Expected precision in future lattice calculations

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Expected precision in future lattice calculations - p.1

By the Super-B factory, experiment will go far ahead of us.

• $|V_{td}|$:

 ΔM_d is known very well (~ 1%), while the lattice calculation of $f_B^2 B_B$ is not (~ 20%). The lattice error has not shrunk in the past decade.

• $|V_{ub}|$

Exclusive decays $B \rightarrow \pi l \nu$, $\rho l \nu$ will be measured very well at Super-B (\leq 5%), while the current lattice calculation suffers from large errors (\sim 20%).

Substantial improvement of the lattice calculation: *needed but possible?*



To be competing with the experiment / to be useful for the flavor physics, we have to achieve < 5% accuracy.

- The CLEO-c report (*the yellow book*) assumed 1% (or a few %) for $f_{D_{(s)}}$ and semileptonic form factors.
 - ⇒ a few % determination of $|V_{cd}|$ and $|V_{cs}|$ without assuming the CKM unitarity.
- The Super-KEKB Lol assumes 5% for $f_B \sqrt{B_B}$ and $B \rightarrow \pi$ form factor. *(conservative?)*



Specific questions (to myself)

- Is the 1% (or a few %) accuracy really achievable in the next several years?
- It must include the effect of dynamical quarks (up, down, and strange). Is it feasible?
- What is needed to achieve this goal?

To consider these questions, let us look back what happened in the past 10 years.



Plan of the talk

- 1. Improvements in lattice QCD
 - Symanzik's improvement
 - HQET/NRQCD
 - renormalized perturbation theory
- 2. Unquenching
 - why so hard?
 - chiral extrapolation
 - fermion actions
- 3. Future Is the 1% feasible?
 - machines



Improvements in lattice QCD

- Introduction
- Symanzik's improvement
- HQET/NRQCD or conventional
- renormalized perturbation theory (or non-perturbation matching)



Lattice QCD = first principles calculation

A regularization of QCD:



lattice spacing *a*

- Numerical simulation is possible.
 path integral ⇒ Monte Carlo
- It gives a nonperturbative formulation of QCD.
 ⇔ Dimensional regularization is defined through perturbation theory.

prediction of LQCD = prediction of QCD



To reproduce the real world, one needs

- unquenched, $N_f = 2+1$.
- *L* = 5 fm.
- a = 0.02 fm;or $a^{-1} = 10 \text{ GeV}.$
- m_{ud} = several MeV, m_s = 100 MeV.
- statistics ~ 10 K.



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Empirial law : the computational demand scales as

$$\left[\frac{m_{\pi}/m_{\rho}}{0.6}\right]^{-6} \left[\frac{L}{3 \text{ fm}}\right]^{5} \left[\frac{a^{-1}}{2 \text{ GeV}}\right]^{7}$$



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For this example, we need 10¹⁰ TFlops · year

Theoretical/algorithmic improvements are crucial.



It is hard to describe the physics at different energy scales on a single lattice.

$m_W \gg m_b > m_c \gg \Lambda_{QCD} \gg m_q$

Lattice QCD deals with the physics at the $O(\Lambda_{QCD})$, leaving the others for effective theories.

- m_W : Weak effective Hamiltonian (4-fermion interactions)
- m_b, m_c : Heavy Quark Effective Theory (HQET)
- m_q : Chiral Perturbation Theory (ChPT)
- 1/a : Symanzik's effective theory (discretization error)



How the discretization error looks like:

 $\mathcal{L}_{lat} \doteq \mathcal{L}_{QCD} + \mathcal{L}_{I}$

 \doteq means "give the same on-shell amplitude." \mathcal{L}_{QCD} is the continuum QCD lagrangian.

• Discretization error is described by local operators \mathcal{L}_I :

$$\mathcal{L}_I = a\mathcal{L}^{(5)} + a^2\mathcal{L}^{(6)} + \cdots$$

Theoretical basis to construct the *improved* actions.



Order counting assuming $\Lambda_{QCD} = 400$ MeV:

a (fm)	0.2	0.1	0.05
1/a (GeV)	1	2	4
$O(a\Lambda_{\rm QCD})$	40%	20%	10%
$O((a\Lambda_{\rm QCD})^2)$	16%	4%	1%
$O((a\Lambda_{\rm QCD})^3)$	6%	1%	< 1%
$O((a\Lambda_{\rm QCD})^4)$	3%	< 1%	< 1%

To achieve the 1% accuracy,

- O(a)-improved action + extrapolation in a^2
- $O(a^2)$ -improved action at a = 0.1 fm.





Heavy quark is static (non-relativistic) in the heavy-light (heavy-heavy) meson. Dynamical degrees of freedom are $\sim O(\Lambda_{\rm QCD})$, which we treat non-perturbatively on the lattice.

$$\mathcal{L}_Q = Q^{\dagger} \left[iD_0 + \frac{\mathbf{D}^2}{2m_Q} + \cdots \right] Q$$

- \cdots an expansion in $\Lambda_{\rm QCD}/m_Q$.
 - HQET: Eichten et al. (1990)
 - NRQCD: Lepage et al. (1992)
 - Fermilab action: El-Khadra, Kronfeld, Mackenzie (1997)



HQET order counting

Assuming $\Lambda_{\rm QCD} =$ 400 MeV:

m_Q	m_b	m_c
(GeV)	4.5	1.5
$O(\Lambda_{ m QCD}/m_Q)$	9%	27%
$O((\Lambda_{\rm QCD}/m_Q)^2)$	1%	7%
$O((\Lambda_{\rm QCD}/m_Q)^3)$	< 1%	2%
$O((\Lambda_{\rm QCD}/m_Q)^4)$	< 1%	< 1%

Т

To achieve the 1% accuracy,

- $O(\Lambda_{\rm QCD}/m_Q)$ or $O((\Lambda_{\rm QCD}/m_Q)^2)$ action for b quark
- $O((\Lambda_{\rm QCD}/m_Q)^3)$ action for c quark



It is also possible to use the conventional fermion action as far as $am_Q \ll 1$. For $m_c = 1.5$ GeV,

a (fm)	0.1	0.05	0.03	0.02
1/a (GeV)	2	4	6.7	10
$O(am_c)$	75%	38%	22%	15%
$O((am_c)^2)$	56%	14%	5%	2%
$O((am_c)^3)$	42%	5%	1%	< 1%

To achieve the 1% accuracy,

- O(a)-improved action at $a \leq 0.03$ fm + extrapolation in a^2 .
- $O(a^2)$ -improved action at a = 0.03 fm.



Example: Continuum extrapolation of f_{D_s}

Juttner, Rolf, PLB560 (2003) 59.

- quenched approximation
- O(a)-improved action
- a = 0.09–0.05 fm

Extrapolation in a^2 :

 $f_{D_s} = 252(9)$ MeV.

(4% error) using f_K as an input for the lattice scale.



Extrapolation to the b quark

Rolf *et al.*, hep-lat/0309072 Continuum extrapolation at (or interpolation) in $1/m_O$. several m_Q ,



Then, another extrapolation



Better controled with a combination with HQET.



Matching of continuum and lattice operators

$$\mathcal{O}^{\overline{\mathrm{MS}}}(\mu) = Z(\mu a)\mathcal{O}^{lat}(a)$$

In most cases, $Z(\mu a)$ is known only at one-loop.

Renormalized lattice perturbation theory

Lepage, Mackenzie (1993),

 $1 + c_1 \alpha_0 + c_2 \alpha_0^2 + \cdots$ poor convergence = $1 + c_1 \alpha_V(q^*) + c'_2 \alpha_V^2(q^*) + \cdots$ much better renormalized coupling



Coupling constant is evaluated at a typical scale $q^* \sim 2/a$.

a (fm)	0.2	0.1	0.05
1/a (GeV)	1	2	4
$\alpha_s(2/a)$	0.26	0.22	0.18
$O(\alpha_s)$	26%	22%	18%
$O(\alpha_s^2)$	7%	5%	3%
$O(lpha_s^3)$	2%	1%	< 1%

To achieve the 1% accuracy,

• two-loop calculation at $a \leq$ 0.1 fm; need automated perturbative calculation.



Or, one may prefer some non-perturbative methods to eliminate the perturbative error.

Heitger, Sommer, hep-lat/0310035.

- Matching the relativistic lattice action and HQET for $am_Q \ll 1$. It is possible if the entire lattice volume is small $L_0 \simeq 0.2$ fm.
- Recursively match the HQET in larger volumes $L_i = 2^i L_0$ until L_i becomes physical volume 2 fm.

Both the perturbative and non-perturbative avenues are to be pursued.



Unquenching

- why so hard?
- chiral extrapolation



An "approximation" to neglect the fermion determinant in the Feynman path integral,

$$Z = \int [dU_{\mu}] \det M^2 e^{-S_G}$$

due to its huge computational demand.

- Most lattice calculations (\lesssim 2000) were within the quenched approximation.
- Its uncertainty is out of control. The only possible solution is to put det back.



Monte Carlo simulation has to deal with

$$Z = \int [dU_{\mu}] \det M^2 e^{-S_G} = \int [dU_{\mu}] [d\phi] e^{-S_G - \phi^{\dagger} (M^{\dagger}M)^{-1} \phi}$$

 $M \equiv \det(\mathcal{D}[U_{\mu}] + m)$ is the fermion matrix; ϕ is a (fictitious) pseudo-fermion field.

- The effective action becomes non-local $\phi^{\dagger}(M^{\dagger}M)^{-1}\phi$; local updation is difficult.
- Matrix inversion $(M^{\dagger}M)^{-1}$ is time-consuming especially for light quarks.

Simulation of light dynamical quarks is very hard: $\sim 1/m_q^3$.



QCD with very small quark masses is described by Chiral Perturbation Theory (ChPT). It can be used to extrapolate lattice data toward the physical point.

 Need overlap region. Perhaps around (500 MeV)²; maybe (300 MeV)²?





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Test with the pion decay constant

Full ChPT

$$\frac{f_{SS}}{f} = 1 - \frac{N_f}{2} y_{SS} \ln y_{SS}$$
$$+ \frac{1}{2} \alpha_5 y_{SS} + \frac{1}{2} \alpha_4 N y_{SS}$$
$$y_{SS} \equiv \frac{m_{SS}^2}{(4\pi f)^2}$$

- chiral log with a known coeffi cient

Quenched ChPT

$$\frac{f_{11}}{f} = 1 + y_{11} \frac{1}{2} \alpha_5.$$

- no quenched chiral log

JLQCD (2002): a high statistics test with the O(a)-improved Wilson fermion.



Data do not show the curvature above (500 MeV) 2 .



Impact on physical quantities

decay constant f_{π}



Possible fit forms:

quadratic fit (no chiral log)



Impact on physical quantities

decay constant f_{π}



Possible fit forms:

- quadratic fit (no chiral log)
- chiral log (with the known coefficient) plus quadratic

curvature cancels in the data region.



Impact on physical quantities

decay constant f_{π}



Possible fit forms:

- quadratic fit (no chiral log)
- chiral log (with the known coefficient) plus quadratic
 curvature cancels in the data region.
- One-loop ChPT formula below μ (μ = 300 MeV and 500 MeV are shown.)

Introduce model dependence; uncertainty of order $\pm 10\%$ in the chiral limit.



Heavy-light meson decay constant

ChPT for the heavy-light decay constant ($N_f = 2$)

Grinstein et al. (1992)

$$\frac{f_B}{f_B^{(0)}} = 1 - \frac{3}{8}(1 + 3g^2) y_{SS} \ln y_{SS}$$
$$+ \text{analytic terms}$$
$$y_{SS} \equiv \frac{m_{SS}^2}{(4\pi f)^2}$$

in the heavy quark mass limit.

 $g: B^*B\pi$ coupling g = 0.59(7) (D^* width, CLEO) JLQCD (2003)



Signifi cant uncertainty depending on the form of chiral extrapolation.



Need even smaller sea quark masses. But how?

 $1 - y \ln y + c_1 y + c_2 y^2$, $y \equiv m_{PS}^2 / (4\pi f)^2$. m_{PS} (MeV) $|y \ln y|$ y^2 $|y^2/(y \ln y)|$ Ŷ 700 0.384 0.368 0.147 40% 0.196 0.319 0.038 12% 500 0.125 0.260 400 0.016 6% 300 0.070 0.186 3% 0.005

To achieve the 1% accuracy,

• $m_{PS} \lesssim 400$ MeV will be needed. Statistical precision of each point is also crucial for a controlled extrapolation.



The problem of chiral extrapolation may be related to the problem of chiral symmetry on the lattice.

- Wilson-type fermions:
 - Add a Wilson term $\frac{1}{2}a\bar{\psi}D^2\psi$ to the action.
 - A conventional choice in the quenched calculations.
 - Chiral symmetry is explicitly broken; massless limit is not determined by any symmetry.
 - ⇒ The computational time $1/(m_q + \Delta m_q)^n$ fluctuates, or even diverges, configuration by configuration.
 - Smallest available sea quark mass is $\sim m_s/2$.



- Staggered fermions:
 - Contains 4 flavors (or 4 *tastes*) of quarks; Chiral U(1) remains out of U(4).
 - Complicated taste structure: 15 pions (1 is NG; others are not), 64 protons *etc.*
 - Take $(\det M)^{1/4}$ per flavor.
 - \Rightarrow Effective action is non-local; inconsistent as a lattice field theory.
 - Effective lattice spacing is $\times 2$ larger; lattice effect could be larger.
 - . Numerically so cheap. Smallest available sea quark mass is $\sim m_s/6.$



Realistic staggered simulations

HPQCD-UKQCD-MILC-Fermilab collaboration (2003)

- 2+1 flavor (u, d and s)
- O(a²)-improved
 staggered fermion
- $m_{u,d} = m_s/2 m_s/6$ chiral extrapolation is done with the data below $m_s/2$.
- lattice spacing 1/8 fm and 1/11 fm.

decay constant





quenched versus unquenched (hep-lat/0304004).



Impressive agreement with experiments. Promising also for *B* and *D* physics.



Other choices

- The best available fermion formulation is the Ginsparg-Wilson fermions (domain-wall or overlap).
 - An exact chiral symmetry on the lattice without introducing fictitious tastes.
 - Tested on the quenched lattices. Simulations with very light quark masses are possible.
 - . The unquenched simulation is extremely demanding (a factor $\times 10\text{--}100$ over the Wilson-type).

Dynamical simulation is already going on at Columbia-RBC with the domain-wall fermion.



Future

- machines
- perspectives and summary



Machine

Moore's law: The computer speed becomes $\times 10$ in 5 years.



Machines available for lattice QCD

Not a complete list:

- SR8000 (KEK): 1.2 TFlops since 2000.
- QCDSP (Columbia + RIKEN-BNL): 1.1 TFlops (total) since 1998.
- QCDOC: 5–10 TFlops in 2004 @ Columbia, RIKEN-BNL, Edinburgh.
- apeNEXT: more than 5 TFlops in 2004 (?) @ INFN, DESY, ...
- many PC clusters @ many places

In 2005–2010, several tens of TFlops will be available for lattice calculations.



I don't see any *fundamental* problems to achieve the goal, *i.e.* a few % accuracy for the *B* physics.

- $O(a^2)$ -improved action at a = 0.1 fm.
- $O((\Lambda_{\rm QCD}/m_Q)^2)$ action for *b* quark. (Without HQET, the *b* quark is not feasible.)
- two-loop matching at $a \leq 0.1$ fm.

All these iterms are within reach. Actually, they are on the program of the HPQCD-UKQCD-MILC-Fermilab group.

This argument is based on an order counting. Scaling test will be needed to convince ourselves (and then others).



There are *practical* problems:

- Two-loop calculation: It is hard. There has been good progress in the past few years, but lots of things are yet to be done.
- Statistics: Present lattice calculations are limited by systematics. But for a few % precision the statistics may be an issue again, especially for unquenched calculations



Computationally most demanding item is the

• dynamical fermion at $m_{u,d} \lesssim m_s/3$.

At present (with O(1) TFlops machines), this is only feasible with the (improved) staggered fermion. Other fermion formulations will need at least $\times 10$ more computer time = five more years to follow.

Therefore,

- short-mid term: More test of the improved staggered fermion (scaling, taste breaking, etc.)
- mid-logn term: Need much faster algorithms for other fermion formulations (especially the GW fermions)



Lattice calculation: ... no fundamental problems to get high accuracy, just take more time.

The *real* question = earlier than the Super-B or later.



1. The problem of chiral extrapolation has recently emerged and added large uncertainty. Do you guarantee that there is no more unknowns?

You can bet! Unquenching is a big step toward the real physics. Remaining improvement will be more like an incremental one.

2. In order to convince non-lattice people, you should give predictions rather then *post*-dictions.

Well, f_B is a prediction. In any case, lattice calculation does not have free parameters to tune.

