

Summary of LQCD123/QCDLAT activities

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Outline

- Down to the physical pion mass
- Flavour physics and SM precision tests
- Including electromagnetism
- Dynamical generation of elementary particle masses
- Improving $N_f = 3$ Wilson fermions

- Disclaimer
 - Slides & info have been provided to me by the LQCD123 & QCDSLAT people

Down to the physical pion mass - I

- $N_f = 2 + 1 + 1$ simulations with twisted clover fermions (ETMC)
 - generating $O(a)$ -improved configurations
 - first low energy results: the pion sector

$N_f = 2 + 1 + 1$ simulations						
a (fm)	Vol	M_π (MeV)	# traj's	# traj's Total 2017	CPU (Mchs) 2017	Machine 2017
0.096	$48^3 \times 96$	170	2.2 k	0.3 k	0.5	Juqueen
	" $32^3 \times 64$	250	2.6 k	2.6 k	4.1	Marconi
	" $24^3 \times 48$	300	5.2 k	5.2 k	4.0	Marconi
	" $24^3 \times 48$	350	5.0 k	5.0 k	3.8	Marconi
0.080	$64^3 \times 128$	139	3.0 k	3.0 k	45.0	SuperMUC
	" $48^3 \times 96$	250	0.5 k	0.5 k	3.2	Marconi

Down to the physical pion mass - II

- $N_f = 4$ simulations for RC calculations
 - mass independent renormalization scheme
 - Z_A, Z_V, Z_P, \dots

$N_f = 4$ simulations						
a (fm)	# ensembles	Vol	# traj's per ens.	# traj's 2017	CPU (Mchs) 2017	Machine 2017
0.096	5	$24^3 \times 48$	3.0 k	2.0 k	0.5	BG/Q Turing
"		"		3.0 k	0.8	Bern cluster
"		"		3.0 k	0.4	Zeuthen
"		"		1.0 k	0.2	Marconi
0.080	5	$24^3 \times 48$	3.0 k	5.5 k	1.3	BG/Q Turing
"		"		2.5 k	0.6	Bern cluster
"		$32^3 \times 64$		1.0 k	0.7	Bern cluster

$N_f = 4$ inversions (RI/S-MOM)					
a (fm)	# ensembles	Vol	# gauges per ens.	CPU (Mchs) 2017	Machine 2017
0.080	2×5	$24^3 \times 48$	200	1.2	Marconi

SM precision tests

Lattice QCD and the phenomenology of Flavor Physics

* The interpretation of experimental data typically requires the precise knowledge of several hadronic parameters

* Lattice QCD provides a first principle approach to the calculation of all the non-perturbative effects of strong interactions

The goal is to achieve a theoretical precision comparable to the experimental one

Flavor Lattice Averaging Group (FLAG): 3rd review EPJC (2017)

quantity	FLAG-3 average	FLAG-3 error (%)	relevance
$\alpha_{\text{MS}}^{(5)}(M_z)$	0.1182 (12)	1.0	QCD parameter
m_{ud} (MeV)	3.373 (80)	2.4	QCD parameter
m_s (MeV)	93.9 (1.1)	1.2	QCD parameter
f_{K^+}/f_{π^+}	1.193 (3)	0.25	V_{us} from K_{l2}
$f_{\pi^+}(0)$	0.9704 (33)	0.34	V_{us} from K_{l3}
\hat{B}_K	0.763 (10)	1.3	$K - \bar{K}$ oscillations
f_{D_s} (MeV)	248.83 (1.27)	0.5	V_{cs} (V_{cd})
f_{B_s} (MeV)	224 (5)	2.2	$B_s \rightarrow \mu^+ \mu^-$
$f_{B_s} \sqrt{\hat{B}_{B_s}}$ (MeV)	270 (16)	5.9	$B - \bar{B}$ oscillations
ξ	1.239 (46)	3.7	$B - \bar{B}$ oscillations



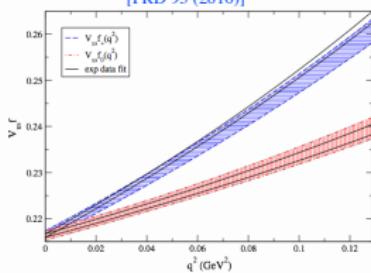
SM precision tests

Two main LQCD activities in RM3

* vector and scalar form factors $f_{+,0}(q^2)$ for the semileptonic decays $K \rightarrow \pi \ell \nu_\ell$ and $D \rightarrow \pi(K) \ell \nu_\ell$ relevant for V_{us} and $V_{cd(s)}$

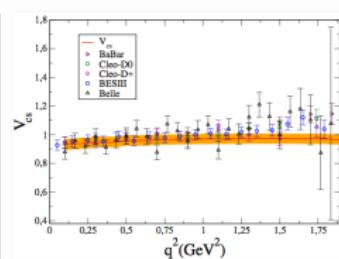
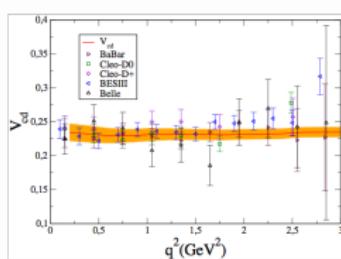
comparison of lattice results with experiments for $K \rightarrow \pi \ell \nu_\ell$

[PRD 93 (2016)]



extraction of V_{cd} and V_{cs} from experimental decay rates using lattice form factors

[PRD 96 (2017) and arXiv:1706.03657]



* more challenging the form factors for the semileptonic decays $B \rightarrow \pi(K, D, D^*) \ell \nu_\ell$ relevant for V_{ub} (V_{cb}) and [R(D), R(D^*)]

- the physical b-quark cannot be simulated on present lattices
- ETMC has developed the “ratio method” to deal with the extrapolation from the physical charm to the physical beauty for many observables
 - JHEP 04 (2010), JHEP 01 (2012)
 - JHEP 03 (2014), PRD 93 (2016)
- the computation of form factors is very demanding as for the memory requirements:
 $V^*T = (48)^3 * 96$, 15 light and heavy quark masses from the c- to the b-quark, 10 values of injected quark momenta (via non-periodic boundary conditions), 4 stochastic sources per gauge conf. ==> ~ 1200 propagators of ~ 6 GB each

~ 70 TB of memory ==> ~ 80 nodes of Marconi A2 (KNL)



Including electromagnetism - The problem

EM and isospin breaking relevant at 1 % accuracy

- Insertion method - expansion in α_{em} and $|m_u - m_q|/\lambda_{QCD}L$
 - IR divergencies in intermediate steps
 - Real and virtual photons
- Full QED+QCD simulation with C^* -bc's
 - Gauge field zero mode (with pbc's)
 - Charged state propagation (Gauss' law)
- Computational bottlenecks
 - Finite size effects
 - Electro-unquenching

Including electromagnetism - Insertion method

* Electromagnetic and strong Isospin Breaking effects due to the up/down quark mass difference and quark electric charges

- RM123/Soton group has developed a new, efficient method to evaluate e.m. and IB effects on hadron masses (IR divergency free) and on hadron decay rates (intermediate IR divergencies)

JHEP 04 (2012)
PRD 87 (2013)
PRD 91 (2015)

meson masses [PRD 95 (2017)]

$$M_{\pi^+} - M_{\pi^0} = 4.21(26) \text{ MeV} \quad [4.5936(5) \text{ MeV}]_{\text{exp.}}$$

$$[M_{K^+} - M_{K^0}]^{\text{QED}}(\bar{MS}, 2 \text{ GeV}) = 2.07(15) \text{ MeV},$$

$$[M_K^- - M_{K^0}]^{\text{QCD}}(\bar{MS}, 2 \text{ GeV}) = -6.00(15) \text{ MeV},$$

$$(\hat{m}_d - \hat{m}_u)(\bar{MS}, 2 \text{ GeV}) = 2.38(18) \text{ MeV},$$

$$\frac{\hat{m}_u}{\hat{m}_d}(\bar{MS}, 2 \text{ GeV}) = 0.513(30),$$

$$\hat{m}_u(\bar{MS}, 2 \text{ GeV}) = 2.50(17) \text{ MeV},$$

$$\hat{m}_d(\bar{MS}, 2 \text{ GeV}) = 4.88(20) \text{ MeV},$$

$$\epsilon_{\rho^0} = 0.03(4),$$

$$\epsilon_{\rho^0}(\bar{MS}, 2 \text{ GeV}) = 0.80(11),$$

$$\epsilon_{K^0}(\bar{MS}, 2 \text{ GeV}) = 0.15(3),$$

$$[M_{D^+} - M_{D^0}]^{\text{QED}}(\bar{MS}, 2 \text{ GeV}) = 2.42(51) \text{ MeV},$$

$$[M_{D^+} - M_{D^0}]^{\text{QCD}}(\bar{MS}, 2 \text{ GeV}) = 3.06(27) \text{ MeV},$$

$$M_{D^+} - M_{D^0} = 5.47(53) \text{ MeV} \quad [4.75(8) \text{ MeV}]_{\text{exp.}}$$

$$\delta M_{D^+} + \delta M_{D^0} = 8.2(9) \text{ MeV},$$

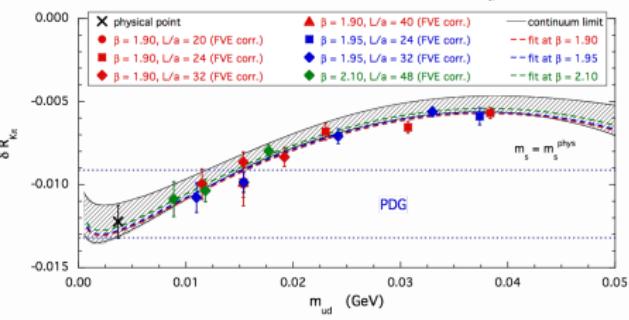
$$\delta M_{D_s^+} = 5.5(6) \text{ MeV},$$

- double expansion in e^2 and $(m_d - m_u)$:

$$\begin{aligned} M_{K^+} - M_{K^0} &= (e_u^2 - e_d^2)c^2\partial_t \left(\text{diagram A} \right) - (e_u^2 - e_d^2)c^2\partial_t \left(\text{diagram B} \right) + \\ &\quad - 2\Delta m_{ud}\partial_t \left(\text{diagram C} \right) - (\Delta m_u^{cr} - \Delta m_d^{cr})\partial_t \left(\text{diagram D} \right) + (e_u - e_d)^2 \sum_j \textcolor{blue}{j} \partial_t \left(\text{diagram E} \right), \end{aligned}$$

first lattice evaluation of leptonic decay rates [arXiv:1711.06537]

$$\frac{\Gamma(K_{l2})}{\Gamma(\pi_{l2})} = \left| \frac{V_{us} f_K^{(0)}}{V_{ud} f_\pi^{(0)}} \right|^2 \frac{M_K^3}{M_K^2} \frac{\left(M_K^2 - m_l^2 \right)^2}{\left(M_\pi^2 - m_l^2 \right)} (1 + \delta R_{K\pi})$$



need of evaluating (fermionic) disconnected diagrams to overcome the quenched QED approximation

$$Tr \left\{ \Gamma S(x, x) \right\}$$

computations are very demanding:
inversions on hundreds of stochastic sources per gauge configuration

Including electromagnetism - C^* bc's

RC* collaboration 1/3

b.lucini, a.patella, a.ramos, n.t, JHEP 1602(2016) 076

- consider C^* boundary conditions (first suggested by wise and polley 91)

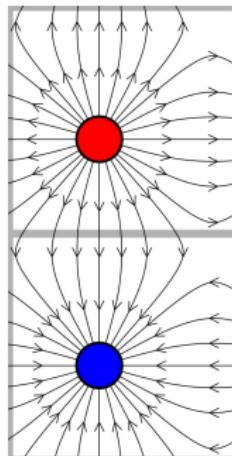
$$\psi_f(x + L\mathbf{k}) = C^{-1} \bar{\psi}_f^T(x)$$

$$\bar{\psi}_f(x + L\mathbf{k}) = -\psi_f^T(x)C$$

$$A_\mu(x + L\mathbf{k}) = -A_\mu(x) , \quad U_\mu(x + L\mathbf{k}) = U_\mu^*(x) ,$$

- the gauge field is anti-periodic ($|\mathbf{p}|_{min} = \pi/L$): no zero modes by construction!
- this means no large gauge transformations and

$$Q = \int_{L^3} d^3x \rho(x) = \frac{1}{e} \int_{L^3} d^3x \partial_k E_k(x) \neq 0$$



- a fully gauge invariant formulation is possible: the electrostatic potential, $\Phi(\mathbf{x})$, is unique and well defined with anti-periodic boundary conditions

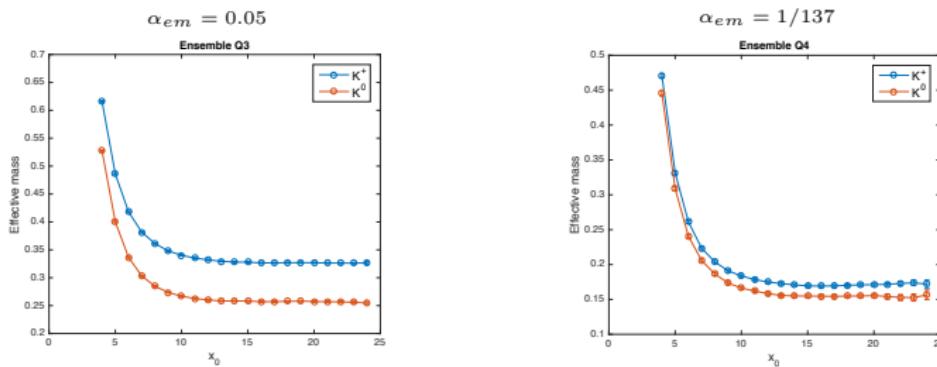
$$\Psi_f(t, \mathbf{x}) = e^{-iq_f \int d^3y \Phi(\mathbf{y}-\mathbf{x}) \partial_k A_k(t, \mathbf{y})} \psi_f(t, \mathbf{x}) , \quad \partial_k \partial_k \Phi(\mathbf{x}) = \delta^3(\mathbf{x})$$



Including electromagnetism - C^* -bc's

RC* collaboration 2/3

m.hansen, b.lucini, a.ramos, a.patella, n.t. in preparation



- the mass of, say, the charged kaon can be extracted from the **fully gauge invariant correlator**

$$\sum_{\omega} \langle \bar{\Psi}_s \gamma_5 \Psi_u(t, \omega) \bar{\Psi}_u \gamma_5 \Psi_s(0) \rangle = \frac{Z_{K^+}(L)}{2M_{K^+}(L)} e^{-M_{K^+}(L)t} + \mathcal{O}[e^{-\Delta(L)t}]$$

- full unquenched simulations of QCD+QED_C (QCD parameters from CLS):

$$24^3 \times 48 , \quad \beta = 3.55 , \quad \kappa_f = \{0.137, 0.137, 0.137\} ,$$

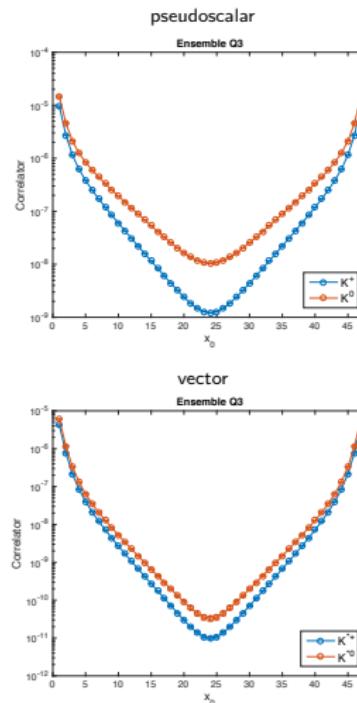
$$a(\alpha_{em} = 0) = 0.0643(7) \text{ fm} , \quad L(\alpha_{em} = 0) = 1.54 \text{ fm} , \quad M_{\pi, K}(\alpha_{em} = 0) = 420 \text{ MeV} ,$$

$$\alpha_{em} = \{0.05, 1/137\} , \quad q_f = \{+2/3, -1/3, -1/3\}$$

Including electromagnetism - C^* bc's

RC* collaboration 3/3

- our results clearly demonstrate the numerical feasibility of a **non-perturbative fully gauge-invariant calculation of charged hadrons masses** within the framework of local constructive quantum field theory
- the **numerical signal** for charged correlators with gauge-invariant interpolating operators is as **good** as in the neutral sector!
- much more numerical work will be needed to obtain results at the physical values of the quark masses, in the continuum and infinite volume limits...
- this is a long-term project of the RC* collaboration: download the **openQCD** code to simulate QCD+QED_C from <http://rcstar.web.cern.ch>
- these results have been obtained by using **60307 node hours** on the KNL partition, i.e. **4.1×10^6 core hours**



Dynamical Generation of Elementary Masses

- Elementary particle masses are (conjectured to be) dynamically generated in a **critical model** where
 - in PT fermions are kept massless by a global symmetry (χ)
 - chiral fermion symmetry ($\tilde{\chi}$) is only broken at the UV scale
- Consider the (χ -invariant) theory Frezzotti Rossi, PRD 92 (2015) 054505

$$\mathcal{L}_{\text{toy}}(Q, A, \Phi) = \mathcal{L}_{\text{kin}}(Q, A, \Phi) + \mathcal{V}(\Phi) + \mathcal{L}_{\text{Yuk}}(Q, \Phi) + \mathcal{L}_{\text{Wil}}(Q, A, \Phi)$$

$$\bullet \mathcal{L}_{\text{kin}}(Q, A, \Phi) = \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \bar{Q}_L \gamma_\mu \mathcal{D}_\mu Q_L + \bar{Q}_R \gamma_\mu \mathcal{D}_\mu Q_R + \frac{1}{2} \text{Tr}[\partial_\mu \Phi^\dagger \partial_\mu \Phi]$$

$$\bullet \mathcal{V}(\Phi) = \frac{\mu_0^2}{2} \text{Tr}[\Phi^\dagger \Phi] + \frac{\lambda_0}{4} (\text{Tr}[\Phi^\dagger \Phi])^2$$

$$\bullet \mathcal{L}_{\text{Yuk}}(Q, \Phi) = \eta (\bar{Q}_L \Phi Q_R + \bar{Q}_R \Phi^\dagger Q_L)$$

$$\bullet \mathcal{L}_{\text{Wil}}(Q, A, \Phi) = \frac{b^2}{2} \rho (\bar{Q}_L \overleftarrow{\mathcal{D}}_\mu \Phi \mathcal{D}_\mu Q_R + \bar{Q}_R \overleftarrow{\mathcal{D}}_\mu \Phi^\dagger \mathcal{D}_\mu Q_L)$$

- Put the theory on a lattice and check the conjecture

DGEM simulation strategy

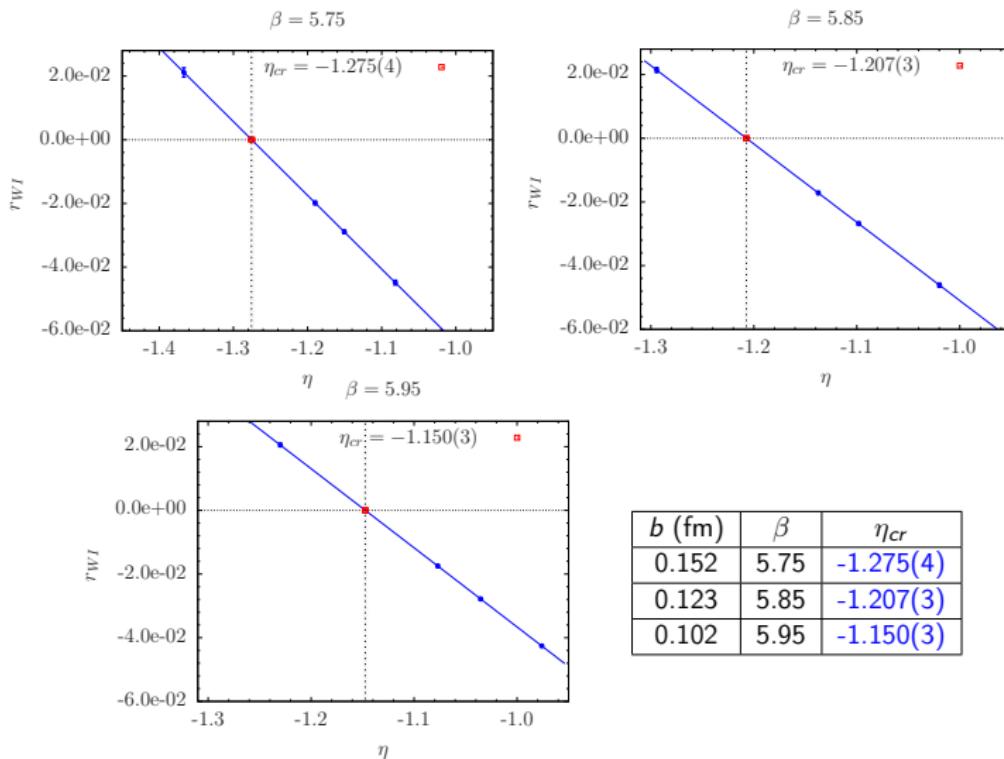
- Determine in Wigner phase (single well $\mathcal{V}(\Phi)$) the value of the Yukawa coupling, η_{cr} , at which fermionic chiral transformations (\tilde{x}) are a symmetry of \mathcal{L}_{toy} by enforcing the WTI

$$\bullet 0 = \partial_0 \langle \tilde{V}_0^3(x) \tilde{D}^3(0) \rangle = (\eta - \eta_{cr}) \langle \tilde{D}^3(x) \tilde{D}^3(0) \rangle + (\text{lat. artefacts})$$

$$\bullet \text{i.e. look for } \eta \text{ such that } r_{WI}(\eta) \equiv \frac{\partial_0 \langle \tilde{V}_0^3(x) \tilde{D}^3(0) \rangle}{\langle \tilde{D}^3(x) \tilde{D}^3(0) \rangle} \Big|_{\textcolor{blue}{W}} = 0$$

- At η_{cr} in Nambu–Goldstone phase (double well $\mathcal{V}(\Phi)$) compute
 - $2m_{PCAC}(\eta_{cr}) \equiv \frac{\partial_0 \langle \tilde{A}_0^1(x) P^1(0) \rangle}{\langle P^1(x) P^1(0) \rangle} \Big|_{\textcolor{blue}{NG}}$ (at η_{cr} Higgs quark mass = 0)
 - From $\partial_0 \langle \tilde{A}_0^1(x) P^1(0) \rangle = 2m_{PCAC}(\eta_{cr}) \langle P^1(x) P^1(0) \rangle + (\text{lat. artefacts})$
 - we interpret $m_{PCAC}(\eta_{cr}) \neq 0$ as a DG quark mass $\rightarrow M_{PS}^2 \neq 0$
 - An alternative to the Higgs mechanism?

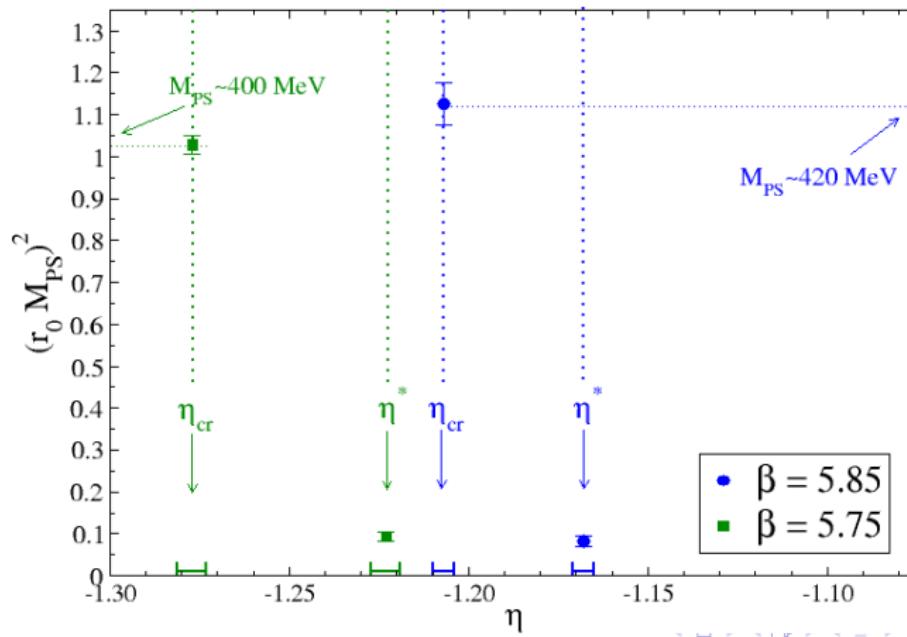
DGEM simulation results - η_{cr} (Wigner phase)



DGEM simulation results - M_{PS}^2 (NG phase)

Recall

- η_{cr} (where $\tilde{\chi}$ -symmetry was enforced) $\rightarrow m_{PCAC}(\eta_{cr}) \neq 0$
- η^* is where $m_{PCAC}(\eta^*) = 0$



DGEM (quenched) simulation cost

DGEM inversions 2017

β	Vol	# inversions (gauge \times scalar)	CPU (Mchs)	Machine
5.75	$16^3 \times 40$	6.0 k	2.0	Marconi
	$16^3 \times 32$	6.0 k	2.0	
5.85	$16^3 \times 40$	10.0 k	3.4	"
5.95	$20^3 \times 48$	2.0 k	0.7	"

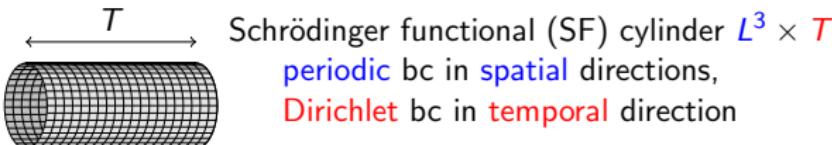
b-coeff's for O(a) improvement of Wilson fermions

Finite volume & mass independent renormalization scheme

- Finite volume and masses fixed by renormalized couplings

$$\left(\mu = 1/L, \frac{M}{\Lambda}\right) = \text{fixed} \iff \left(g_R^2(L), m_R(1/L)L\right) = \text{constant}$$

- Finite volume requires boundary conditions:



- In $O(a)$ improved & mass-independent schemes
bare quantities must be renormalized with mass-dependent terms

$$g_R^2 = Z_g(\tilde{g}_0^2, a\mu) \tilde{g}_0^2$$

$$\tilde{g}_0^2 = (1 + b_g(g_0^2) am_q) g_0^2$$

$$m_R = Z_m(\tilde{g}_0^2, a\mu) \tilde{m}$$

$$\tilde{m} = (1 + b_m(g_0^2) am_q) m_q$$

$$X_R = Z_X(\tilde{g}_0^2, a\mu) \tilde{X}$$

$$\tilde{X} = (1 + b_X(g_0^2) am_q) X_I$$

b-coeff's for O(a) improvement of Wilson fermions

Improvement condition

- (non-singlet) PCAC relation free of $O(a)$ violations

$$\tilde{\partial}_\mu \langle A_R^{ij}(x) \mathcal{O}^{ji} \rangle = (m_{R,i} + m_{R,j}) \langle P_R^{ij}(x) \mathcal{O}^{ji} \rangle + O(a^2)$$

- Standard renormalization pattern of improved lattice operators (for $\hat{m}^{(\text{sea})} \sim 0$)

$$A_R^{ij} = Z_A (1 + b_A a m_{q,ij} + \cancel{b_A a \text{tr } \hat{m}^{(\text{sea})}}) \{ A_\mu^{ij} + c_A a \tilde{\partial}_\mu P^{ij} \}$$

$$P_R^{ij} = Z_P (1 + b_P a m_{q,ij} + \cancel{b_P a \text{tr } \hat{m}^{(\text{sea})}}) P^{ij}$$

$$m_{R,i} = Z_m \left\{ m_{q,i} (1 + b_m a m_{q,i} + \cancel{b_m a \text{tr } \hat{m}^{(\text{sea})}}) + x \text{tr } \hat{m}^{(\text{sea})} + y a \text{tr } \hat{m}^{2(\text{sea})} + z a (\text{tr } \hat{m}^{(\text{sea})})^2 \right\}$$

$$x = (r_m - 1)/N_f, \quad y = (r_m d_m - b_m)/N_f, \quad z = (r_m \bar{d}_m - \bar{b}_m)/N_f$$

$$A_\mu^{ij} = \bar{\psi}_i \gamma_\mu \gamma_5 \psi_j, \quad P^{ij} = \bar{\psi}_i \gamma_5 \psi_j$$

$$m_{q,ij} = \frac{1}{2}(m_{q,i} + m_{q,j}), \quad m_{q,i} = m_{0,i} - m_c = \frac{1}{2a} \left(\frac{1}{\kappa_i} - \frac{1}{\kappa_c} \right)$$

Numerical definitions of $b_A - b_P$, b_m , Z

$$m_{ij}(x_0) = \frac{\tilde{\partial}_0 f_A^{ij}(x_0) + ac_A \partial_0^* \partial_0 f_P^{ij}(x_0)}{2 f_P^{ij}(x_0)}$$

$$\begin{aligned} f_A^{ij}(x_0) &\equiv -a^3 \sum_x \left\langle A_0^{ij}(x) \mathcal{O}^{ji} \right\rangle \\ f_P^{ij}(x_0) &\equiv -a^3 \sum_x \left\langle P^{ij}(x) \mathcal{O}^{ji} \right\rangle \\ \mathcal{O}^{ji} &\equiv a^6 \sum_{u,v} \bar{\zeta}_j(u) \gamma_5 \zeta_i(v) \end{aligned}$$

$$R_{AP} = \frac{2(2m_{12} - m_{11} - m_{22})}{(m_{11} - m_{22})(am_{q,1} - am_{q,2})} = b_A - b_P + O(am_{q,1} + am_{q,2})$$

$$R_m = \frac{4(m_{12} - m_{33})}{(m_{11} - m_{22})(am_{q,1} - am_{q,2})} = b_m + O(am_{q,1} + am_{q,2})$$

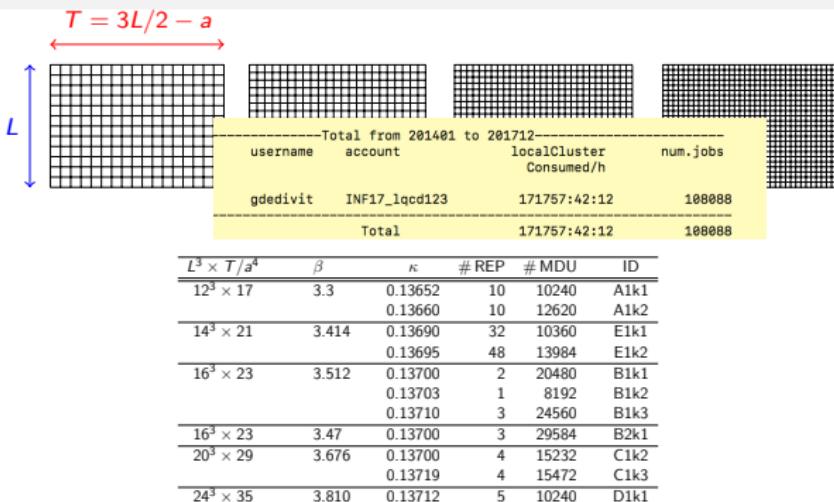
$$\begin{aligned} R_Z &= \frac{m_{11} - m_{22}}{m_{q,1} - m_{q,2}} + (R_{AP} - R_m)(am_{11} + am_{22}) = Z + O(a \text{tr } \hat{m}^{(\text{sea})}) \\ Z &= Z(g_0) = \frac{Z_m(g_0, L) Z_P(g_0, L)}{Z_A(g_0)} \end{aligned}$$

$$L \approx 1.2 \text{ fm} \quad Lm_{11} \approx 0.0$$

$$Lm_{22} \approx 0.25, 0.5, 0.75, 1.0$$

$$m_{0,3} = \frac{1}{2}(m_{0,1} + m_{0,2})$$

Contractions on Galileo cluster at CINECA: 0.17MCH



- $L \approx 1.2 \text{ fm}$, $Lm_{11} \approx 0.0$, $Lm_{22} \approx 0.25, 0.5, 0.75, 1.0$

- $a \approx 0.09 \text{ fm} \longrightarrow 0.045 \text{ fm}$

Parameters span the common range of bare couplings in large volume simulations of 3-flavour lattice QCD

Allocated CPU time

- PRACE 2016_143304
 - “Lattice QCD simulations at the physical point with $N_f = 2 + 1 + 1$ dynamical flavors”
 - 48 Mchs on Marconi A2
- LQCD123 2017
 - 34.3 Mchs on Marconi A2
 - 1.5 Mchs on Marconi A1

Thanks for the attention