Computational Aspects of Lattice Gauge Theory

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Outline

Lattice gauge theory as a numerical problem

- path integral formulation of quantum field theory

$$\langle \mathcal{O} \rangle = \frac{\int dA_\mu d\psi d\overline{\psi} e^{-S_E} \mathcal{O}[A_\mu, \psi, \overline{\psi}]}{\int dA_\mu d\psi d\overline{\psi} e^{-S_E}} \tag{1}$$

- infinite dimensional integral problem
- Monte Carlo method for numerical integral
- importance sampling

$$\langle \mathcal{O} \rangle \sim \frac{1}{N} \sum_i \mathcal{O}[A_i] \tag{2}$$

Lattice gauge theory as a numerical problem

- caveats :

  fermion doubling problem

  integration of Grassmann variables

  breaking of continuous spacetime symmetry

Lattice gauge theory as a numerical problem

- fermion doubling problem: staggered fermion, wilson fermion, domain wall fermion, overlap fermion

- analytic integration of grassmann variables: effective action

- point symmetry group for global symmetry: different lattice meson and baryon representation with a same continuum limit

Lattice gauge theory as a numerical problem

- Lattice QCD is based on

$$\langle \mathcal{O} \rangle = \frac{\int D\phi\, \mathcal{O} e^{-\int d^4x \mathcal{L}_E}}{\int D\phi\, e^{-\int d^4x \mathcal{L}_E}} \tag{1}$$

- Lattice QCD is defined on discrete space-time lattices

$\rightarrow$ various scales

a_τ, a_s (UV cutoff)

$\frac{1}{M_q}$ (Compton wavelength)

$N_s a_s$ (spatial IR cutoff)

$N_\tau a_\tau$ (temporal IR cutoff)

Lattice gauge theory as a numerical problem

$$a_\tau << \frac{1}{M_q} << (N_s a_s, N_\tau a_\tau)$$

- for bottomonium, $M_q = M_b(\sim 4.65\mathrm{GeV})$,

  $\frac{1}{M_q} \sim 0.04$ fm and spatial size ~ 1 fm.

  if $a_s \sim 0.01$ fm, $N_s \sim 100$

Lattice gauge theory as a numerical problem

- finite volume effect

- finite lattice spacing effect

- quark mass effect (e.g., physical pion mass? or chiral extrapolation? or is it heavy enough?)

- light quark vacuum polarization

Lattice gauge theory as a numerical problem

- bound state dynamics in quarkonium $\sim \mathcal{O}(100)$ MeV

$n^{S+1}L_J$	State	$a_\tau M$	$E_0 + M$ (MeV)	$M_{\rm expt}$ (MeV)
$1^1\mathrm{S}_0$	η_b	0.20549(4)	9409(12)	9398.0(3.2)
$2^1\mathrm{S}_0$	η_b'	0.311(3)	10004(21)	9999(4)
$1^3\mathrm{S}_1$	Υ	0.21460(5)	9460*	9460.30(26)
$2^3\mathrm{S}_1$	Υ'	0.318(3)	10043(22)	10023.26(31)
$1^1\mathrm{P}_1$	h_b	0.2963(4)	9920(15)	9899.3(1.0)
$1^3\mathrm{P}_0$	χ_{b0}	0.2921(4)	9896(15)	9859.44(52)
$1^3\mathrm{P}_1$	χ_{b1}	0.2964(4)	9921(15)	9892.78(40)
$1^3\mathrm{P}_2$	χ_{b2}	0.2978(4)	9928(15)	9912.21(40)

Table: comparison from FASTSUM

- large energy scale separation between M_b and binding enery
- sub-percent level accuracy required

Lattice gauge theory as a numerical problem

- Effective Field Theory (EFT) : $M_b,\ M_b v,\ M_b v^2$
- NRQCD : M_b scale is "integrated away"

  bottom quark is "point-like" ($M_b a \sim 1$)
- pNRQCD : $M_b, M_b v$ scales are "integrated away"

  bottom quark is "point-like"
  and bottomonium is also "point-like"
  ("Bohr radius" is also an expansion parameter)
- our choice is lattice NRQCD

Lattice gauge theory as a numerical problem

- temperature is an additional scale

$$T = \frac{1}{N_\tau a_\tau} \tag{1}$$

- for consistent lattice NRQCD, $M_b a_\tau \sim 1$

- to keep NRQCD remain valid as an effective field theory, $T << M_b$

- in summary, a consistent lattice NRQCD for bottomonium ($M_b = 4.65$ GeV) requires

$$a_\tau \sim \frac{1}{4.65}(\mathrm{GeV}^{-1}) \tag{2}$$

and

$$T = \frac{1}{N_\tau a_\tau} \sim \frac{4.65\mathrm{GeV}^{-1}}{N_\tau} \tag{3}$$

- if we are interested upto $\sim 2T_c(\sim 300$ MeV for $N_f = 2+1)$,

$N_\tau \sim \mathcal{O}(10)$

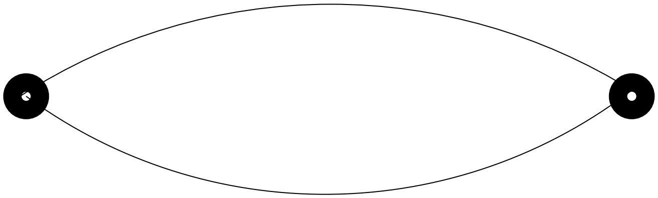
Lattice gauge theory as a numerical problem

• for the study of EoS (entropy density, pressure, energy density etc), $N_\tau \sim \mathcal{O}(10)$ doesn't pose a problem

• for the study of in-medium bottomonium, bottomonium correlator is important

$$G(\tau) = \sum_{\vec{x}} \langle \phi^\dagger(\vec{x},\tau;\vec{0},0)\phi(\vec{x},\tau;\vec{0},0)\rangle \tag{1}$$

• spectral information (mass shift, thermal broadening etc) needs to be obtained from $G(\tau)$ evaluated at $N_\tau \sim \mathcal{O}(10)$ of τ position



bottomonium correlator, $G(\tau, \mathbf{x})$

Lattice gauge theory as a numerical problem

- Step 1: generate Monte Carlo data of “important” gauge configurations

- Step 2: compute observables using these configurations

- Step 3: analyze observables (and other post processing, renormalization and etc)

High Performance Computing - Grid

- EP (Embarassingly Parallel) problem

- Two-color QCD : a model for QCD in finite baryon density (S.Hwang, H. Kim, S.K, Comput. Phys. Commun. 182 (2011) 277

- QCD with imaginary chemical potential : analytic continuation for QCD in finite baryon density (J.T. Mosciki et al, Comput. Phys. Commun. 181 (2010) 1715)

- suitable for parameter scan

High Performance Computing - Parallel Computing

- large problem with data dependency
- most of large scale problem
- parallel programming required : MPI, OpenMP, CUDA
- data parallel or message passing
- data decomposition, surface-to-volume ratio

Step 1: $N_f = 2 + 1$ gauge configuration with $m_\pi = 161$ MeV

- uses gauge field configurations generated by HotQCD collaboration (A. Bazavov et al, PRD85 (2012) 054503)
- $T = 0$ gauge configurations : 32^4 lattice, 48^4 lattice, $48^3 \times 64$ lattice
- $T \neq 0$ gauge configurations : $48^3 \times 64$ lattice
- HiSQ action for quark + tree level improved Symanzik action for gauge field
- hardware : IBM BG/P and BG/Q supercomputers
- takes a few years to generate

Step 2: quarkonium correlator

- NRQCD quark correlator and quarkonium correlator computed on a conventional cluster computer at J-Lab

- purely serial code

- need to run on 400 configurations at $4-7\beta$ values and need to repeat 2 for $T=0$ run : 5600 runs

- need to run on 400 configurations at 14β values and need to repeat 2 for $T\neq 0$ run : 11200 runs

- one run takes 40 hours on 1 node of J-Lab cluster

Step 3: reconstruction of spectral function

- In NRQCD, with $\omega = 2M + \omega'$ and $T/M << 1$, $K(\tau, \omega) \to e^{-\omega\tau}$

$$G(\tau) = \int_{-2M}^{\infty} \frac{d\omega'}{2\pi} \exp(-\omega'\tau)\rho(\omega') \tag{1}$$

- numerical inverse Laplace transform problem
- serial code
- need to repeat for all the β's at $T = 0$ and $T \neq 0$
- Bayesian reconstruction algorithm

Step 1: $N_f = 0$ gauge configurations on $16^3 \times 256$

- uses gauge field configurations generated in-house

- $16^3 \times 256$ lattice ($\sim$ 300 MBytes per configuration) and $20^3 \times 256$ lattice ($\sim$ 600 MBytes) : 400 configurations

- 1 configurations takes 1 hours on 8-node

- parallel code (written in MPI)

- 1-plaquette wilson action

- hardware : 64 + 4 + 6 + 2 + 16 node cluster

Step 1: $N_f = 0$ gauge configurations on $16^3 \times 256$

- multi-hit metropolis + over-relaxation algorithm
- 1000 sweeps separation per configuration
- coding example

Step 2: stoponium correlator

• NRQCD squark correlator and stoponium correlator computed on in-house cluster computer

• need to run on 400 configurations for 8 Ma parameters : 3200 runs

• each run takes 4.2 hours on 1 node of Sejong U. cluster

Step 3: correlator fitting

- correlator fitting

$$G(\tau) = \langle 0|\chi^\dagger \psi(x)\psi^\dagger \chi(0)|0\rangle \tag{2}$$

$$G(\tau) = A_0 e^{-E_0\tau} + A_1 e^{-E_1\tau} + \cdots \tag{3}$$

- χ^2 minimization

Discussion

- use a well developed code : MILC code, Chroma code (and many more)

- develop your own code : serial vs parallel

- dedicated hardware resources vs computer center