

Scientific opportunities & Computing challenges in Hot & Dense Lattice QCD

中国格点QCD第一届年会@华南师范大学, online 202I.IO.30



Heng-Tong Ding (丁亨通) Central China Normal University (华中师范大学)



Lattice QCD at nonzero temperature & density Differences from T=0 lattice QCD



Quark Gluon Plasma Ordinary nuclear (QGP) matter μ_{B}

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



 $T = (aN_{\tau})^{-1}$ with smaller temporal extent

anti-periodic boundary conditions in the temporal direction

Equilibrium & near-equilibrium properties of strong-interaction matter in extreme conditions

> high T, large baron density, strong magnetic field...







超高温或高密度: 激发强相互作用真空、找寻丢失的对称性



"

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.



NUCLEAR PHYSICS A

Nuclear Physics A590 (1995) 11c-28c

RHIC and QCD: an overview

T. D. Lee

Columbia University,

Two Puzzles Of Modern Physics

Vacuum As a Condensate

RHIC Physics and QCD

Phase Transitions Present Theoretical Limitations

A New Theoretical Approach

Elimination of Spurious Fermion Solutions Noncompact Formulation of Lattice QCD







Columbia plot, QCD critical point, In-medium hadron properties...





Nonzero T: First numerical lattice simulations



string tension 1.0 $\beta = \frac{4}{e^2}$ Low T

Michale Creutz @BNL

PRD 1980, cited by 1112 records





Michale Creutz on the beach

Spawned golden age in lattice QCD





(Most likely) the first LQCD simulation at nonzero T in China

高能物理与核物理 第13卷第6期 Vol. 13, No. 6 1989 年 6 月 HIGH ENERGY PHYSICS AND NUCLEAR PHYSICS June, 1989

二维和三维空间 SU(2) 规范群的 Wilson 圈平均值*

李志兵 郑维宏 郭硕鸿

(中山大学,广州)

摘 要

本文采用改进了的 Monte Carlo 方法在二维和三维空间计算了 SU(2) 格 点规范理论的 nxm Wilson 圈平均值,并与分立子群 Y120 以及二维的准确结 果作了比较.

THE WILSON LOOP EXPECTATION VALUES IN 2-AND 3-DIMENSIONAL SU(2) LGT

LI ZHIBING ZHENG WEIHONG GUO SHUOHONG (Zhongshan University, Guangzhou)

ABSTRACT

An improved Monte Carlo scheme is applied to the computation of the expectation values of nxm Wilson loops in both 2-and 3-dimensional SU (2) lattice gauge theories. The results are compared with those simulated by the discrete group Y120 and the exact results in two dimensions.

在哈密顿形式格点理论中¹¹,三维空间的 Wilson 圈与胶球质量、弦张力和玻色凝量 等有非常密切的关系^[2]. 因为维数比拉氏形式格点理论少一维,所需的 Monte Carlo 模 拟时间就大大减少(代价是增加了解析运算量).这一点给在大中型计算机上获取较好的 结果提供了机会.

研究三维纯规范场的另一个很重要的理由涉及到有限温度 QCD 的性质. 三维纯规 范场理论作为极高温(或高密度) FQCD 的极限理论,在描述早期宇宙和高能重离子碰 撞中可能找到其应用^[3]。

常用的模拟 SU(2) 群的方法主要有 Metropolis 方法¹⁵¹和 Creutz 提出的 heat bath 方法^[6]. Cabibbo 和 Marinari 等在模拟 SU(2) 的基础上,把 Creutz 的方法推广到 SU(N) 群的模拟^[7]. 最近 Y. F. Deng 改进了他们的方法^[8],进一步提高了 MC 叠代的 效率. 本文采用 Deng 的方法对二维和三维的 SU(2) 规范群进行了 Monte Carlo 模 拟,并改进了 Wilson 圈的测量方法,使测量时间约缩短三分之一.







^{*} 本工作得到中山大学高等学术中心基金会和国家教委科学基金会的资助. 本文 1988 年 6 月 11 日收到.





Lattice QCD group@CCNU

现课题组成员: 1名教授+1名工程师+2名博士后+3名博士生+5名直博生(硕士阶段)+1名硕士



丁亨通,教授 2013-至今,华中师大



李胜泰, 工程师, 2021-至今,华中师大 核科学计算中心软件负责人



刘俊宏,博士后



黄玮平,华博计划博士生



李文汐,直博生





张英杰,直博生







高翔,博士后

汪晓丹,华博计划博士生 施岐,华博计划博士生









罗冉, 直博生

张丹, 直博生

张成,直博生







Previous group members 已毕业硕士5名、博士3名,出站博士后2名

原课题组成员:



Prasad Hegde, 博士后 (2013-2016) 美国纽约州州立大学石溪分校 博士,出站后被国际著名教育 研究单位——印度科学研究院 (IISc, Banglore) 聘为副教授



Akio Tomiya, 博士后 (2015 - 2018)日本大阪大学博士 出站后赴RIKEN-BNL美国 分部做博士后



QCD EoS at nonzero μ_B

Strong magnetic field

Quarkonia



Chiral phase transition T



张瑜,博士生 (2016-2021)博士毕业后赴日本理 化研究所RIKEN-Kobe做博后

> Axial UI anomaly





S 华中师范大学核科学计算中心 NuclearScience Computing CenteratCCNU

N: Nuclear S: Science C^3 : Color 3 -> QCD "道生一,一生二,二生三,三生万物。"—《道德经》老子600 BC





2018年成立运行, 2PFlops/s, 5 papers published in PRL (LQCD, 2)

Sun, Oct. 31 16:50-17:20



Mon, Nov. 1 15:00-15:30



Quarkonia and heavy quark diffusion in the hot gluonic medium

L. Altenkort, A. M. Eller, O. Kaczmarek, L. Mazur, G. D. Moore, 舒海涛, PRD103 (2021) 1, 014511 丁亨通, O. Kaczmarek, A.-L. Lorenz, H. Ohno, H. Sandmeyer, **舒海涛**, arXiv: 2108.13693.

Mon, Nov. 1 15:30-16:00



Fluctuations of conserved charges in strong magnetic fields 丁亨通,李胜泰,施岐,汪晓丹, EPJA 57 (2021) 6, 202, 丁亨通,**刘俊宏**,李胜泰,汪晓丹, in preparation

Mon, Nov. I 16:00-16:30



Tue, Nov. 2 16:30-16:50



Axial U1 anomaly

丁亨通,李胜泰,复谷昭夫, S. Mukherjee,汪晓丹, **张瑜**, PRL 126 (2021) 082001

Chiral properties of QCD in strong magnetic fields at T=0

丁亨通, 李胜泰, 复谷昭夫, 汪晓丹, 张瑜, PRD 104 (2021) 1

Machine learning spectral functions in lattice QCD

陈世阳,丁亨通,刘非易,G. Papp,杨纯斌, arXiv: 2110.13521





Chiral crossover/phase transition temperature at physical point and $m_q \rightarrow 0$

Rigorous definition from O(4) universality class



A. Bazavov, HTD, P. Hegde et al. [HotQCD], Phys. Lett. B795 (2019) 15, 被引259次

Chiral crossover transition T=156.5(1.5) MeV

Consistent results from Wuppertal-Budapest, PRL125 (2020) 052001





HTD, P. Hegde, O. Kaczmarek et al.[HotQCD], Phys. Rev. Lett. 123 (2019) 062002, 被引93次

Chiral phase transition T is a possible upper bound of T_{CEP} 李胜泰, 晨光杯二等奖





丁亨通,李胜泰,复谷昭夫,S. Mukherjee,汪晓丹,张瑜, PRL 126 (2021) 082001

Axial U1 anomaly



- At a single T~205 MeV
- HISQ/tree action
- $N_{\rm f}=2+1$:
 - ✓ Nt=8,12,16 (a=0.12,0.08,0.06 fm) $M_{s}^{phy}/m_{l} = 20, 27, 40, 80, 160$
 - $m_{\pi} \approx 160, 140, 110, 80, 55 \text{ MeV}$

\swarrow 9 \ge N_s/N_t \ge 4

Novel method to compute the quark mass derivative of Dirac Eigenvalue spectrum









Topological susceptibility at nonzero T SU(3)2+I+I flavor QCD 10² 10⁻¹ 200 -10⁰ 10^{-2} Ŧ ± ± + Ŧ Ŧ 10⁻² 10^{-3} $\chi_{t}^{1/4}/MeV$ 150 · 10⁻⁴ χ [fm⁻⁴] Ŧ 10^{-4} 150 200 250 100 10⁻⁶ 重 $T_2=296 MeV$ 100 10⁻⁸ 重 重 10⁻¹⁰ Ŧ 50 -10⁻¹² 1.5 0.0 0.5 2.0 1.0 200 500 1000 2000 100 T/T T[MeV] 熊光仪,张剑波,陈莹,刘川,刘玉斌,马建平, Borsanyi et al, [WB collaboration], Phys.Lett.B 752(2016)34 Nature 539(2016)7627,69-71 程贞, 张剑波, Chin.Phys.C 45 (2021) 7, 073103







B pointing to the z direction & Gauge link multiplied by a U(1) factor

$$u_x(n_x, n_y, n_z, n_\tau) = \begin{cases} \exp[-\frac{1}{2} \end{bmatrix}$$

$$u_y(n_x, n_y, n_z, n_ au) = \exp[iqa^2Bn_x],$$

 $u_z(n_x, n_y, n_z, n_ au) = u_t(n_x, n_y, n_z, n_ au) = 1.$

Quantization of the magnetic field

$$qB = rac{2\pi N_b}{N_x N_y} a^{-2}$$
 qu=2/3e,

CCNU LQCD group has developed GPU/C++ codes for LQCD simulations at eB=/=0 contributors: Akio Tomiya, 李胜泰, 汪晓丹, 李韶荣, 张瑜 Made in EPJ Web Conf. 175 (2018) 07041, PoS LATTICE2018 (2019) 163, *PoS* LATTICE2019 (2020) 250, *Phys.Rev.D* 102 (2020) 5 Eur. Phys. J.A 57 (2021) 6, 202, Phys. Rev. D 104 (2021) 1, Acta Phys. Polon. Supp. 14 (2021) 403

Lattice QCD in strong magnetic fields No sign problem

 $[-iqa^2 B N_x n_y] \qquad (n_x = N_x - 1)$ (otherwise)

qd=-1/3e, qs=-1/3e
$$eB = \frac{6\pi N_b}{N_x N_y} a^{-2}$$



First LQCD study on GMOR relation at $eB \neq 0$ and T=0



丁亨通,李胜泰,复谷昭夫,汪晓丹,张瑜, PRD 104 (2021) 1

Mon, Nov. 1 16:00-16:30 李胜泰



$$4m_u \langle \bar{\psi}\psi \rangle_u = 2f_{\pi_u^0}^2 M_{\pi_u^0}^2 (1-\delta_{\pi_u^0})$$

$$4m_d \langle \bar{\psi}\psi \rangle_d = 2f_{\pi_d^0}^2 M_{\pi_d^0}^2 (1-\delta_{\pi_d^0}).$$

$$(m_u + m_d) (\langle \bar{\psi}\psi \rangle_u + \langle \bar{\psi}\psi \rangle_d) = 2f_{\pi}^2 M_{\pi}^2 (1-\delta_{\pi})$$

neutral pion remains as a Goldstone boson with eB up to $\sim 3.5 \text{ GeV}^2$





Probe to detect the existence of Mon, Nov. 1 magnetic field in Heavy Ion collision 15:30-16:00 刘俊宏

Heavy-Ion collision



 $1 \text{ Gauss} = 1.95 \times 10^{-14} \text{ MeV}^2$

Fluctuations of conserved charges





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Charm and beauty in hot medium







L. Altenkort, A. M. Eller, O. Kaczmarek, L. Mazur, G. D. Moore, 舒海涛, PRD103 (2021) 1, 014511 丁亨通, O. Kaczmarek, A.-L. Lorenz, H. Ohno, H. Sandmeyer, 舒海涛, arXiv: 2108.13693







Explorative study on the inverse problem using machine learning

$$\begin{split} G(\tau,T) &= \sum_{\substack{x,y,z \\ \mathcal{O}(10)}} \left\langle J_H(0,\vec{0}) J_H^+(\tau,\vec{x}) \right\rangle_T \\ \end{split}$$

Trained to obtain the most probable spectral function:



Production process:

Tue, Nov. 2 16:30-16:50 陈世阳 $O(10^3)$ sVAE: Variational autoencoder including an information entropy $S = \int_{0}^{\infty} d\omega \left(\rho(z) - \rho_{gt} - \rho(z) \log \left(\frac{\rho(z)}{\rho_{gt}}\right)\right)$ $egin{pmatrix} ho(z) o G[ho(z)] \ lpha(z) \end{pmatrix}$ $E_Q[\log P(\rho|z,G)]$ $\left(Q(z|G_{gt}, ho_{gt}) ight)$ sampling zDecoder P(z|G)KL divergence Loss function $egin{array}{l} ho(z) \ lpha(z) \end{array}$ P(z|G)sampling zDecoder

陈世阳, 丁亨通, 刘非易, G. Papp, 杨纯斌, arXiv: 2110.13521











Challenges in mapping out the QCD phase diagram



What is the structure of the QCD phase diagram at nonzero baryon density? Does it, like that of water, feature a critical end point at large baryon density?



Lattice QCD at nonzero baryon density



HTD, F. Karsch, S. Mukherjee, arXiv:1504.05274 Sign Problem at μ_B=/=0 Taylor Expansion Imaginary μ_B Taylor expansion of the QCD pressure:

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

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

Taylor expansion coefficients at μ=0 are computable in LQCD

fluctuations of conserved charges:

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







Mesonic correlators at non-zero baryon chemical potential



S. Choe,...,刘玉斌 et al., [QCD-TARO Collaboration], *Phys.Rev.D*65(2002)054501



G. Aarts,..,吴良凯 et al., [FASTSUM collaboration], arXiv: 2001.04415, *PoS* LATTICE2019(2020)077





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Indirect evidence on



Bielefeld-BNL-CCNU, PRL 113 (2014) 072001 V. Koch, A. Majumder, and J. Randrup, PRL95 (2005) 182301 HRG: Hadron Resonance Gas PDG: Particle Data Group QM: Quark Model



Pressure difference



A. Bazavov, HTD. P. Hegde et al., [HotQCD], Phys.Rev.D 95 (2017) 5, 054504, cited by 303 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 $\mu_B/T \leq 2$ or $\sqrt{s_{NN}} \geq 12$ GeV

QCD Equation of State at small baryon density





Chiral crossover transition temperature at small baryon density



Bazavov, HTD, P. Hegde et al. [HotQCD], Phys. Lett. B795 (2019) 15, cited by 259 records

Consistent results from Wuppertal-Budapest, PRL125 (2020) 052001



Chiral crossover transition temperature at small baryon density



Bazavov, HTD, P. Hegde et al. [HotQCD], Phys. Lett. B795 (2019) 15, cited by 259 records

Consistent results from Wuppertal-Budapest, PRL125 (2020) 052001

ALICE data point: $T_f = 156.5(1.5) \text{ MeV}$

STAR data points:

Adamczyk et al., Phys. Rev. C 96 (4) (2017) 044904







LQCD meets experiment

LQCD data are obtained at $T_{pc}(\mu_B)$ in NNLO



Bazavov, Bollweg, HTD et al., [HotQCD], Phys. Rev. D 101 (2020) 7, 074502, cited by 53 records



General trend of kurtosis R_{42} & skewness R_{31} ratios are consistent

High statistics data at 54.4 GeV are in good agreement





LQCD meets experiment



Bazavov, Bollweg, HTD et al., [HotQCD], Phys. Rev. D 101 (2020) 7, 074502, cited by 53 records



Outlook: Mapping out the QCD phase diagram

RHIC Beam Energy Scan, Phase II (BES-II)

2019-2021: at least 10 times more statistics for each $\sqrt{s_{NN}}$

Lattice QCD: higher accuracy for the 8th & 10th or even higher order Taylor expansion coefficients



in particular for T<135 MeV





CEP search

(for Nt=8 and T=125 MeV, 2PFlops*year)



LQCD: Upto 10th order coefficients known soon! Next step in 5 years

- Exscale PFLOPS
- TFLOPS
- GFLOPS



based on A. Ukawa, 2013 HPC summer school



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Ongoing/Future heavy ion collision experiments



RHIC@BNL:

BES II: 2019-2021, FXT: 2021**s**PHENIX

SALICE/LHCb/CMS/ATLAS@LHC

CEE@Lanzhou, FAIR@GSI, NICA@JINR, J-PARC...







实验



理论









谢谢

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