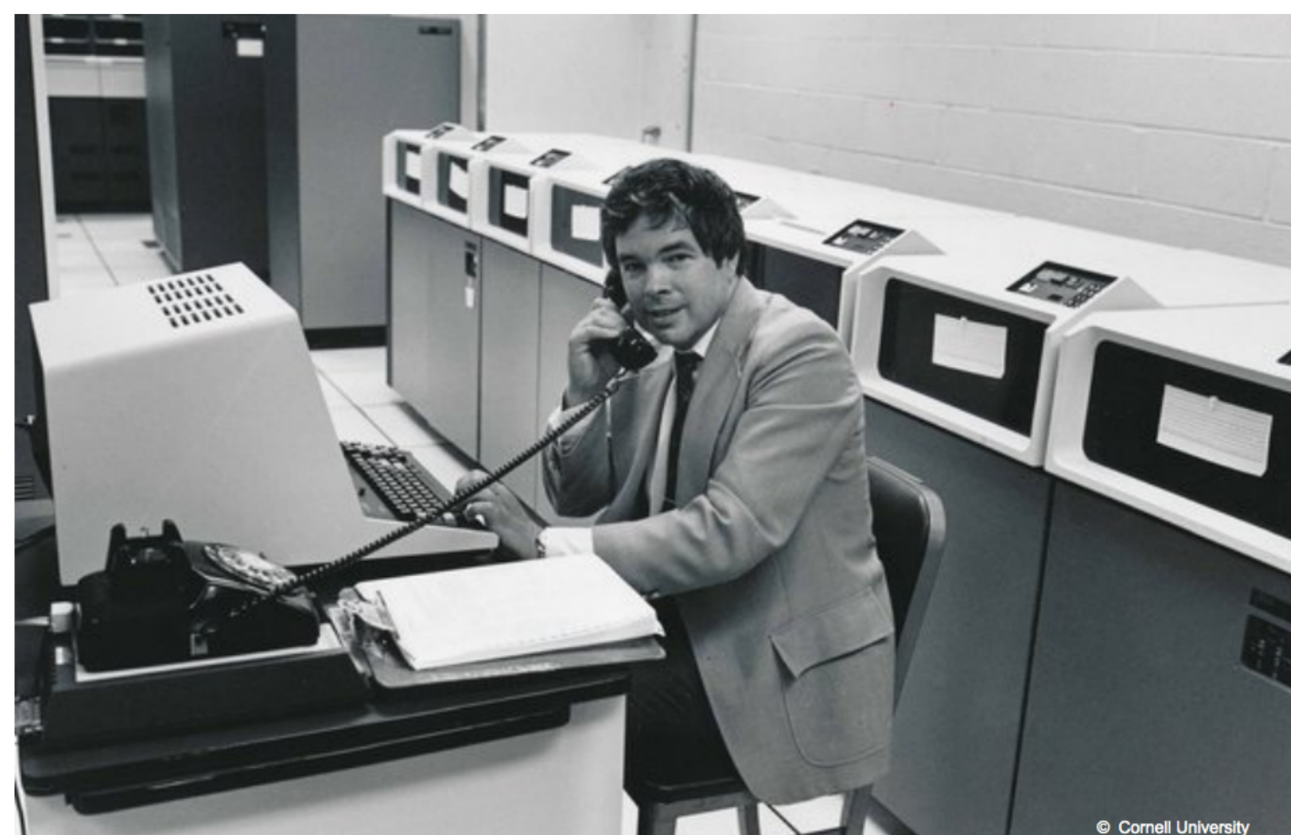
用来理解自然界中
为什么不存在自由的夸克

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

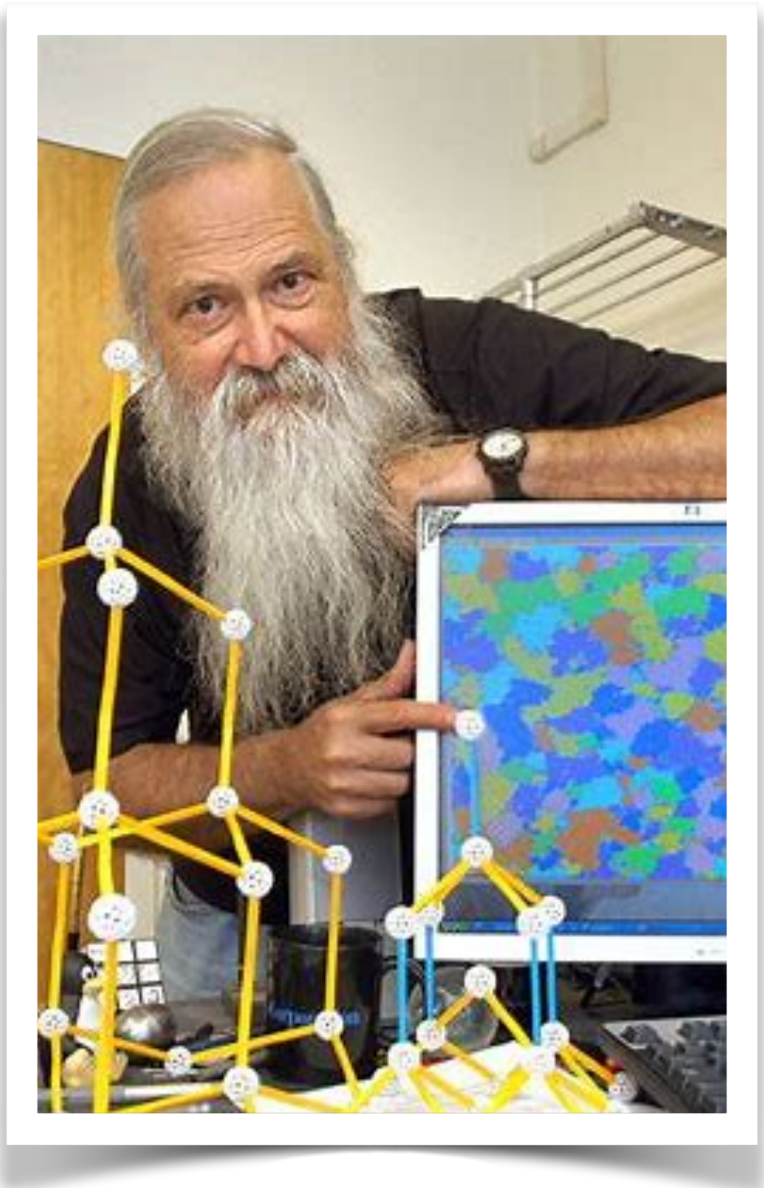
1982



First numerical lattice simulations

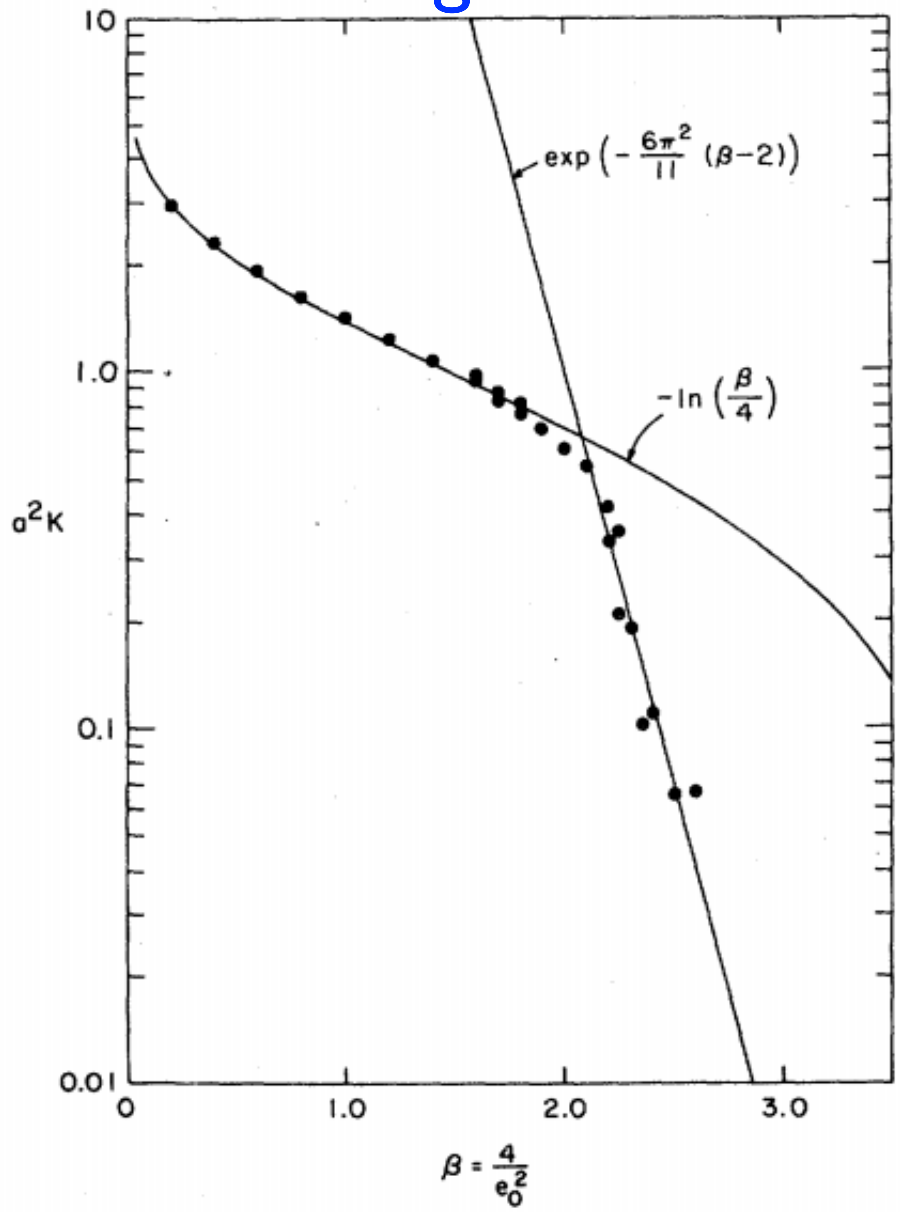
Spawned golden age in lattice QCD

M. Creutz, PRD 1980



Michale Creutz
@BNL

string tension



lattice gauge coupling

Michale Creutz
on the beach

arXiv: hep-lat

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

arXiv.org

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- General Relativity and Quantum Cosmology (**gr-qc**
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- High Energy Physics - Lattice (**hep-lat** new, recent,
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格点量子色动力学在中国

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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。

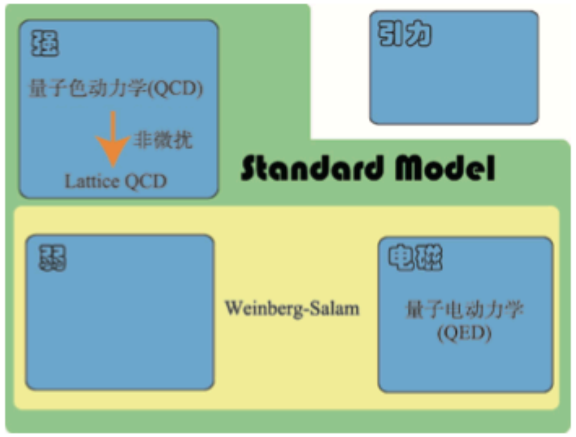


图1 格点QCD在标准模型中的相对位置的示意图

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

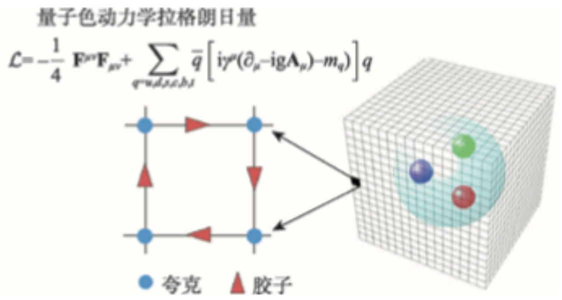


图2 格点QCD中,夸克和反夸克场被定义在格点上,而规范场则定义在相邻两格点间的链接上

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

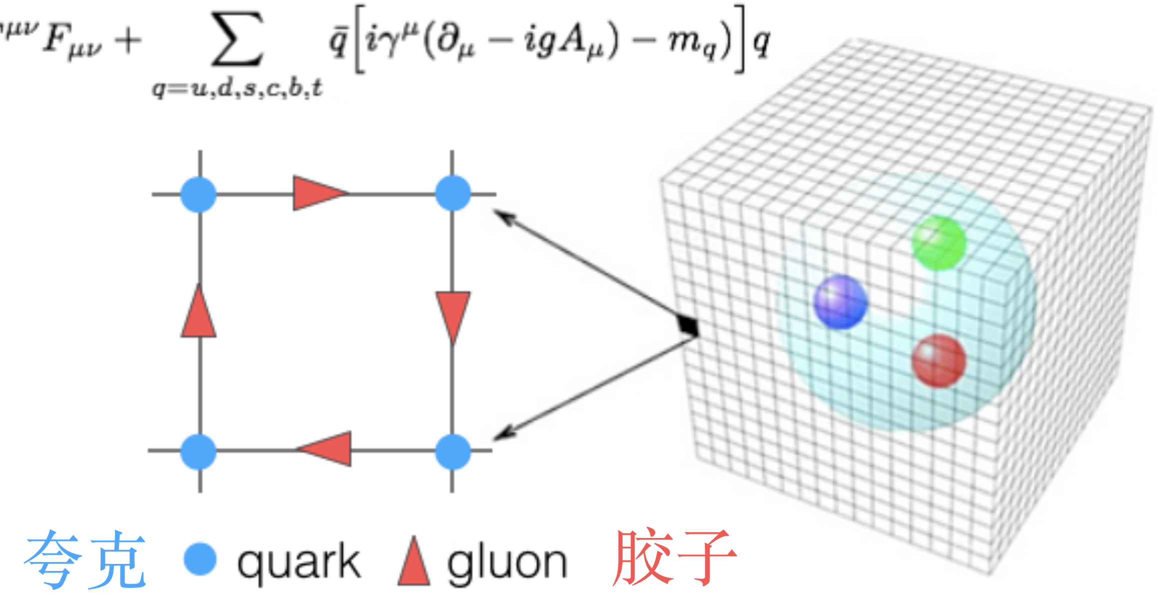
主办单位：华中师范大学
协办单位：北京大学, 清华大学, 南开大学, 浙江大学, 四川大学, 湖南师范大学, 江苏大学, 西安工业大学, 台湾交通大学, 中科院高能物理研究所，中科院近代物理研究所, 中科院理论物理研究所

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

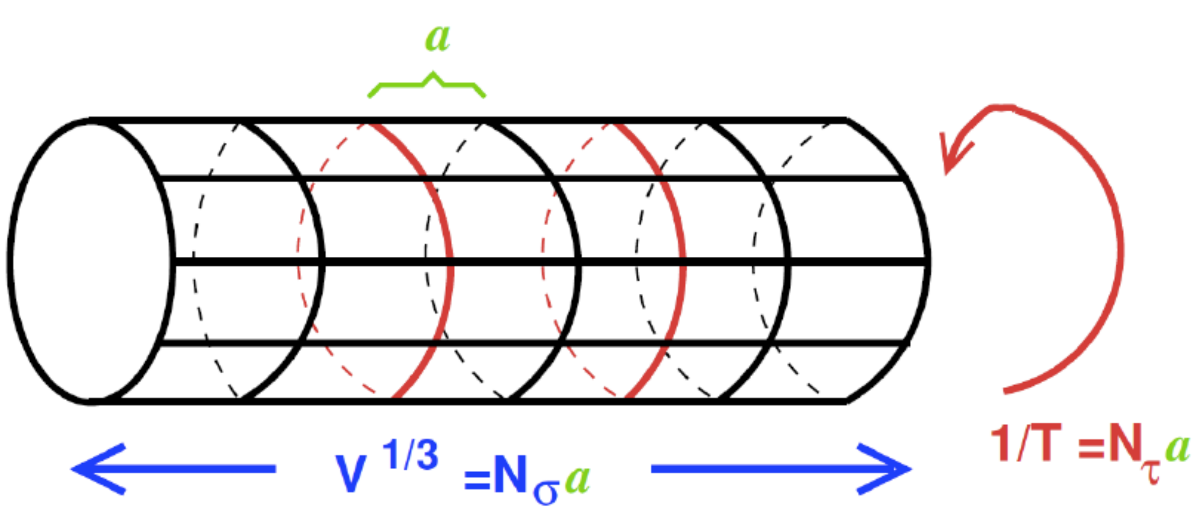
QCD Lagrangian 量子色动力学拉格朗日量

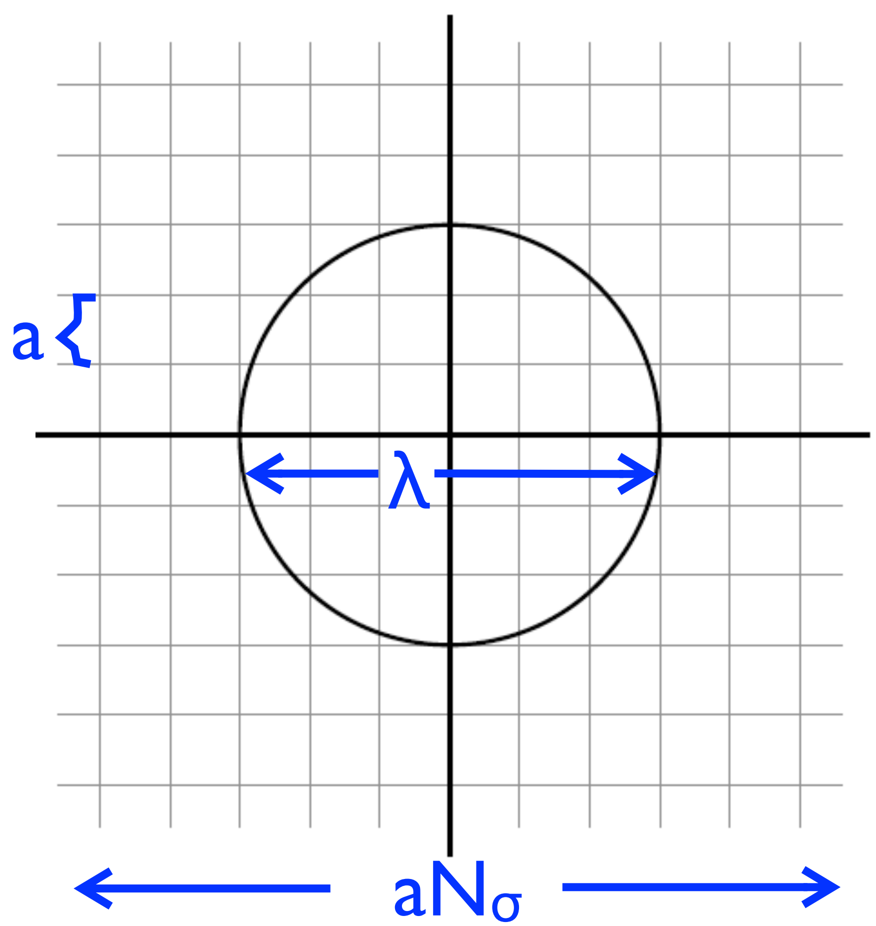
$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q}\left[i\gamma^{\mu}(\partial_{\mu} - igA_{\mu}) - m_q\right]q$$



- 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

setup of Lattice QCD simulations





- Four dim. Euclidean lattice
  $N_\sigma^3 \times N_\tau$
- Temperature $T = 1/(N_\tau a)$
- $a \ll \lambda \ll N_\sigma a$

Thermodynamic limit: V→0
Continuum limit: a→0

Input parameters

- lattice gauge coupling: $\beta (= 6/g^2)$
- quark masses
- lattice size: $N_\tau,\ N_\sigma$

No free parameters
input bare parameters of QCD Lagrangian
fixed by reproducing physics at T=0

格点量子色动力学：高维度数值积分

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\mathcal{U}\, \mathcal{D}\psi\, \mathcal{D}\bar{\psi}\, \mathcal{O}\, \exp(-S_{LQCD})$$

- Z：配分函数
- $\mathcal{D}$：路径积分
- $\mathcal{U}$：胶子场
- ψ：夸克场
- $\bar{\psi}$：反夸克场
- S_{LQCD}：格点QCD作用量

路径积分维度： $N_c \otimes N_f \otimes N_{spin} \otimes N_d \otimes N_s^3 \otimes N_t \gtrsim 10^9$

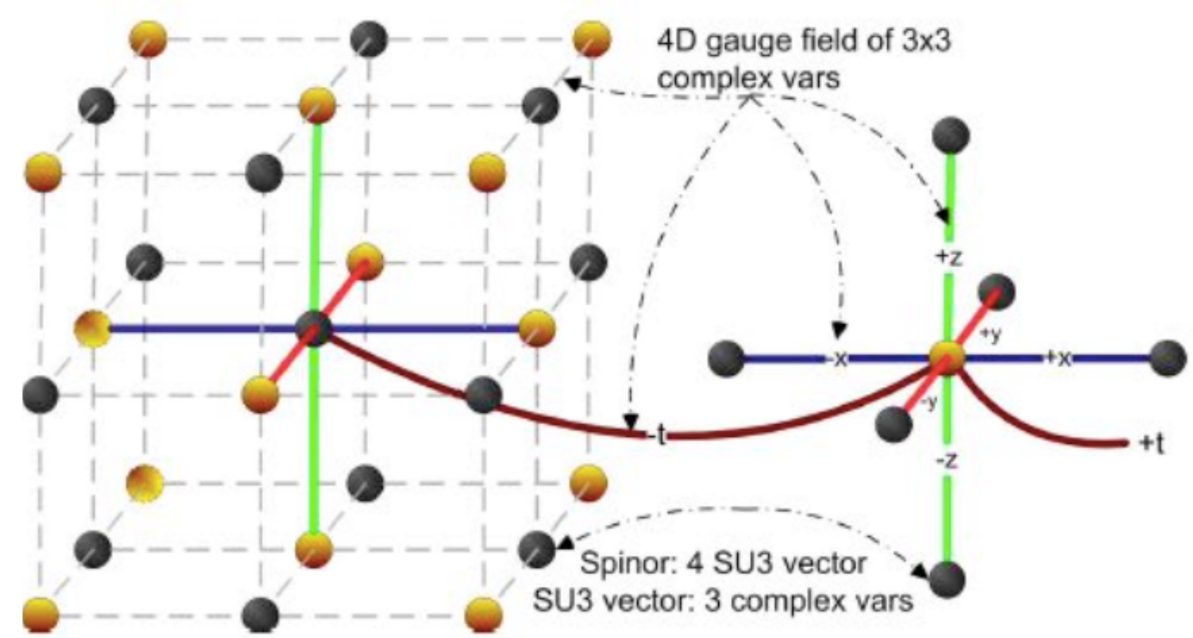
颜色	味道	自旋	维度	空间点数	时间点数
3	3	2	4	～48	～12

格点量子色动力学：高维度数值积分

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \, \mathcal{D}\psi \, \mathcal{D}\bar{\psi} \, \mathcal{O} \, \exp(-S_{LQCD})$$

配分函数 路径积分 胶子场 夸克场 反夸克场 格点QCD作用量

- 4 dimensional grid (=Lattice)
    - quarks live on lattice sites
    - gluons live on the links
- typical sizes 24^3x6 to 256^4
    - parallelization over lattice sites (10^5 to 10^9)



格点量子色动力学模拟

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

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

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

Un: 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对化学势能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

最简单的情形: 对矩阵的逆求迹

- 二次平均: 组态平均+随机平均

I. 组态平均

$$\langle \mathrm{Tr} M^{-1} \rangle = \lim_{N_{conf}\to\infty} \frac{1}{N_{conf}} \sum_{k=1}^{N_{conf}} \left(\mathrm{Tr} M^{-1}\right)_k$$

N_{conf}: ~20000
组态(configuration)数目

II: 随机平均：Random Noise Method

$$\left(\mathrm{Tr} M^{-1}\right)_k = \lim_{N_{rv}\to\infty} \frac{1}{N_{rv}} \sum_{j=1}^{N_{rv}} \eta_j^\dagger M_k^{-1} \eta_j$$

N_{rv}: ~2000
随机向量(random noise vector)数目

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} \eta_{ki}^* \eta_{kj} = \delta_{ij}$$

一般需要10^7次求逆

Challenges in computations of higher order fluctuations

8th order susceptibility/ fluctuation

$$\frac{\partial^8 \ln\det M}{\partial\mu^8} = \mathrm{tr}\left(M^{-1}\frac{\partial^8 M}{\partial\mu^8}\right) - 8\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^7 M}{\partial\mu^7}\right)$$
$$-28\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^6 M}{\partial\mu^6}\right) - 56\mathrm{tr}\left(M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial^5 M}{\partial\mu^5}\right)$$
$$-35\mathrm{tr}\left(M^{-1}\frac{\partial^4 M}{\partial\mu^4}M^{-1}\frac{\partial^4 M}{\partial\mu^4}\right) + 56\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^6 M}{\partial\mu^6}\right)$$
$$+168\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^5 M}{\partial\mu^5}\right) + 168\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^5 M}{\partial\mu^5}\right)$$
$$+280\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial^4 M}{\partial\mu^4}\right) + 280\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^4 M}{\partial\mu^4}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$
$$+420\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^4 M}{\partial\mu^4}\right) + 560\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$
$$-336\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^5 M}{\partial\mu^5}\right)$$
$$-840\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^4 M}{\partial\mu^4}\right)$$
$$-840\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^4 M}{\partial\mu^4}\right)$$
$$-840\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^4 M}{\partial\mu^4}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$
$$-1120\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$
$$-560\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$
$$-1680\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$

M: fermion matrix

Challenges in computations of higher order fluctuations

8th order susceptibility/ fluctuation

Too many inversions!

$$-1680\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$-1680\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$-630\mathrm{tr}\left(M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$+1680\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^4 M}{\partial\mu^4}\right)$$

$$+3360\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$

$$+3360\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$

$$+3360\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$+3360\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$+5040\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$+5040\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$-6720\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)$$

M: fermion matrix

$$-10080\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$-10080\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$-5040\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$+20160\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)$$

$$-5040\mathrm{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}\right)$$

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

—Norman Christ, Columbia

New Computer Architectures For Lattice QCD

Peter Batacan

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

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Peter Batacan

1989

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—Thomas Nash, Fermilab

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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！

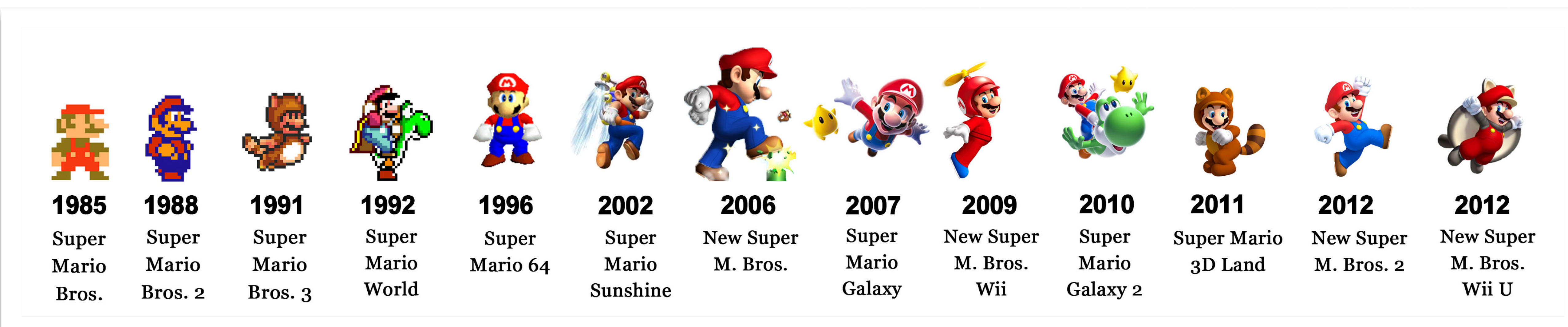
Lattice QCD as a video game

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



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

- 简称： **NSC³**

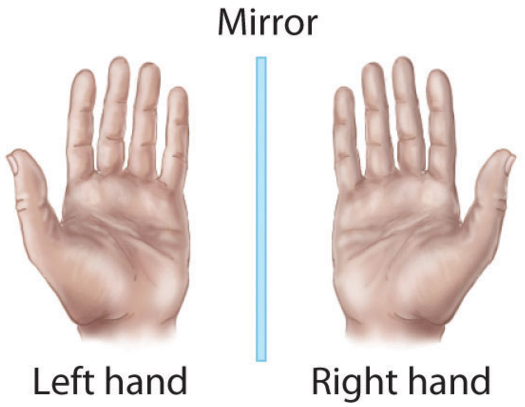
N: Nuclear， **S**: Science， **C³**: Color 3 -> QCD

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 禁闭

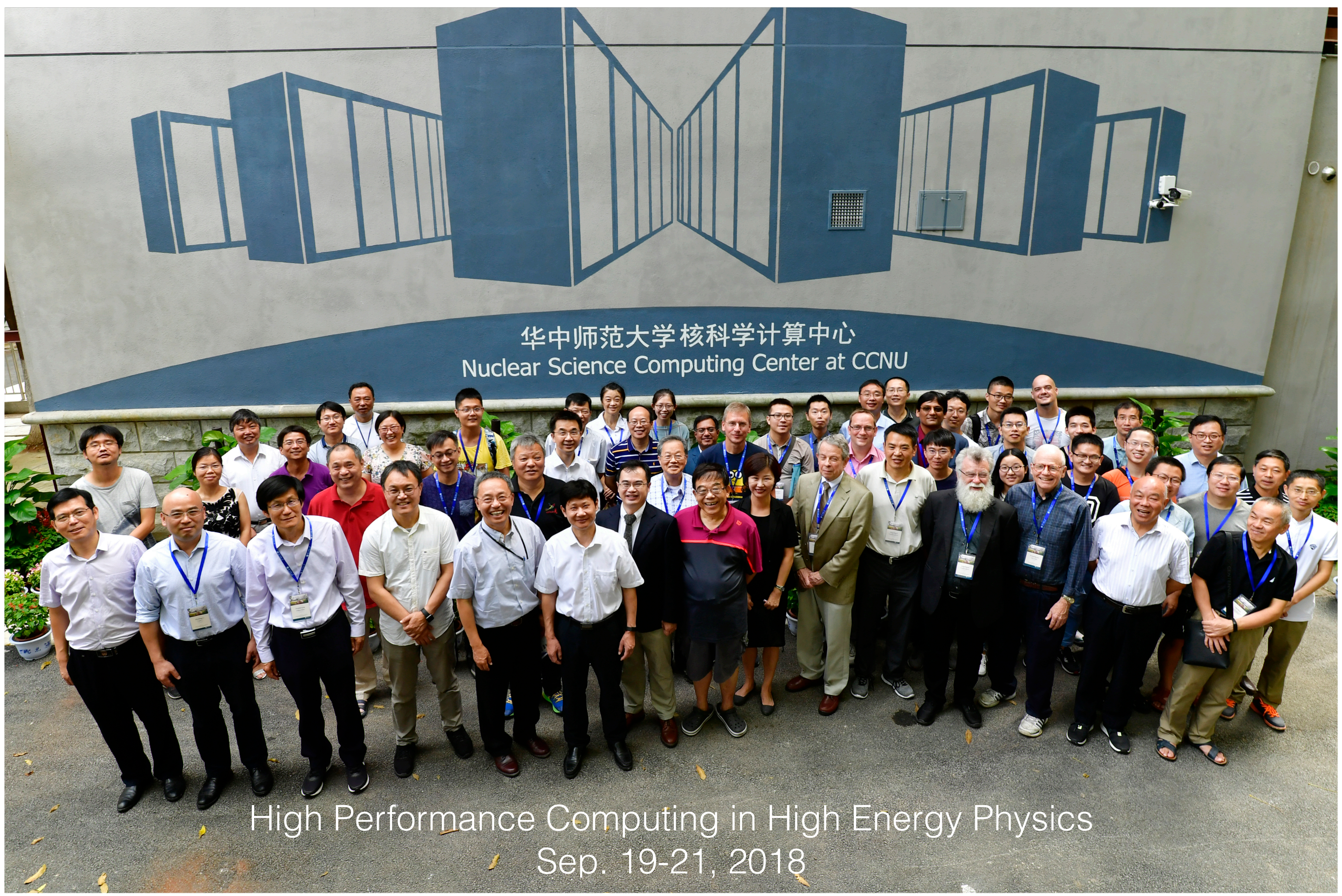
Chirality 手征



Criticality 临界行为

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

国内首个格点QCD专用超算平台，国内最快！



38 computing nodes
(304 V100 GPUs)
Peak performance:
2 PFlops/s
(每秒2千万亿次浮点运算)
Storage:
1 PB

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

计算决定未来

国内首个格点QCD专用超算平台，国内最快！

38 computing nodes
(304 V100 GPUs)
Peak performance:
2 PFlops/s
(每秒2千万亿次浮点运算)
Storage:
1 PB

June, 2021
TOP 500 The List.
The GREEN 500

国内首个格点QCD专用超算平台，国内最快!

8 nodes in each rack
8 GPUs in each node
On 1-single GPU:
64^3x16, 72^3x12

38 computing nodes
(304 V100 GPUs)
Peak performance:
2 PFlops/s
(每秒2千万亿次浮点运算)
Storage:
1 PB

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

国内首个格点QCD专用超算平台，国内最快！

GPU Hackathon（黑客马拉松）

- 针对人群：
  1）想优化GPU应用程序的研究团队
  2）想把CPU程序移植到GPU上的研究团队
- 指导专家：英伟达公司及业内GPU和计算机专家
- 时间：每年春天
- 地点：华中师范大学核科学计算中心

GPU Hackathon 2020
http://physics.ccnu.edu.cn/info/1045/3637.htm

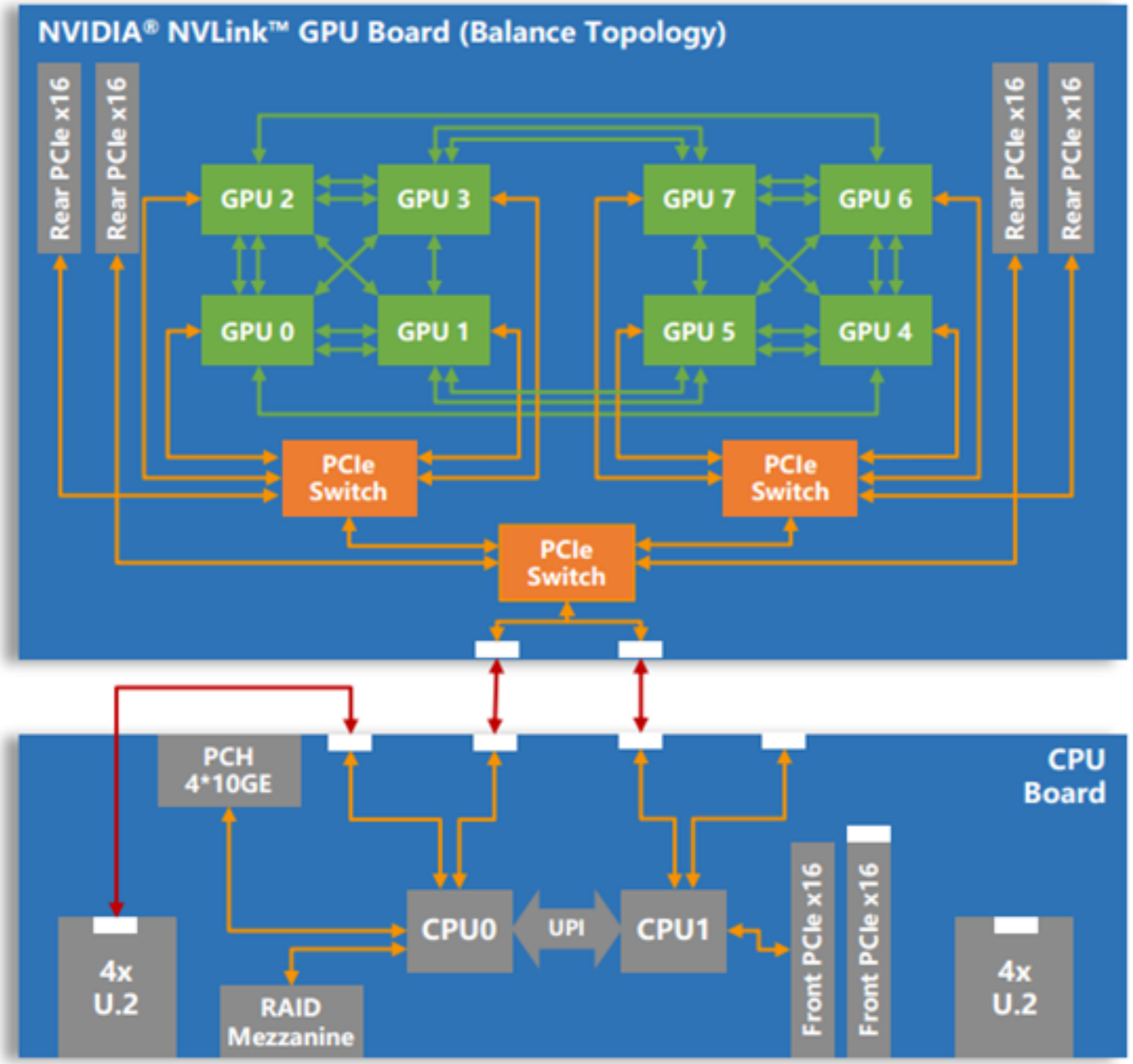
GPU Hackathon 2021
http://qlpl.ccnu.edu.cn/info/1093/2403.htm

38 computing nodes
(304 V100 GPUs)
Peak performance:
2 PFlops/s
(每秒2千万亿次浮点运算)
Storage:
1 PB

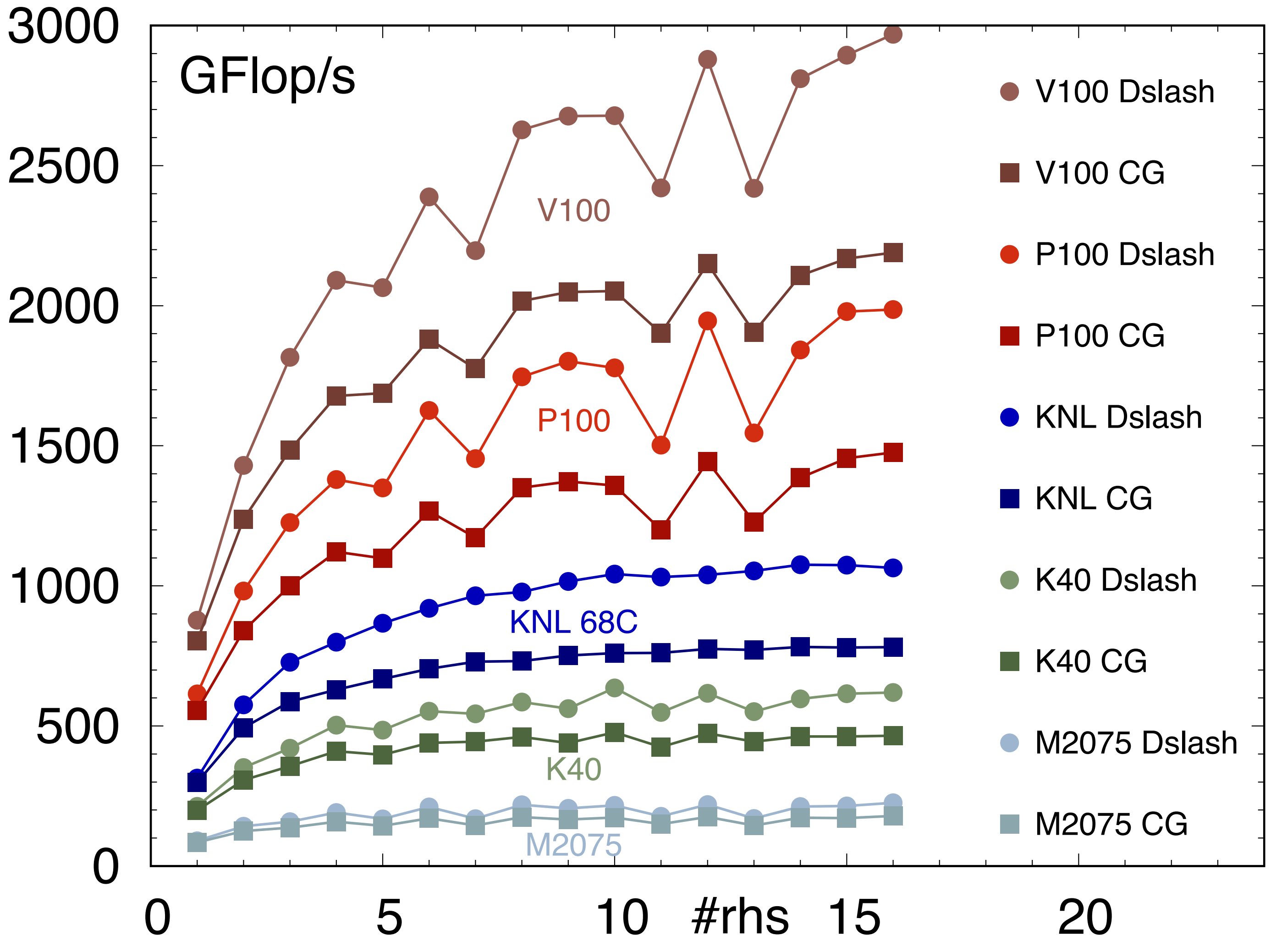
June, 2021
TOP 500 The List.
The GREEN 500

国内首个格点QCD专用超算平台，国内最快！

8卡V100 服务器架构

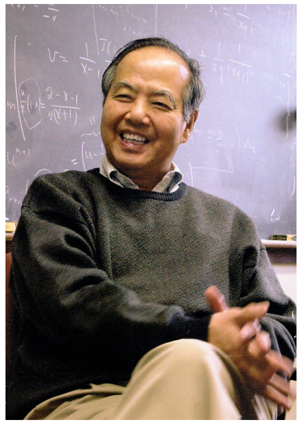


优化的GPU代码在不同架构上的运算速度



宇宙终极问题? 42?

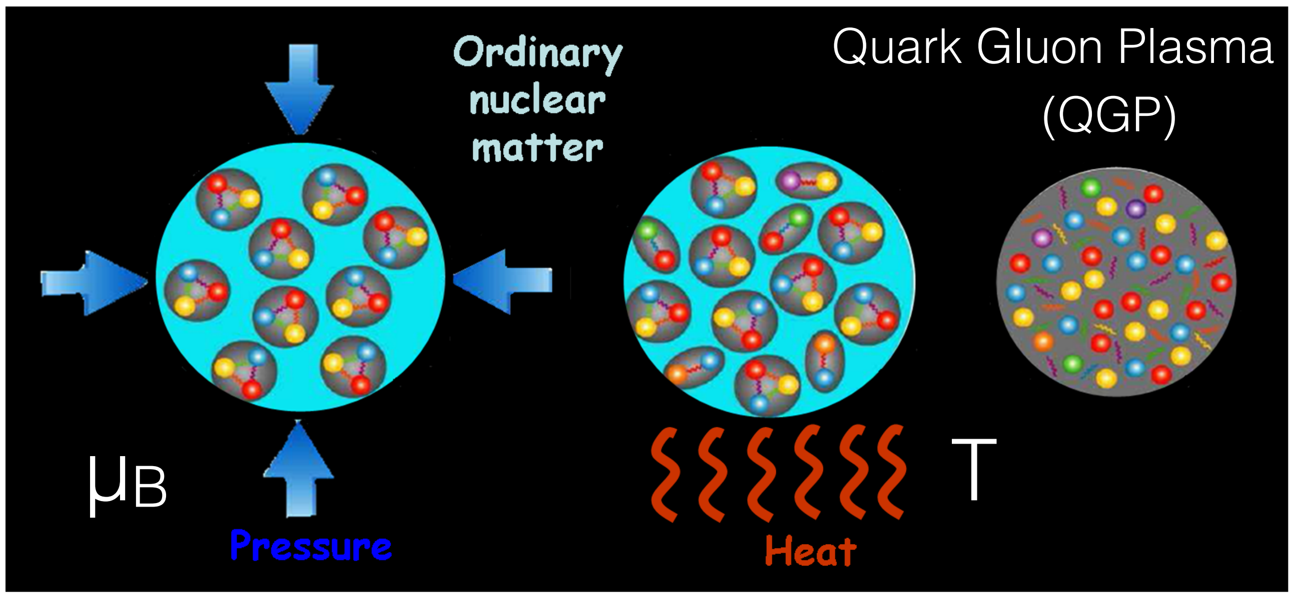
from The Hitchhiker's Guide to the Galaxy (2005) 《银河系漫游指南》



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



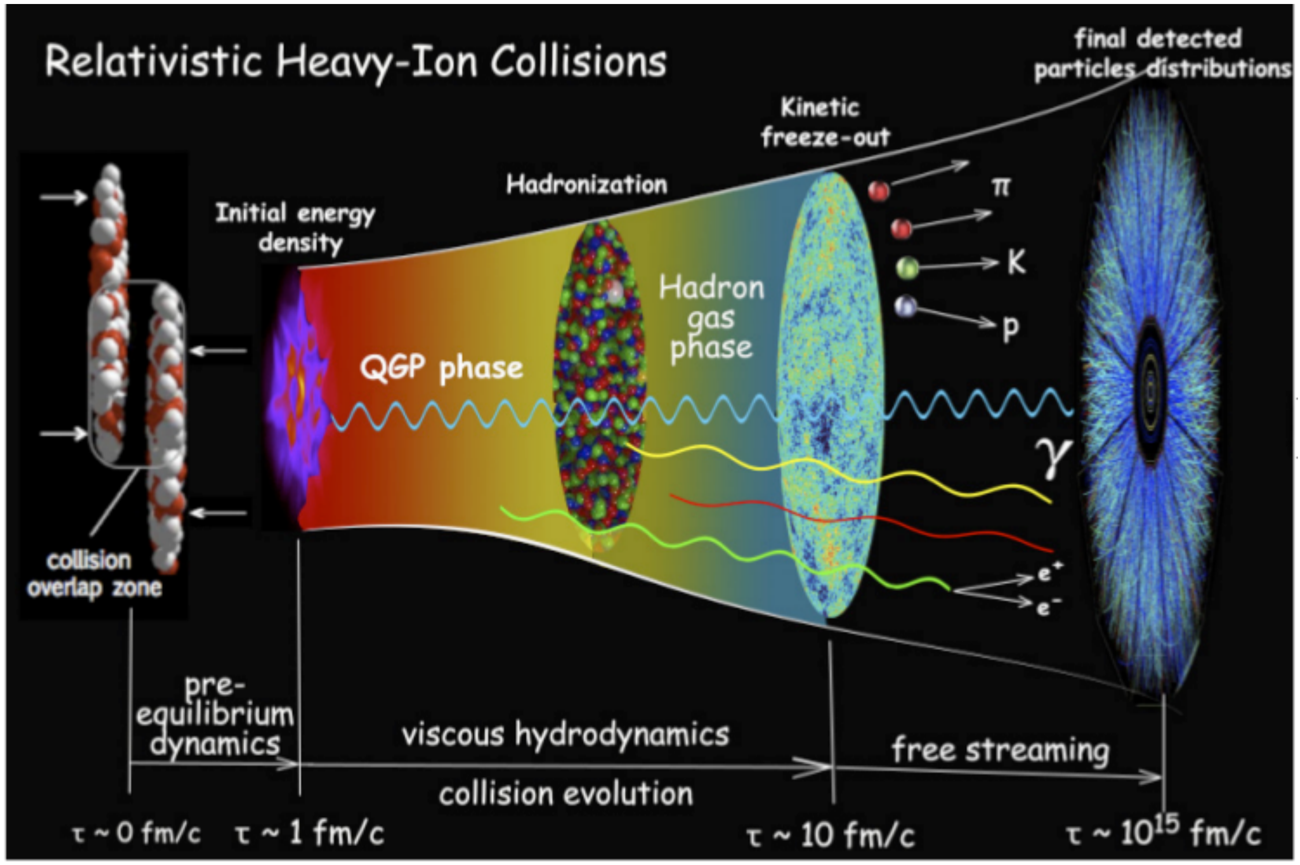
“The whole is more than sum of its parts.”
Aristotle, Metaphysica 10f-1045a

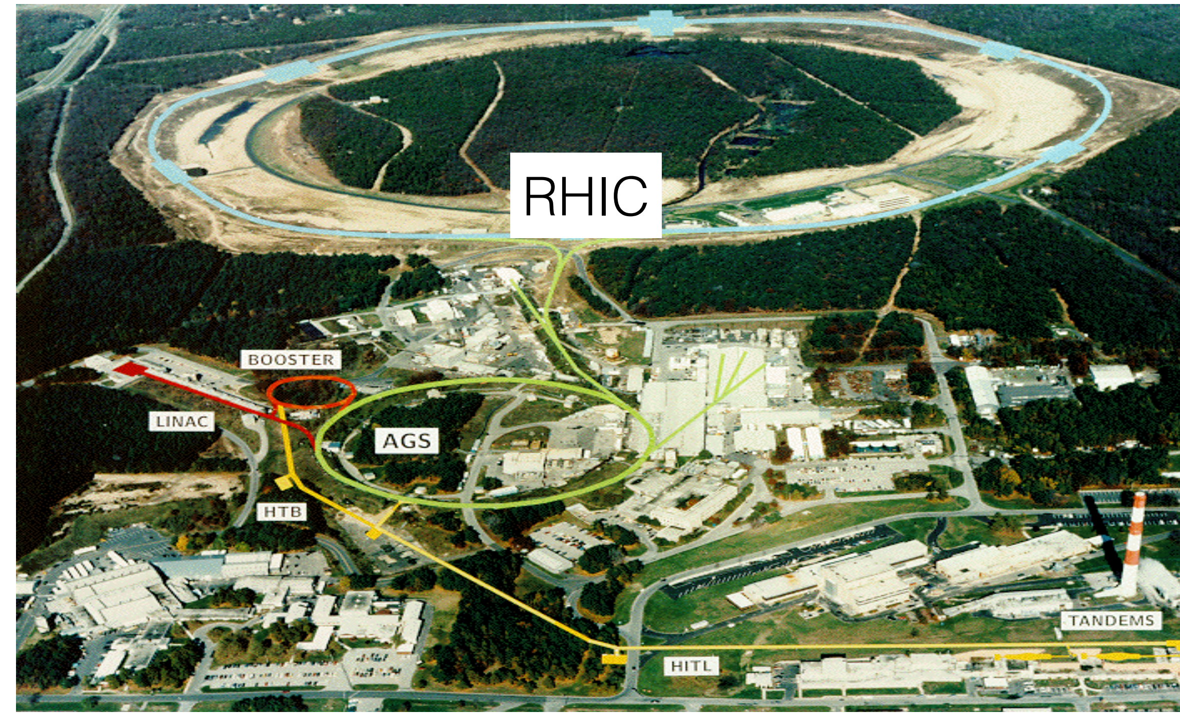
从还原论到整体论

“核子重如牛，对撞生新态。”

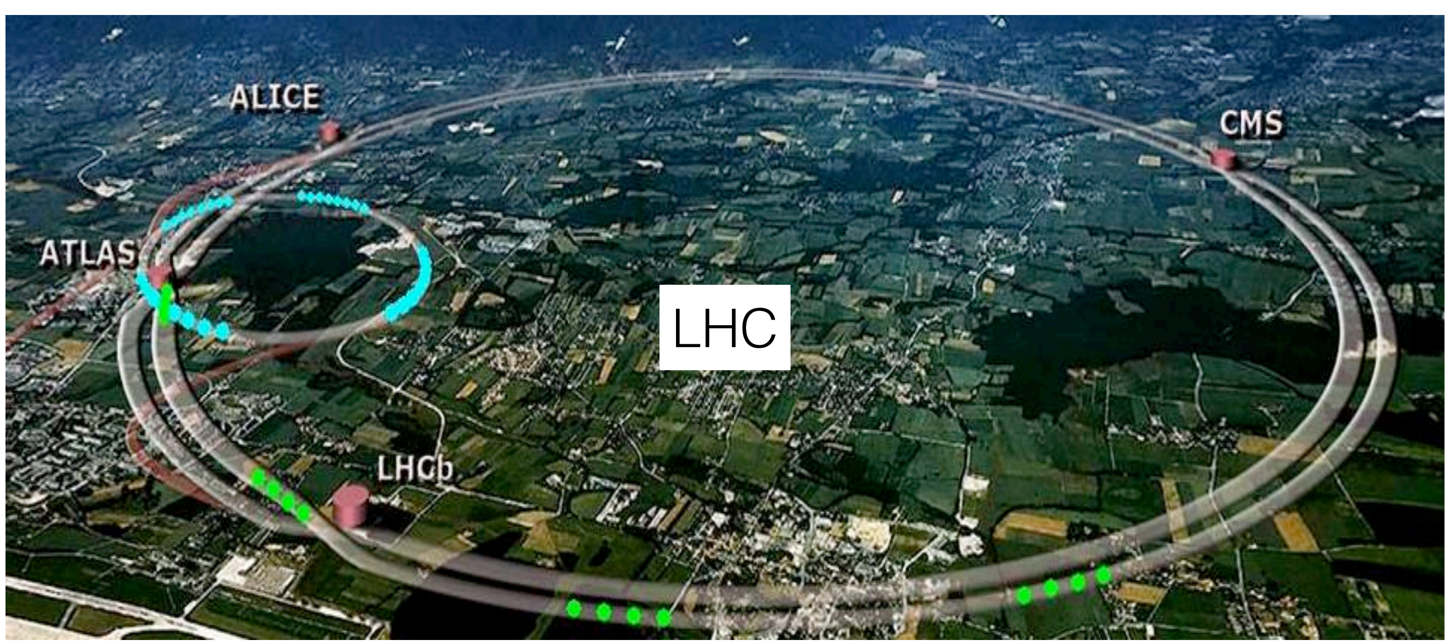
Ink painting masterpiece 1986:
"Nuclei as Heavy as Bulls, Through Collision
Generate New States of Matter”,
by Li Keran,
reproduced from open source works of T.D.Lee.

实验室中的“小爆炸”: 重新产生夸克胶子等离子体

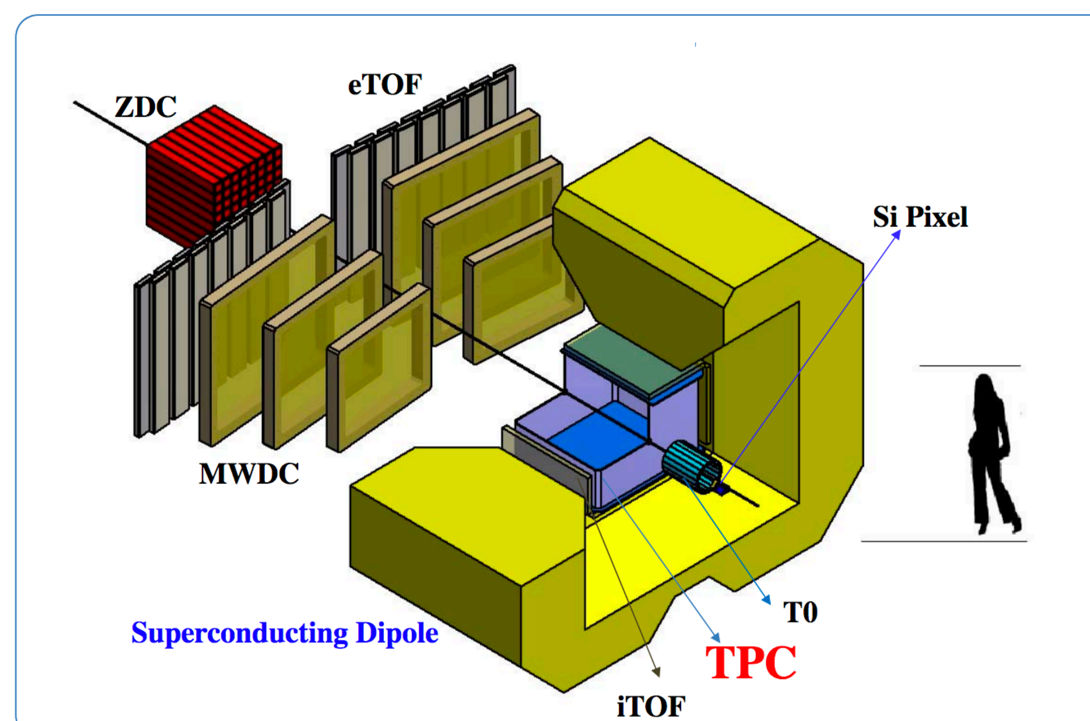




相对论重离子对撞机 (Relativistic Heavy Ion Collider)
@美国布鲁克海文国家实验室



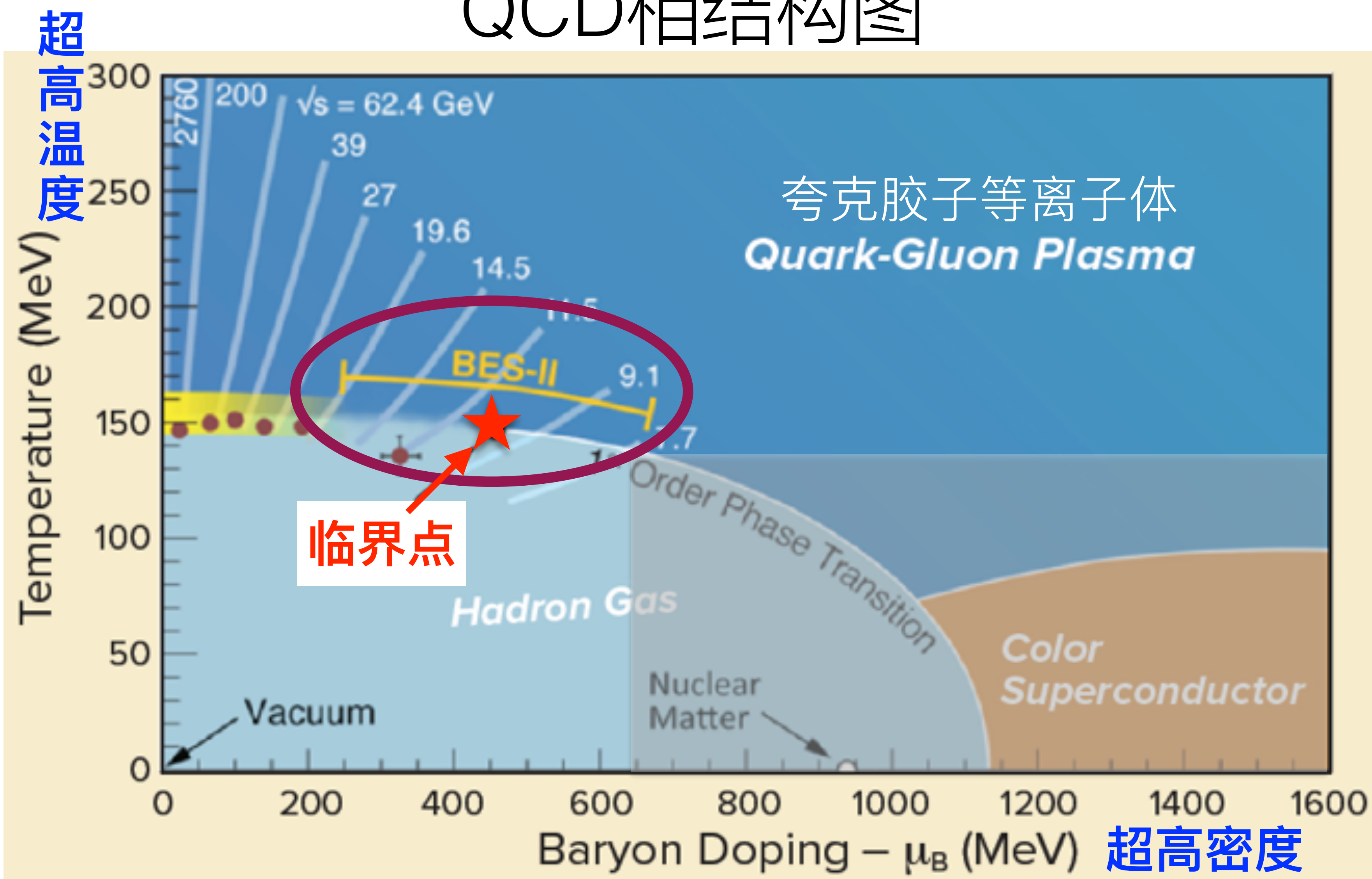
大型强子对撞机(Large Hadron Collider)@欧洲核子研究中心



冷密核物质测量谱仪(CEE)@中科院近代物理研究所

热密核物质：探索QCD相结构, 寻找QCD 临界点

QCD相结构图



- 从强子相到夸克胶子等离子的相变温度
- QCD 临界点(critical point) — Criticality

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

Physics Department, Brookhaven National Laboratory, Upton, NY 11973, USA
and
Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany

Swagato Mukherjee

Physics Department, Brookhaven National Laboratory, Upton, NY 11973, USA

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, Int.J.Mod.Phys. E24 (2015) no.10, 1530007
https://arxiv.org/pdf/1504.05274

ESI(前1%)高被引文章

Famous plots

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

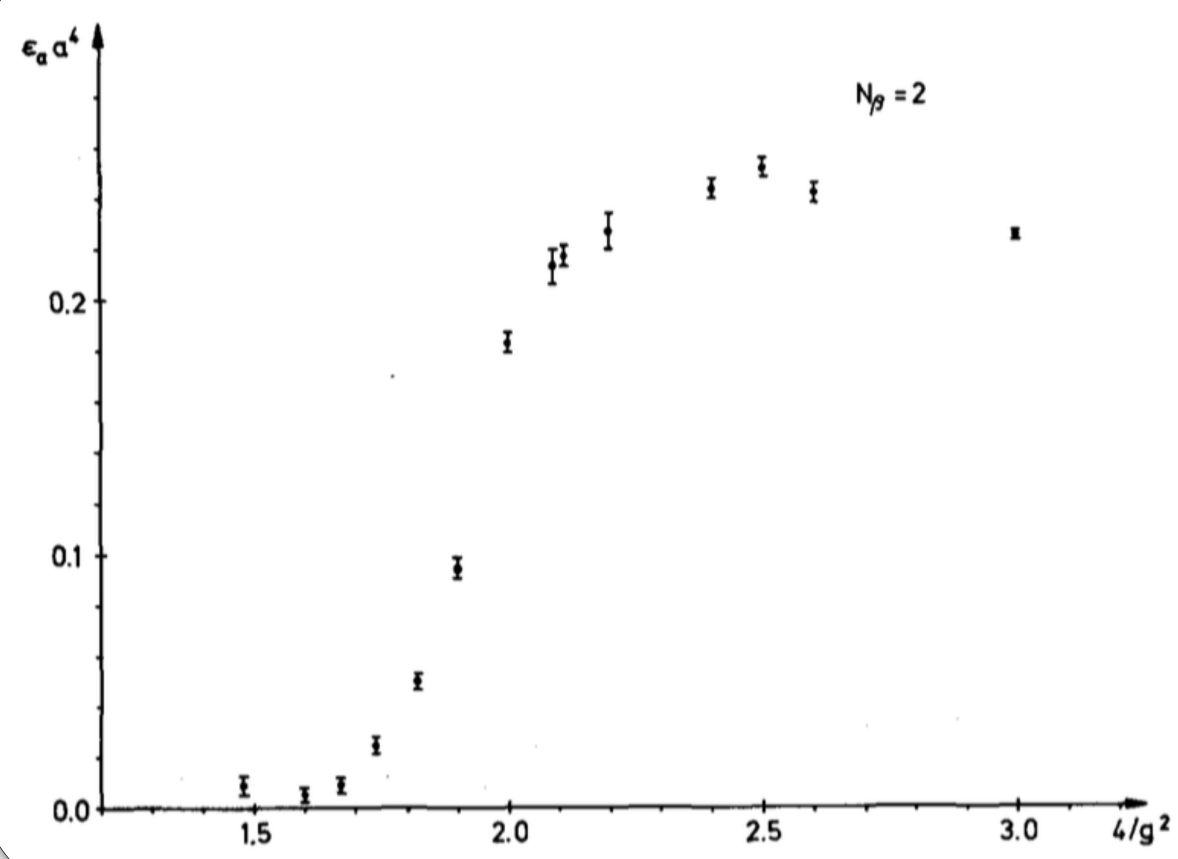
#2: At what temperature a QGP can be formed ?

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

Famous plots #1:

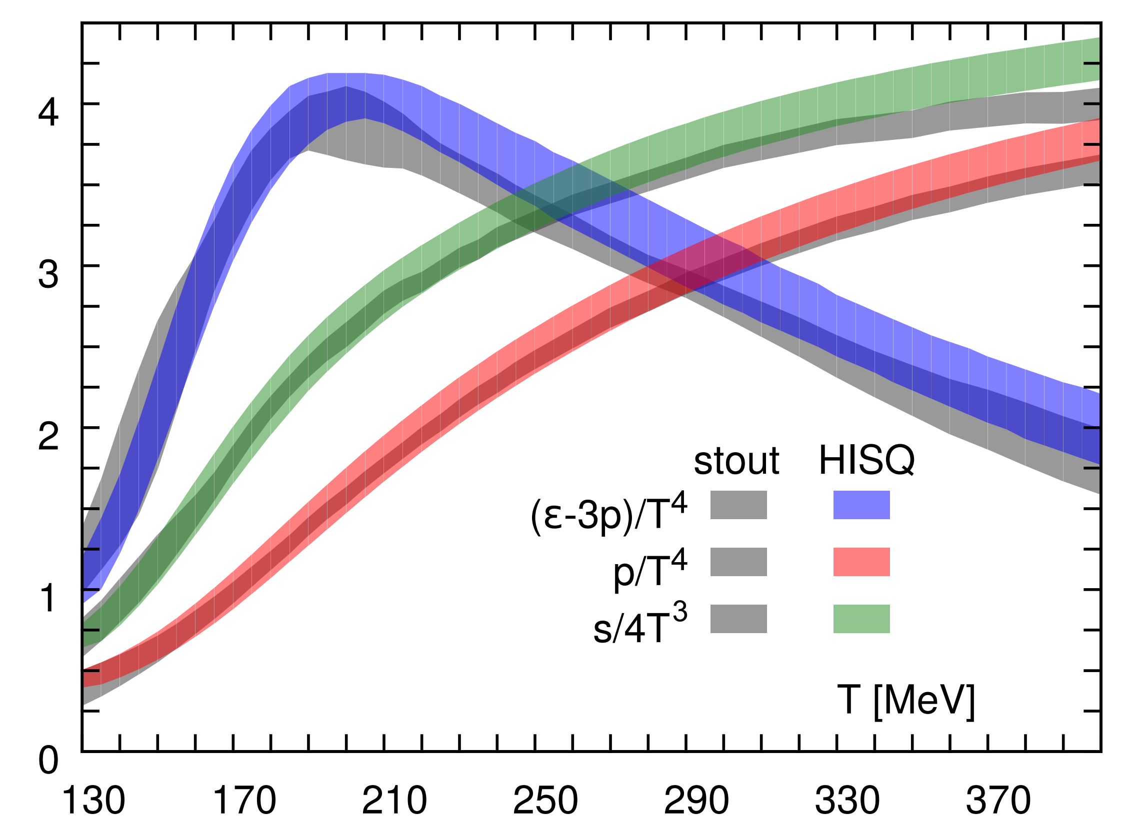
Lattice QCD calculation of EoS at μ_B =0

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



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

N_f=2+1, physical point
continuum extrapolated



HotQCD, PRD 90 (2014) 094503
Cited by 872 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
Grassman variables

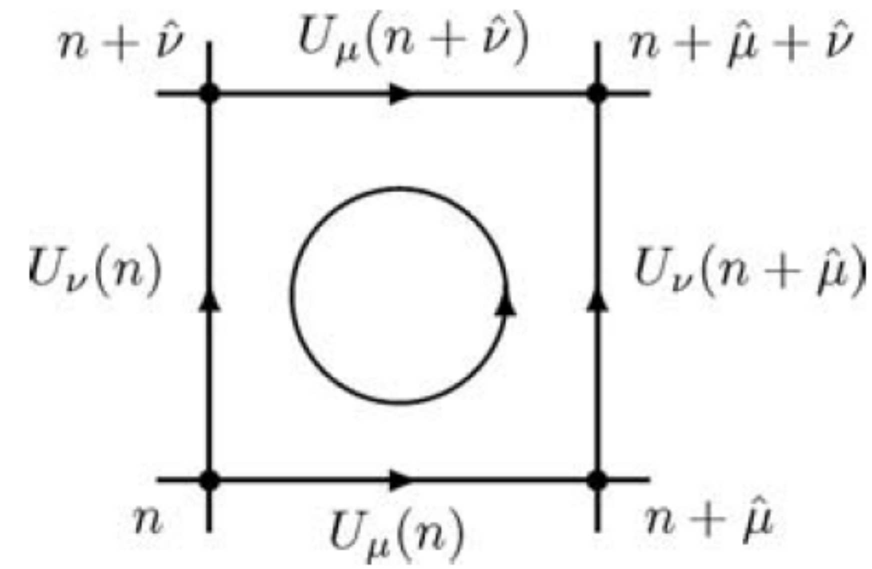
$$< \mathcal{O} >= \frac{1}{Z} \int \mathcal{D}U\, \mathcal{O}\, e^{-S_G} \prod_{f=u,d,s,\cdots} \det M_f$$

- **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

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:

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

Reproduce the gauge action in the continuum limit with an order a^2 correction

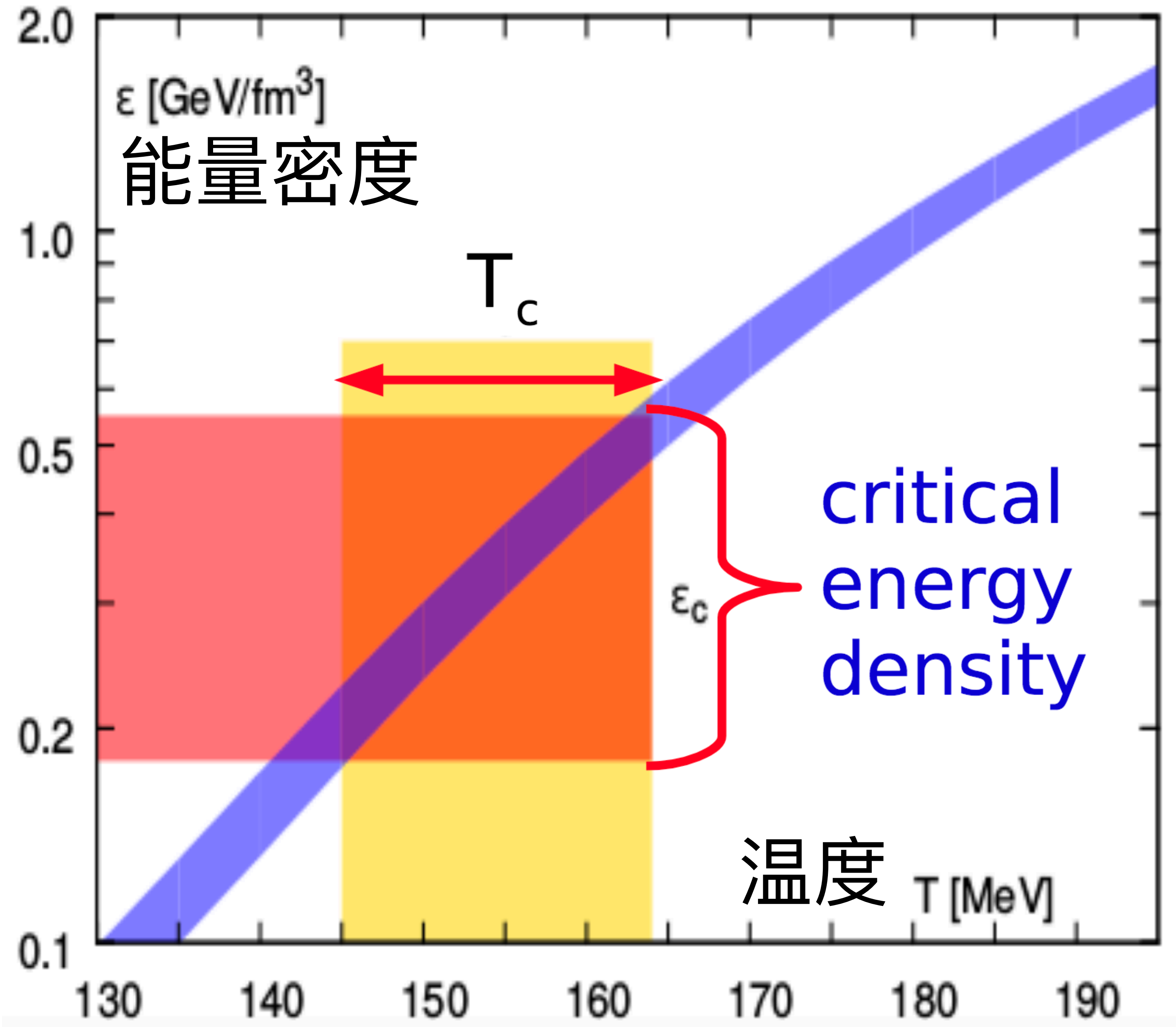
$$S_G[U] = \frac{a^4}{2\,g^2} \sum_{n\in\Lambda} \sum_{\mu,\nu} \mathrm{tr}[F_{\mu\nu}(n)^2] + \mathcal{O}(a^2)$$

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

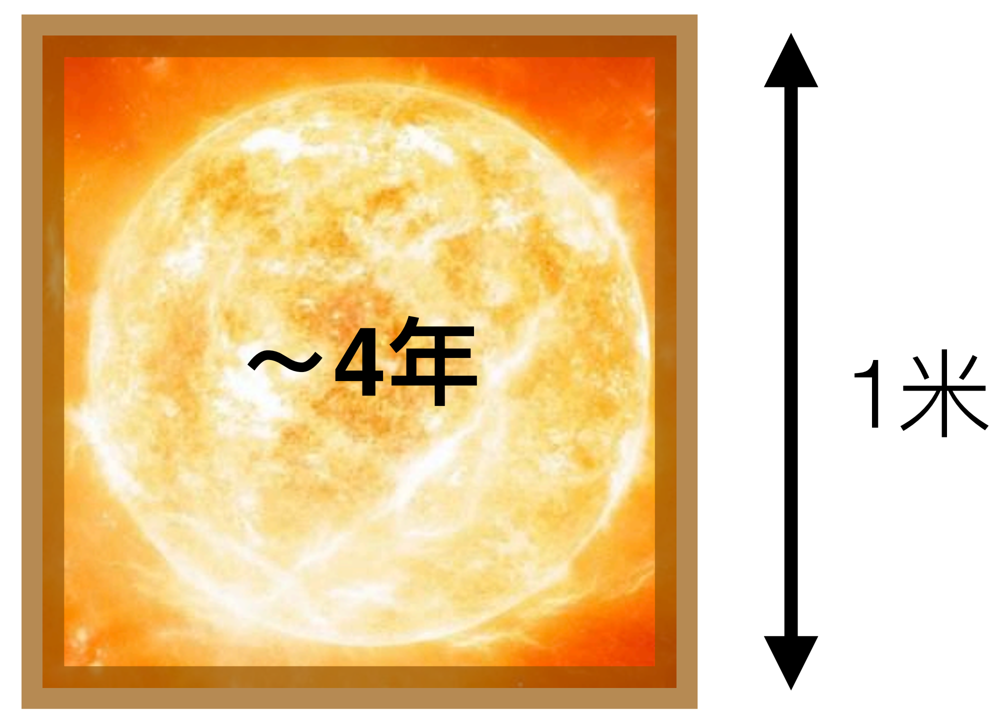
$$U_\mu(n) = \exp\left(\mathrm{i}\, a A_\mu(n)\right), \quad \exp(A)\,\exp(B) = \exp\left(A + B + \frac{1}{2}[A,B] + \cdots\right)$$

夸克胶子等离子体的能量密度

N_f=2+1 QCD at physical point



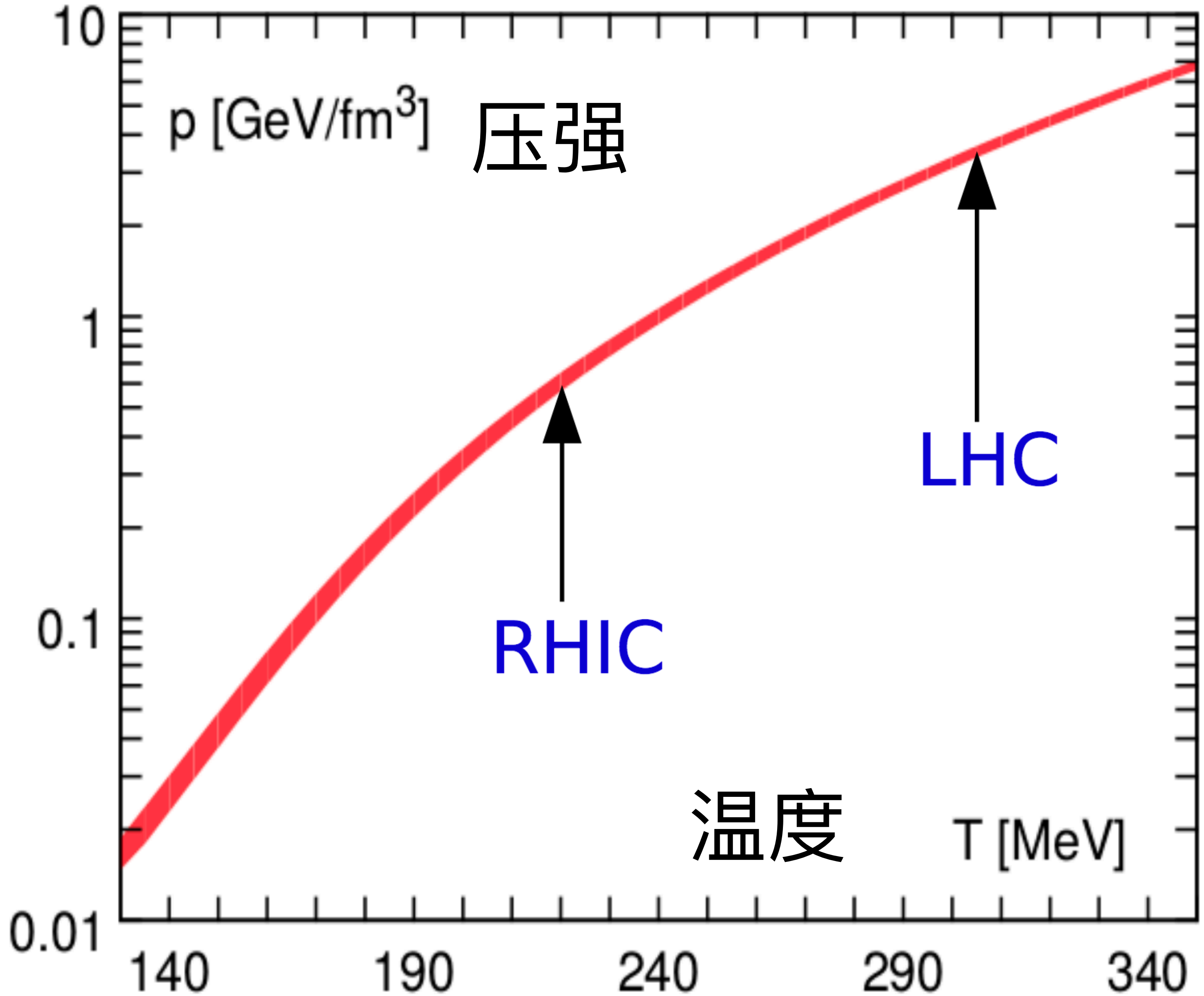
$\varepsilon_c \simeq 5\text{x}10^{34}$ J/m^3



A.Bazavov,...**丁亨通** et al.[HotQCD], Phys.Rev. D90 (2014) 094503
总被引872次

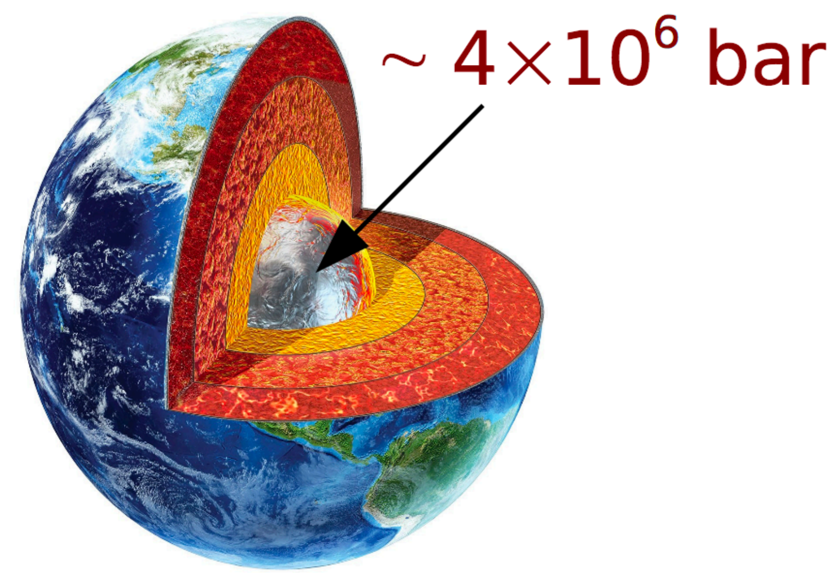
夸克胶子等离子体内的压强

N_f=2+1 QCD at physical point



A.Bazavov,…**丁亨通** et al.[HotQCD], Phys.Rev. D90 (2014) 094503
总被引872次

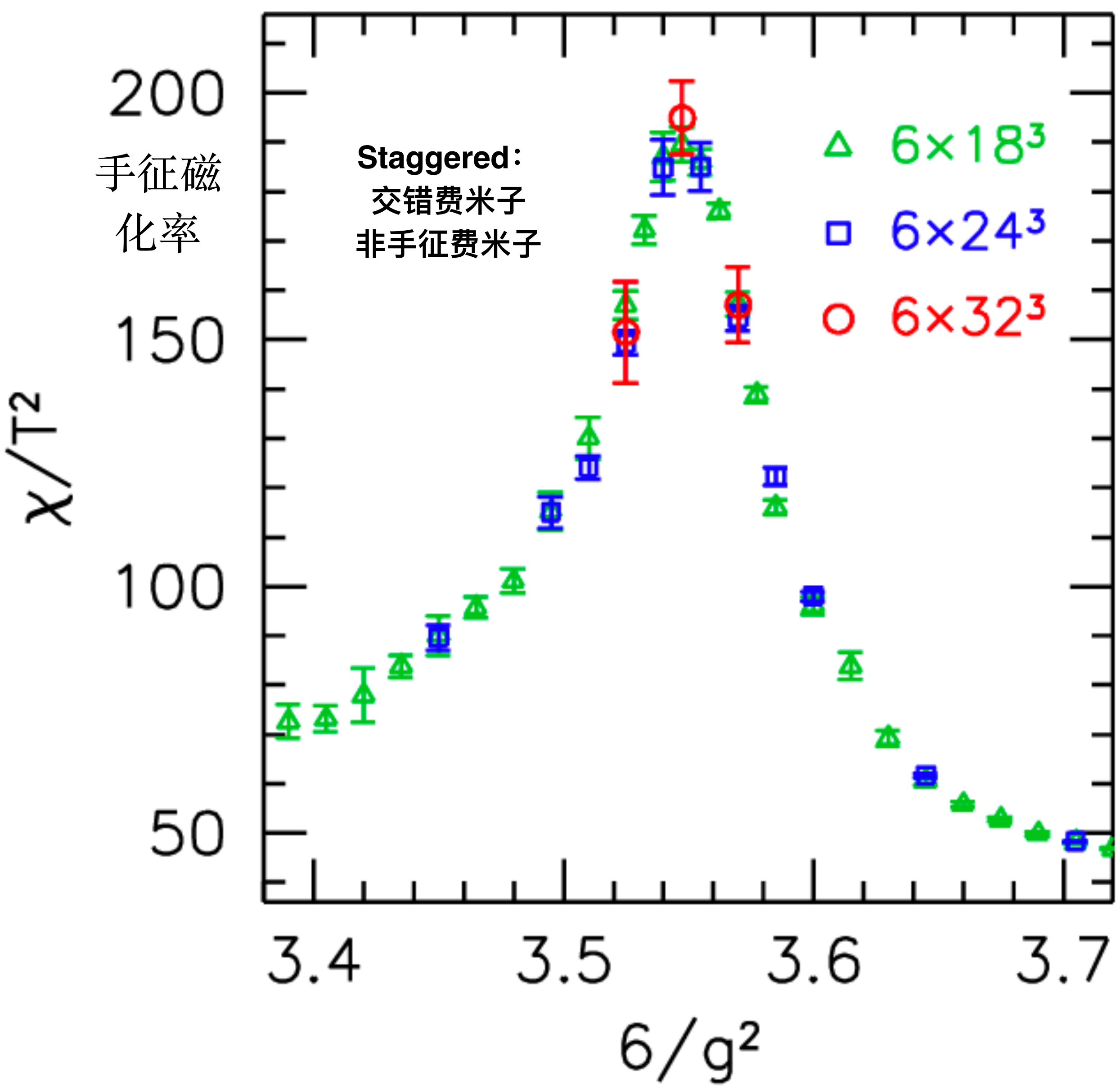
RHIC: p $\simeq 10^{30}$ bar



Famous plots #2:

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

crossover transition

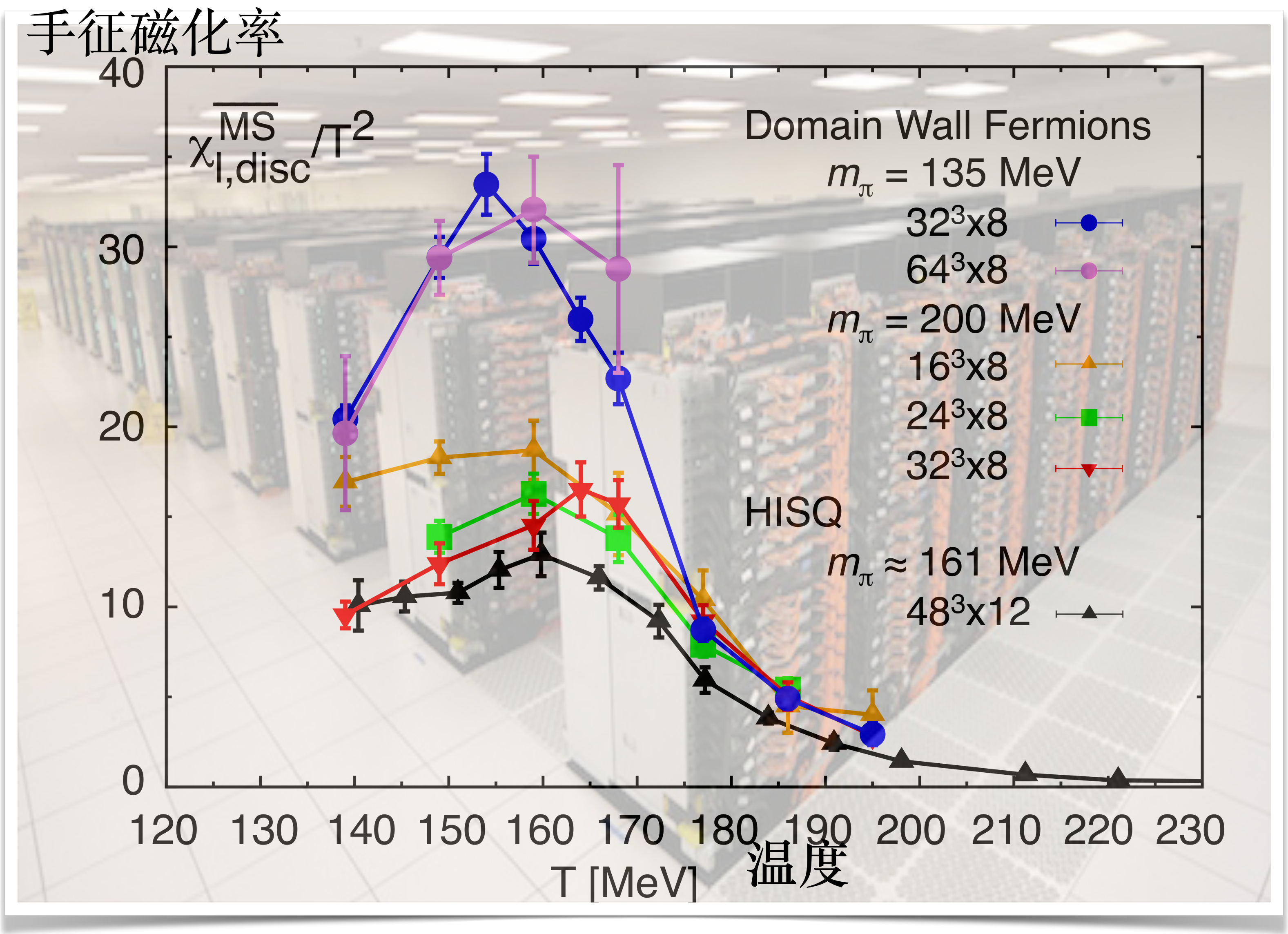


Y. Aoki et al., Nature 443 (2006) 675-678
Cited by 1516 records

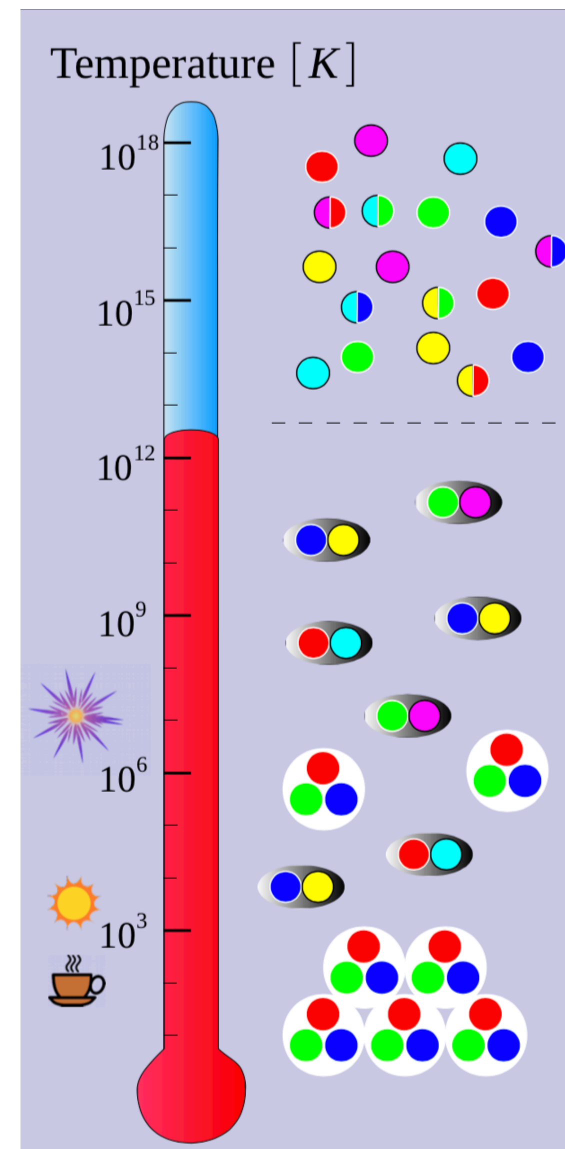
实验中是否产生新的物质形态——夸克胶子等离子体

强相互作用核物质平滑过渡到夸克胶子等离子体的相转变温度为

155(1)(8) MeV ～1.8x10^{12} K



背景为IBM BGQ超级计算机



室温：
293.15 K

太阳表面温度：
～5.8x10^3 K

太阳中心温度：
～1.57x10^7 K

《物理评论快报》编辑推荐阅读并被美国物理学会《观点》杂志报道

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

ESI(前1%)高被引文章

Doubler problem & Wilson fermion action

Naïve fermion action in the free limit:

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

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

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

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

$\lim_{x\to 0} \sin(x) = x$

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

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

Different discretization schemes

- Wilson fermions: free of the doublers but break the chiral symmetry explicitly
- Staggered fermions: preserve part of the chiral symmetry and partially get rid of the doublers
- Domain Wall fermions: live in 5D, preserve exact chiral symmetry as the extent of the 5th-d going to infinity
- Overlap fermions: preserve exact chiral symmetry

Current hot & dense lattice QCD simulations

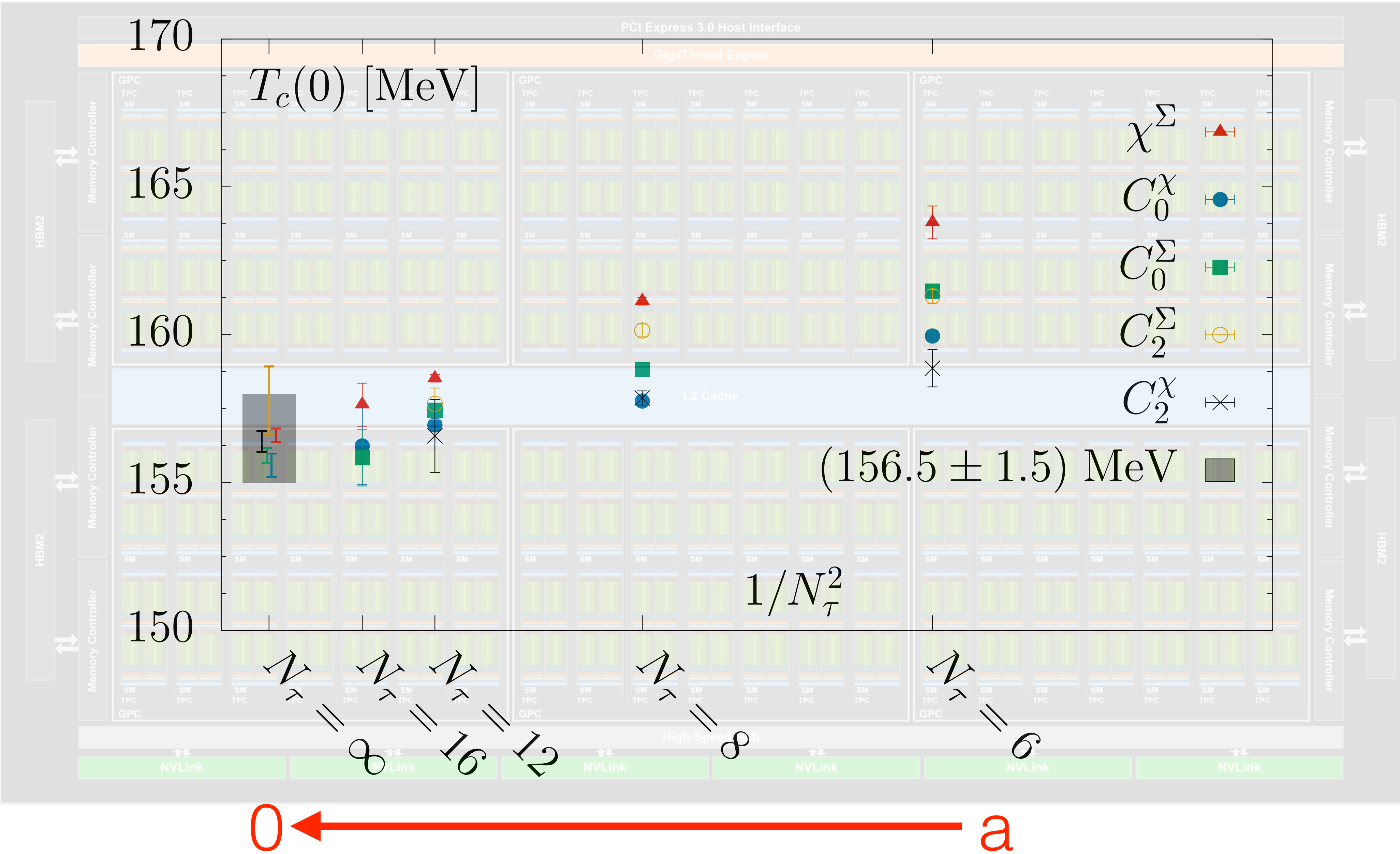
Lattice QCD: discretized version of QCD on a Euclidean space-time lattice, reproduces QCD when lattice spacing $a \to 0$ (continuum limit)

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

- Staggered actions at $a \neq 0$: 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 $a \neq 0$
  - preserves full flavor symmetry and chiral symmetries
  - computationally expensive to simulate, currently starts to produce interesting results on QCD thermodynamics

更精准地得到了相转变温度

$T_c(0)$=156.5(1.5)MeV



连续外推结果

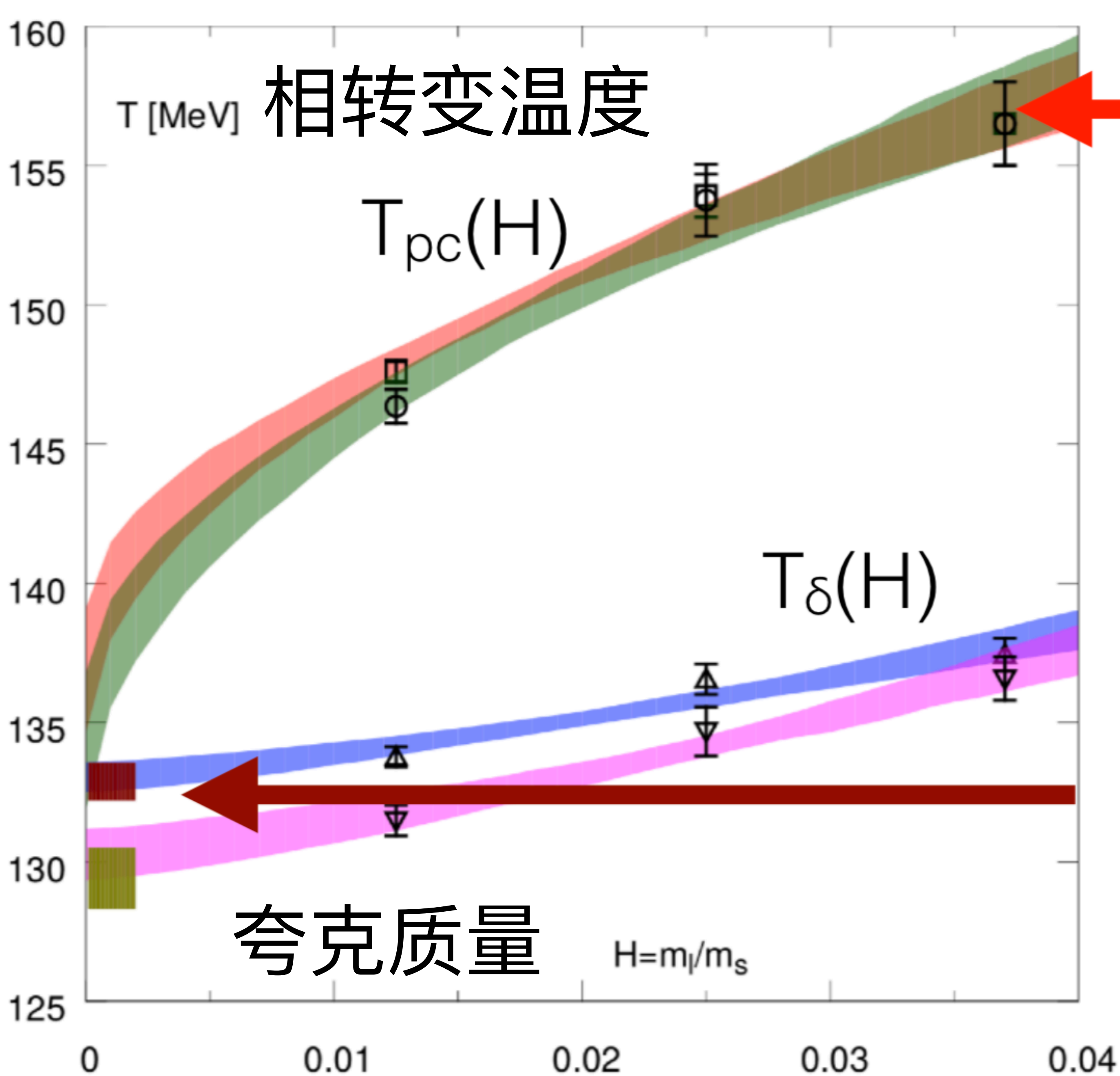
背景为V100
图形处理器(GPU)

A. Bazavov, **丁亨通**, P. Hegde et al. [HotQCD],
Phys. Lett. B795 (2019) 15, 总被引228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

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

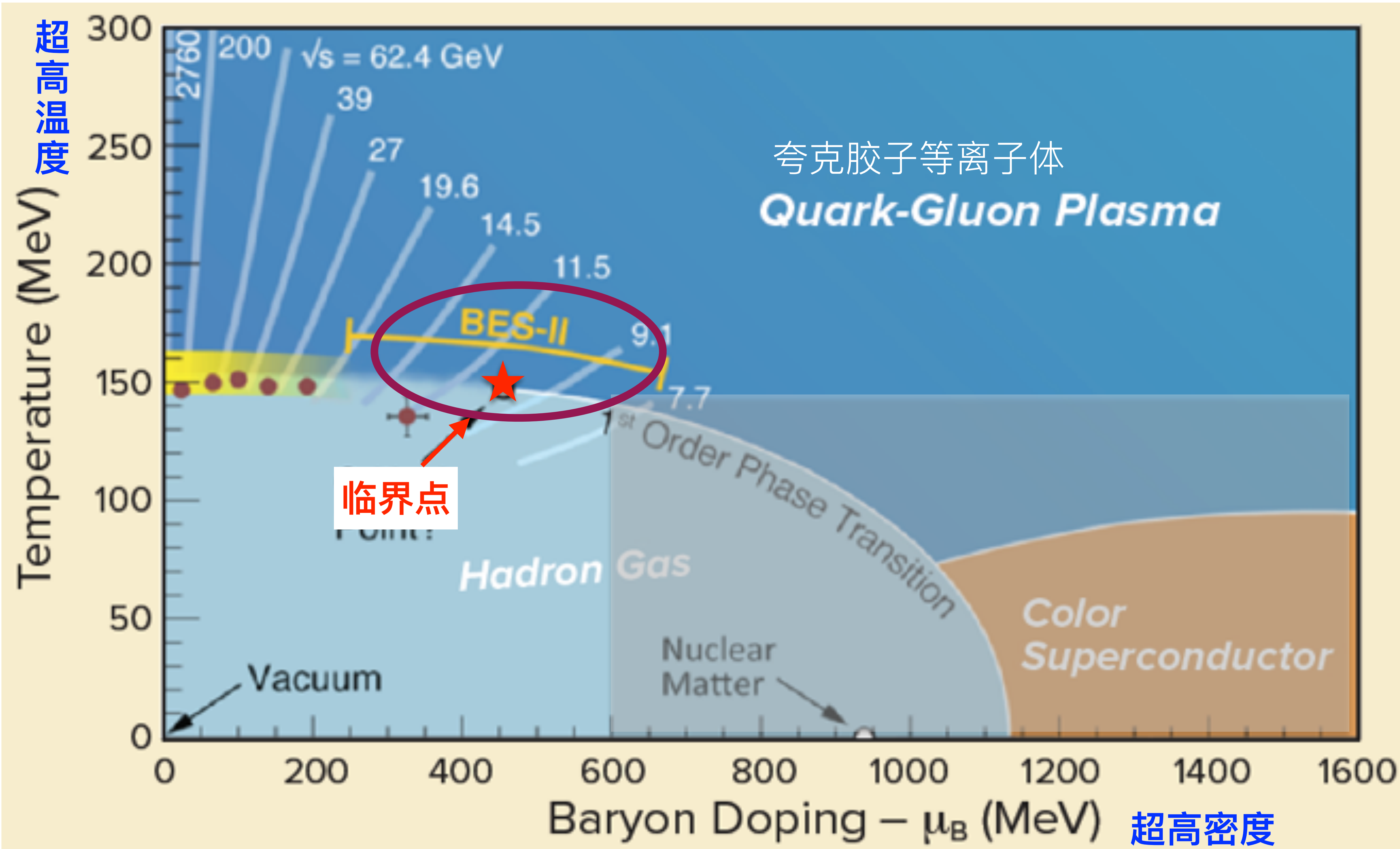
二阶相变,O(4)群普适类

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80次

净重子数目不为零时的QCD 相结构



非零重子化学势能下的格点QCD模拟

符号问题

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

为复数　　不正定

- 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

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

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

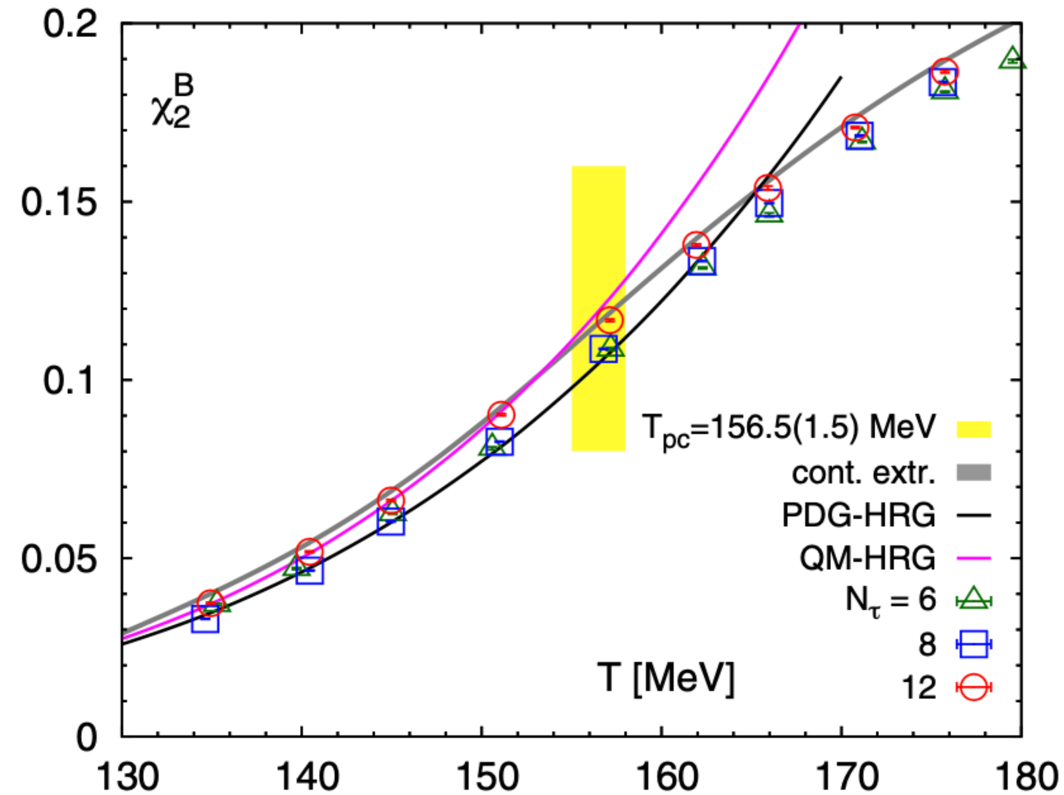
☑ Taylor expansion coefficients at μ=0 are computable in LQCD

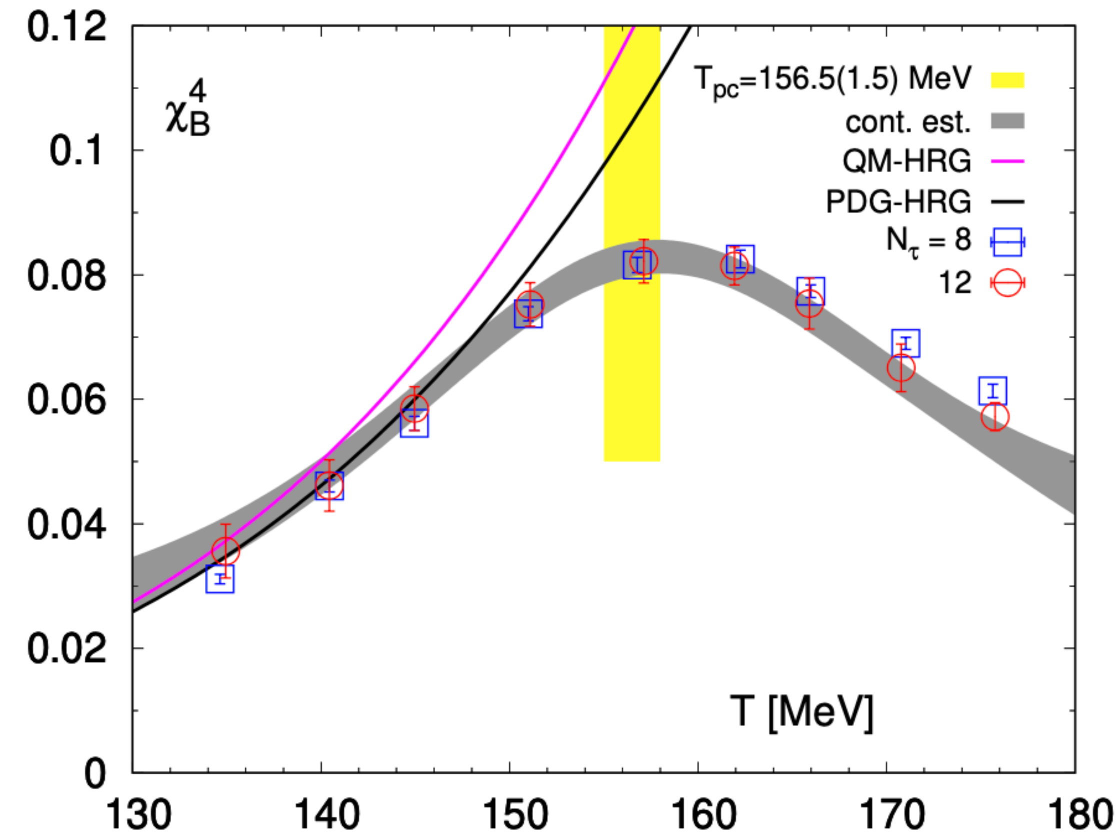
$$\chi_{ijk}^{BQS} \equiv \chi_{ijk}^{BQS}(T) = \frac{1}{VT^3}\frac{\partial P(T,\hat{\mu})/T^4}{\partial\hat{\mu}_B^i\partial\hat{\mu}_Q^j\partial\hat{\mu}_S^k}\Big|_{\hat{\mu}=0}$$

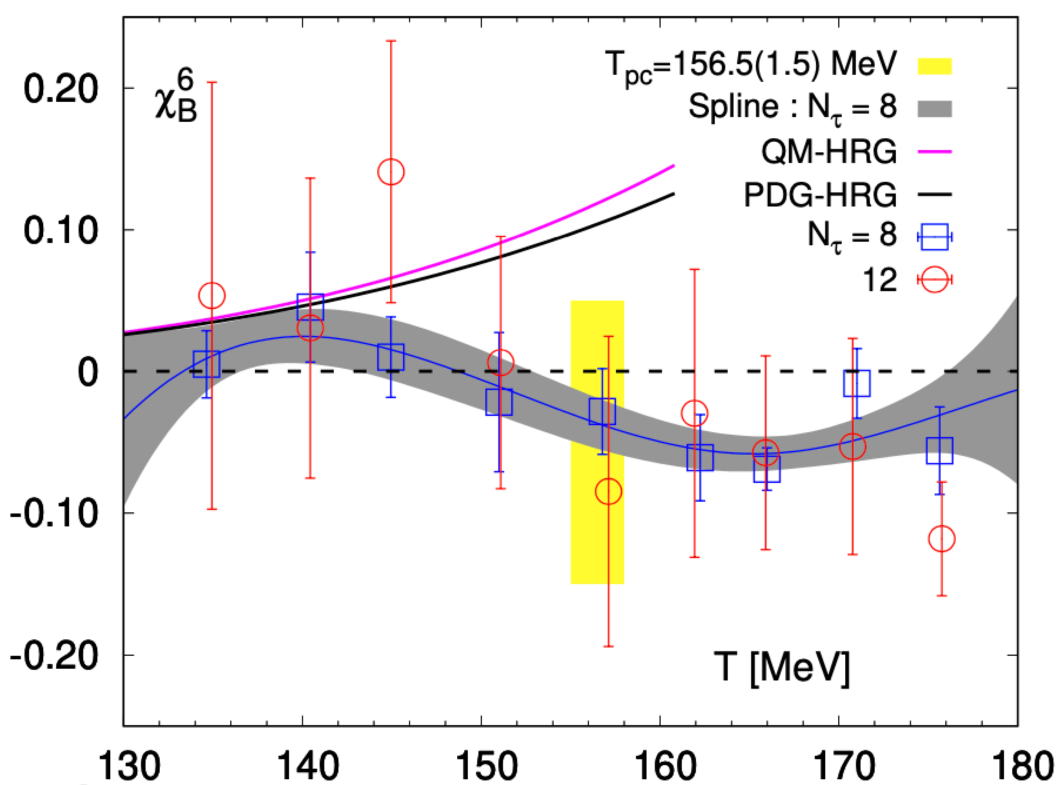
☑ Thermodynamic quantities can be obtained using relations, e.g.

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

Taylor expansion coefficients at μ_B=0



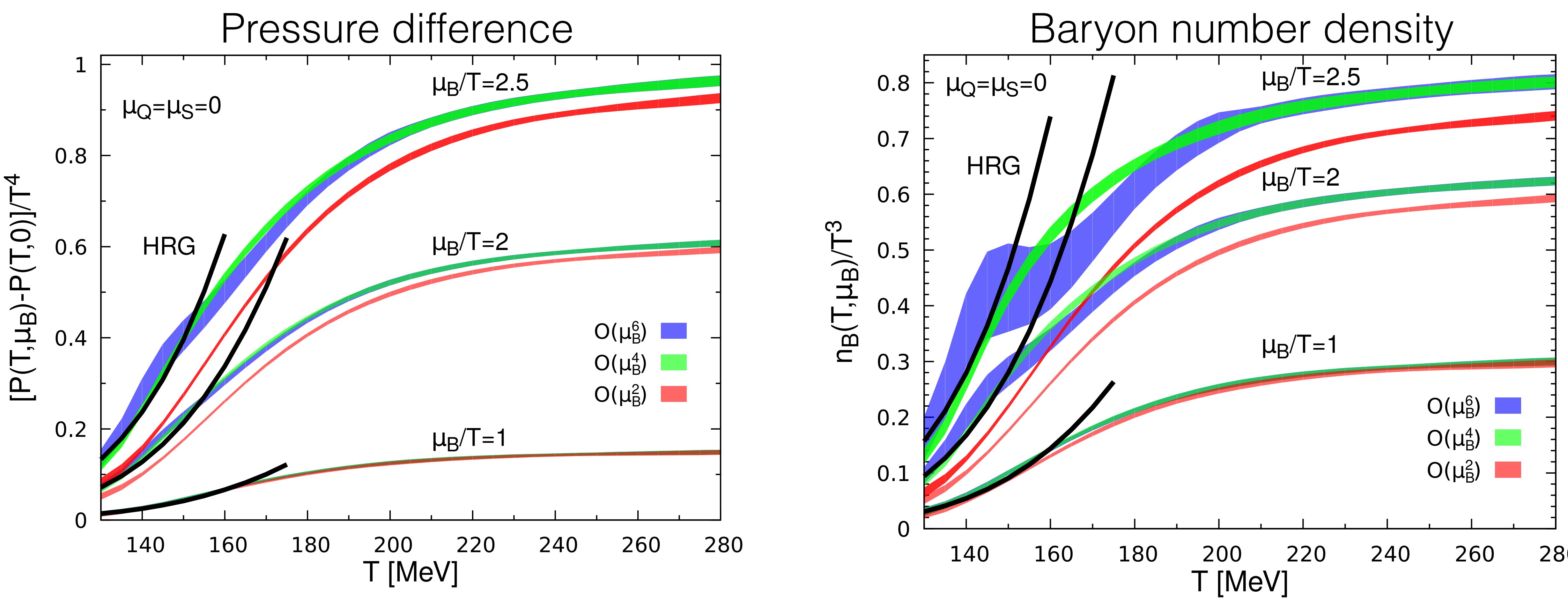




$$\chi_n^B(T) = \frac{\partial^n P(T,\mu_B)/T^4}{\partial \hat{\mu}_B^n}\Big|_{\hat{\mu}_B=0}$$

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 287 records

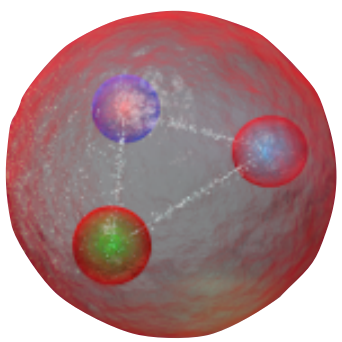
$$\frac{P(T,\mu_B)-P(T,0)}{T^4}=\sum_{n=1}^{\infty}\frac{\chi_{2n}^B(T)}{(2n)!}\left(\frac{\mu_B}{T}\right)^{2n}=\frac{1}{2}\chi_2^B(T)\hat{\mu}_B^2\left(1+\frac{1}{12}\frac{\chi_4^B(T)}{\chi_2^B(T)}\hat{\mu}_B^2+\frac{1}{360}\frac{\chi_6^B(T)}{\chi_2^B(T)}\hat{\mu}_B^4+\cdots\right)$$

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

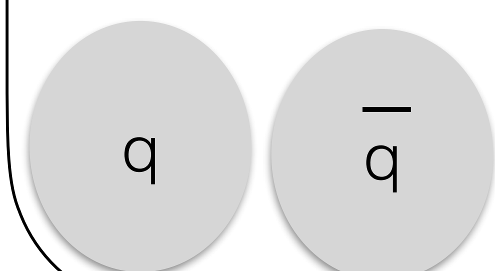
Baryon number fluctuation —> B^2



Bound state of quarks

B=1, -1

B^2=1

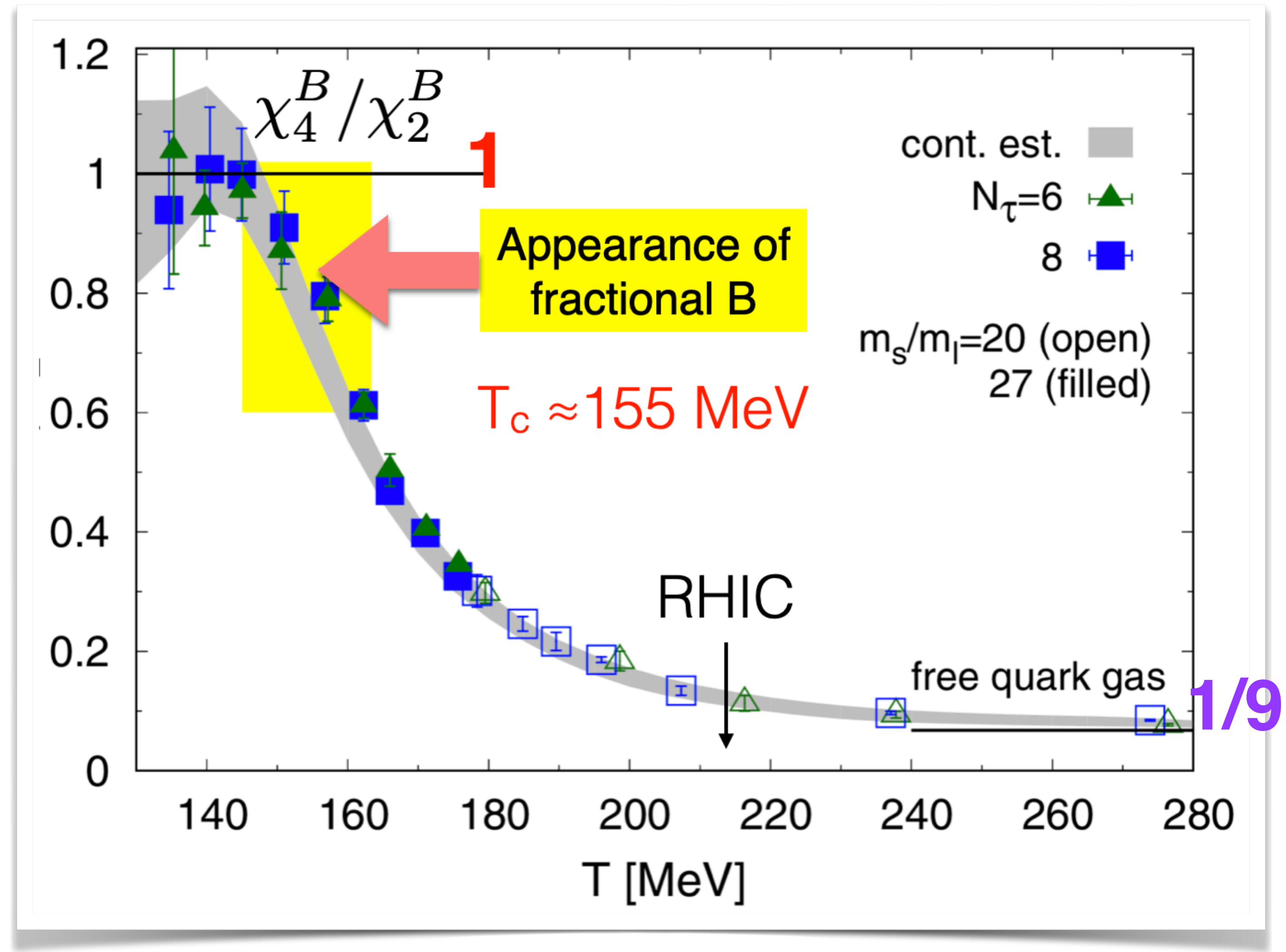


Unbounded quarks

B=1/3, -1/3

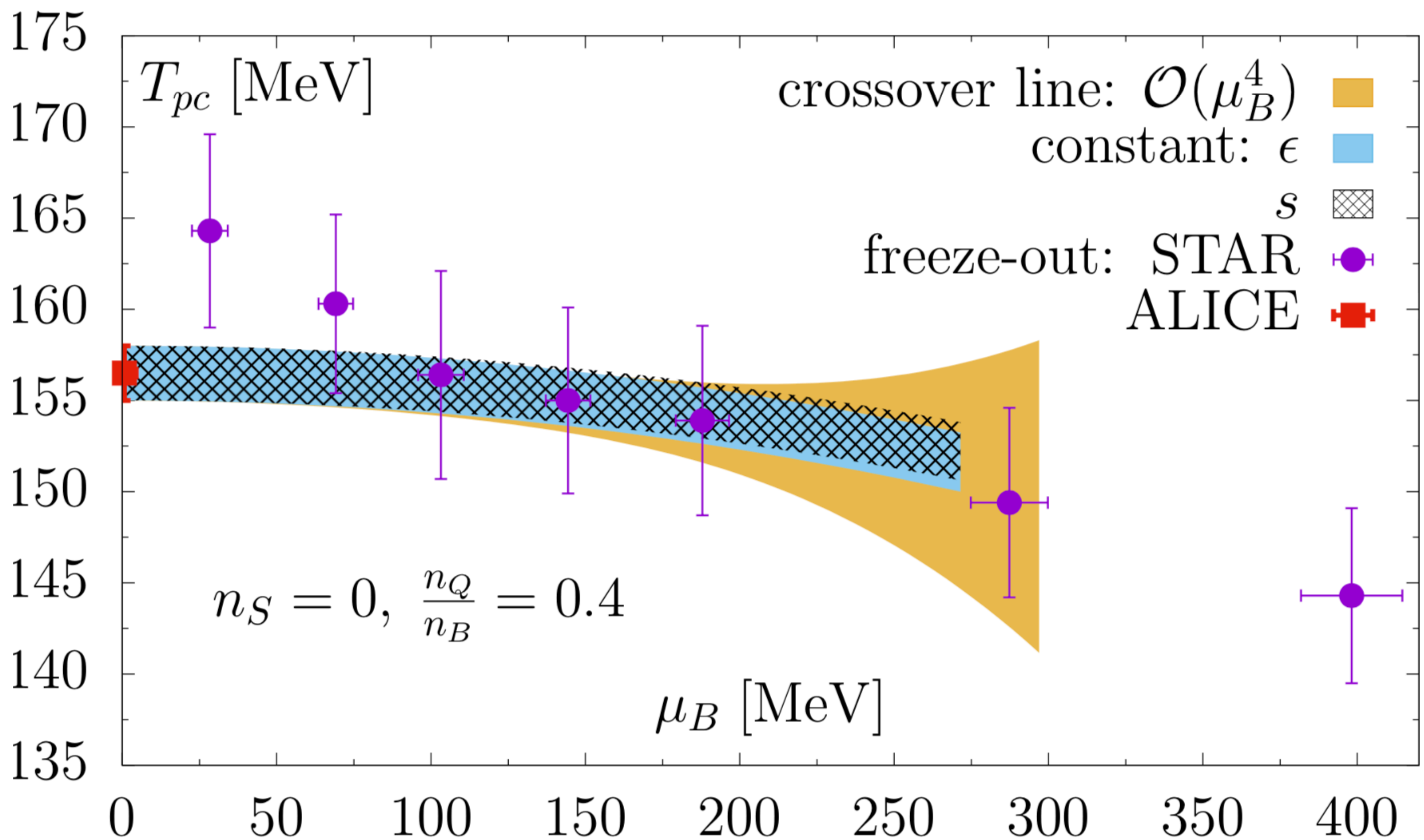
B^2=1/9

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228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

Books & literatures

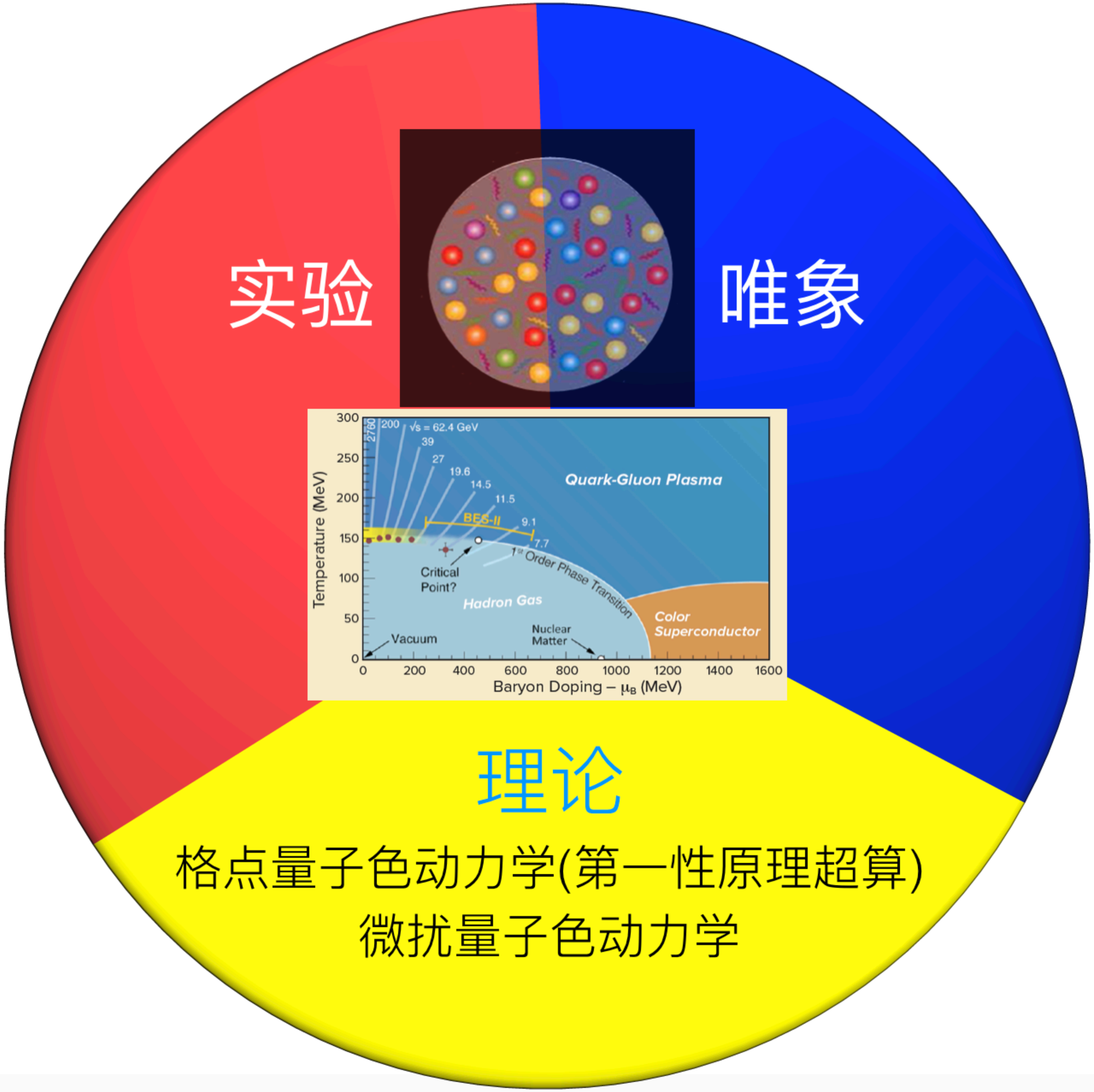
✤ “Quantum Chromodynamics on the Lattice”,
C. Gattringer and C. B. Lang, Springer 2010

✤ “Lattice QCD for Novices”,
G. Peter Lepage, arXiv:hep-lat/0506036

✤ “Thermodynamics of strong-interaction matter from Lattice QCD”,
HTD, F. Karsch, S. Mukherjee, arXiv:1504.05274

✤ Conference proceedings in the annual “lattice conference”

- Lattice 2017, Granda, Spain
- Lattice 2018, Michigan, USA
- Lattice 2019, CCNU, Wuhan, China
- …


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
Temperature (MeV)
Baryon Doping – μ_B (MeV)
Quark-Gluon Plasma
Hadron Gas
Color Superconductor
Critical Point?
1st Order Phase Transition
BES-II
Vacuum
Nuclear Matter
√s = 62.4 GeV
2760
200
39
27
19.6
14.5
11.5
9.1
7.7
0
50
100
150
200
250
300
400
600
800
1000
1200
1400
1600

Backup

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: $m\,\overline{\psi}'\psi' = m\,\overline{\psi}\,\mathrm{e}^{i2\alpha\gamma_5}\,\psi$

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

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

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

chiral symmetry on the lattice

- Massless Wilson Dirac operator breaks chiral symmetry

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

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

- The Ginsparg-Wilson equation

$$D\,\gamma_5 + \gamma_5\,D = a\,D\,\gamma_5\,D$$

lattice space a ->0

$$D\,\gamma_5 + \gamma_5\,D = 0$$

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

chiral rotation on the lattice

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

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

chiral symmetry on the lattice

- Massless Wilson Dirac operator breaks chiral symmetry

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

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

- The Ginsparg-Wilson equation

$$D\,\gamma_5 + \gamma_5\,D = a\,D\,\gamma_5\,D \quad \xrightarrow{\text{lattice space a ->0}} \quad D\,\gamma_5 + \gamma_5\,D = 0$$

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

chiral rotation on the lattice

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

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

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

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

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

QCD action

- Gauge action:

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

$$F^{(i)}_{\mu\nu}(x) = \partial_\mu A^{(i)}_\nu(x) - \partial_\nu A^{(i)}_\mu(x) - f_{ijk}A^{(j)}_\mu(x)A^{(k)}_\nu(x)$$

- Fermion action:

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

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

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

Sign problem at μ_B =/=0

QCD: $$Z = \mathrm{Tr}\left[e^{-(H-\mu N)/T}\right] = \int [\mathrm{d}A] \det[D + m_q + i\mu\gamma_4]\, e^{-S(A)}$$

det D[μ]

- γ_5-hermiticity does not hold and instead: $D^\dagger(-\mu) = \gamma_5 D(\mu)\gamma_5$

det D[μ] is a complex number

- Toy model for demonstration of the sign problem

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

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

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

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

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

→ $$N \gg e^{2(f-f_0)V/T}$$

Staggered fermions

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 fermions:

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

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

16 -> 4 tastes (doublers)

chiral fermions on the lattice

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

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

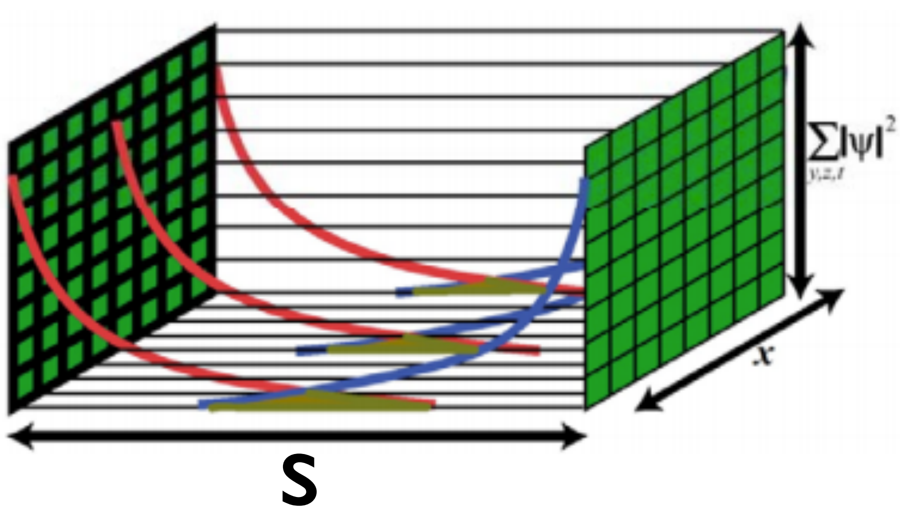
A denotes some suitable γ_5-hermitian “kernel” Dirac operator

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 N_5. Residual symmetry breaking is quantified by the additive renormalization factor m_{res} to the quark mass



costs > N_5 x costs of Wilson formulation

Ns = 16-64

Monte Carlo simulation

Expectation value: $$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[U]\, e^{-S_G[U]} \det[D_u] \det[D_d]\ O$$

Partition function: $$Z = \int \mathcal{D}[U]\ \mathrm{e}^{-S_G[U]}\ \det[D_u]\ \det[D_d]$$

- Treat the fermion determinant as a weight factor

U_n is distributed according to: $$\frac{1}{Z}\,\mathrm{e}^{-S_G[U]}\ \det[D_u]\ \det[D_d]$$

Should be real and nonnegative as a probability

$$\langle O \rangle \approx \frac{1}{N} \sum O[U_n]$$

- γ_5-hermiticity: $(\gamma_5 D)^\dagger = \gamma_5 D$ or $D^\dagger = \gamma_5 D \gamma_5$

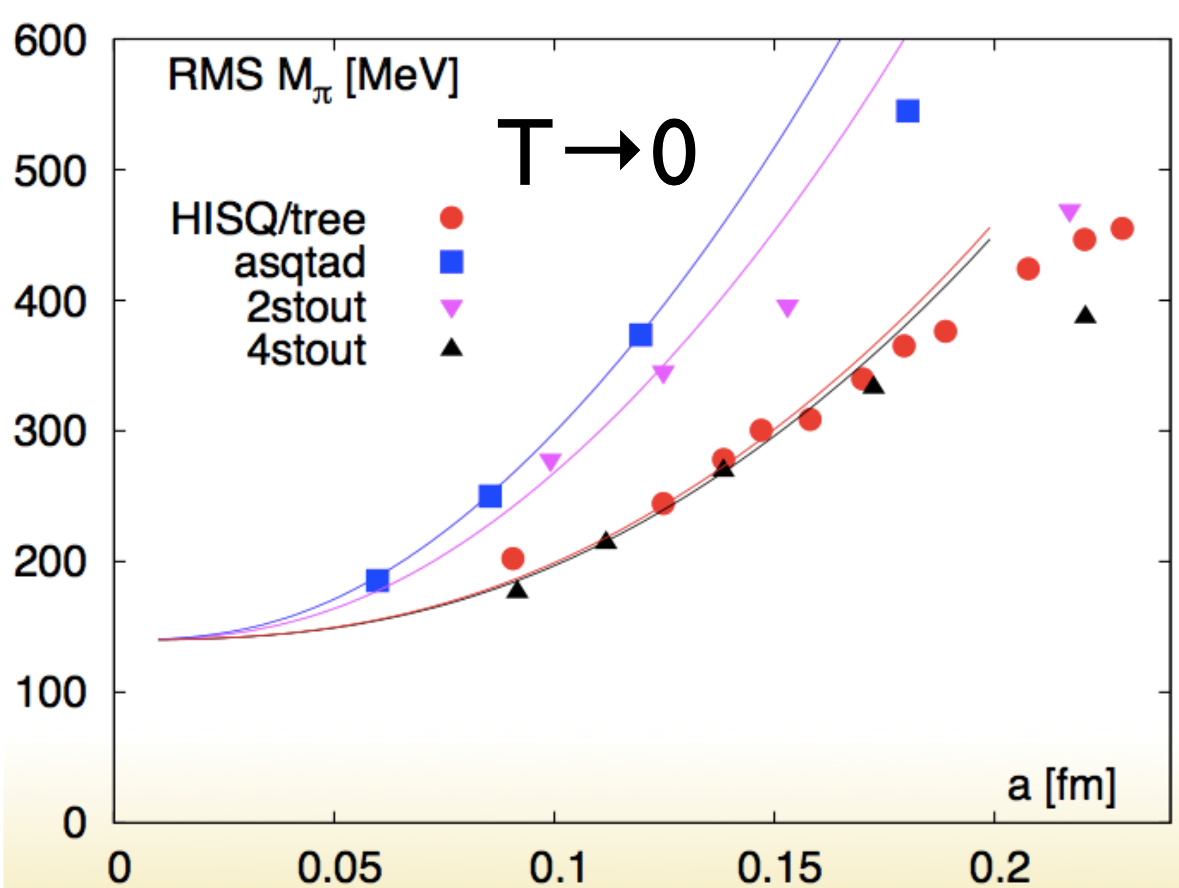
$$\det[D]^* = \det[D^\dagger] = \det[\gamma_5\, D\, \gamma_5] = \det[D] \quad \Rightarrow \quad \det D \in \mathbb{R}$$

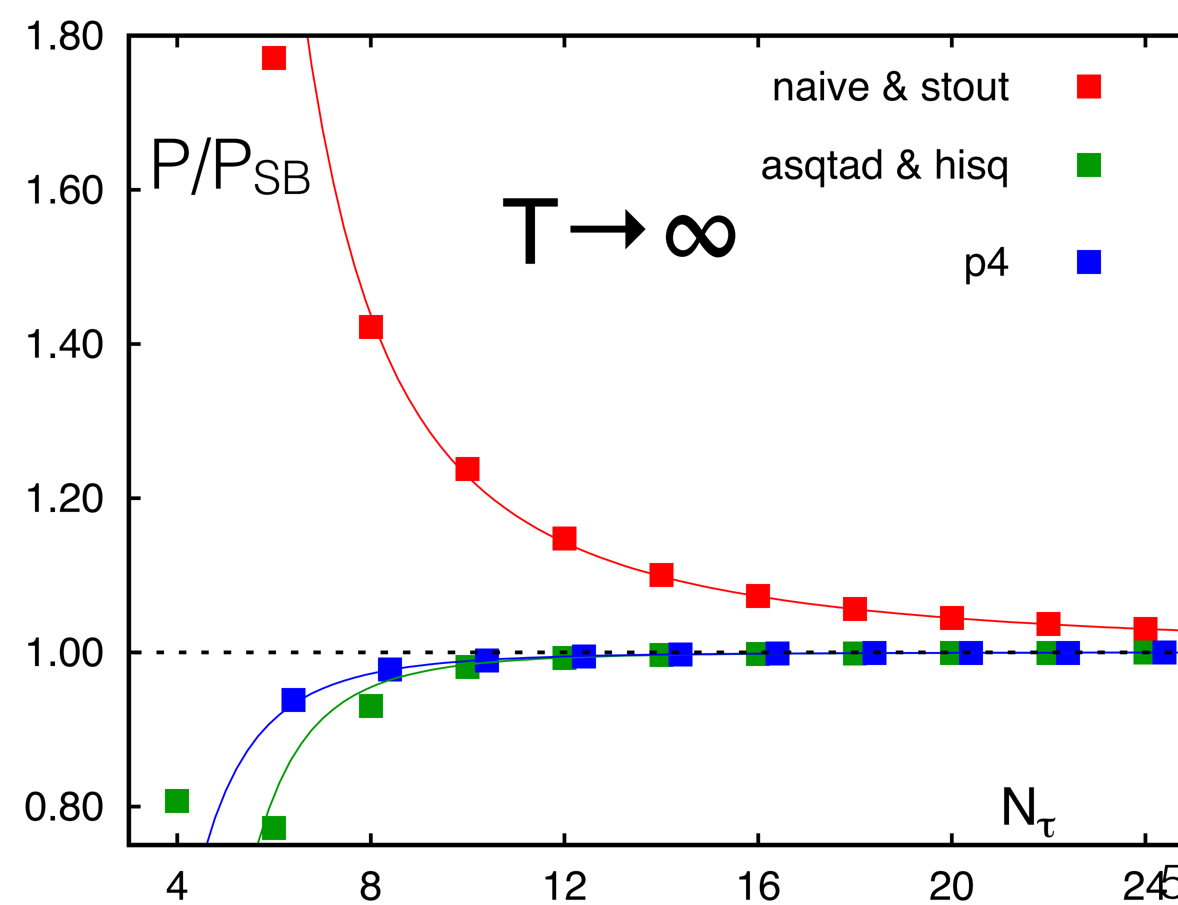
$$0 \le \det[D]\ \det[D] = \det[D]\ \det[D^\dagger] = \det[D\, D^\dagger]$$

Wilson fermion matrix (page 18) satisfy γ_5-hermiticity

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





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:

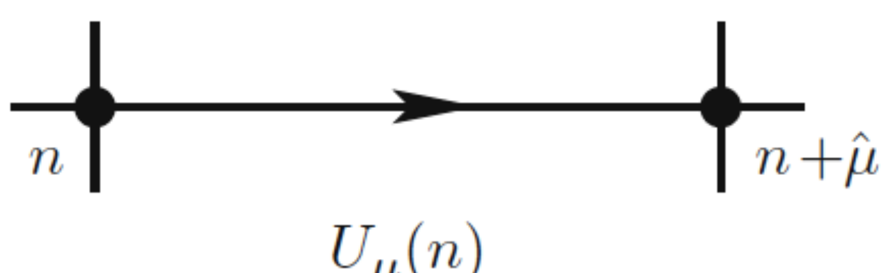
$$\psi(x) \rightarrow \psi'(x) = \Omega(x)\psi(x) \qquad \overline{\psi}(x) \rightarrow \overline{\psi}'(x) = \overline{\psi}(x)\Omega(x)^\dagger$$

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

- Introduction of a gauge link：

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

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



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

Pure gauge theory (N_f=0)

center transformation: $A_4(\mathbf{x}, x_4) \to z\, A_4(\mathbf{x}, x_4)$, $z \in Z(N_c)$

- The gauge action is invariant under the center transformation
- Polyakov loop: $\ell = \frac{1}{N_c} \mathrm{Tr} \left[\mathcal{P} \exp \left(-ig \int_0^\beta \mathrm{d}x_4\, A_4(\mathbf{x}, x_4) \right) \right]$

$$\ell \to z\ell \implies \langle \ell \rangle = \frac{1}{3} \langle \ell + z\ell + z^2 \ell \rangle = 0$$

- Polyakov loop is related to the heavy quark (pair) potential:

$$|\langle \ell \rangle| \propto e^{-f_q/T}, \quad \langle \ell^\dagger(r)\ell(0) \rangle \propto e^{-f_{q\bar{q}}(r)/T}$$

	Confined (Disordered) Phase	Deconfined (Ordered) Phase
Free Energy	$f_\mathrm{q} = \infty$	$f_\mathrm{q} < \infty$
	$f_{\bar{\mathrm{q}}\mathrm{q}} \sim \sigma r$	$f_{\bar{\mathrm{q}}\mathrm{q}} \sim f_\mathrm{q} + f_{\bar{\mathrm{q}}} + \alpha \frac{\mathrm{e}^{-m_\mathrm{M} r}}{r}$
Polyakov Loop	$\langle \ell \rangle = 0$	$\langle \ell \rangle \neq 0$
$(r \to \infty)$	$\langle \ell^\dagger(r)\ell(0) \rangle \to 0$	$\langle \ell^\dagger(r)\ell(0) \rangle \to |\langle \ell \rangle|^2 \neq 0$