Ginsparg-Wilson fermions: practical aspects and applications

Pilar Hernández

- **Introduction**
- **Why chiral symmetry in lattice QCD at finite a ?**
- **Progress in implementations of GW fermions**
- **Physics results**

Introduction

Lattice Dirac operators can be constructed which are local, do not suffer from the doubling problem and satisfy the Ginsparg–Wilson (GW) relation:

$$\boxed{\{D, \gamma_5\} = D\gamma_5 D \quad \leftrightarrow \quad \{D^{-1}, \gamma_5\} = \gamma_5}$$

This relation ensures that Ward identities associated with a standard chiral transformation are satisfied on shell at finite a:

$$\langle \delta S_f(x)\, O(y) \rangle = 0, \qquad |x - y| \neq 0$$

Ginsparg, Wilson, Hasenfratz

Furthermore it implies an exact symmetry :

$$\delta\Psi = \epsilon\, \gamma_5 (1 - aD)\Psi \qquad \delta\bar{\Psi} = \epsilon\bar{\Psi}\gamma_5 \quad \rightarrow \delta S_f = 0$$

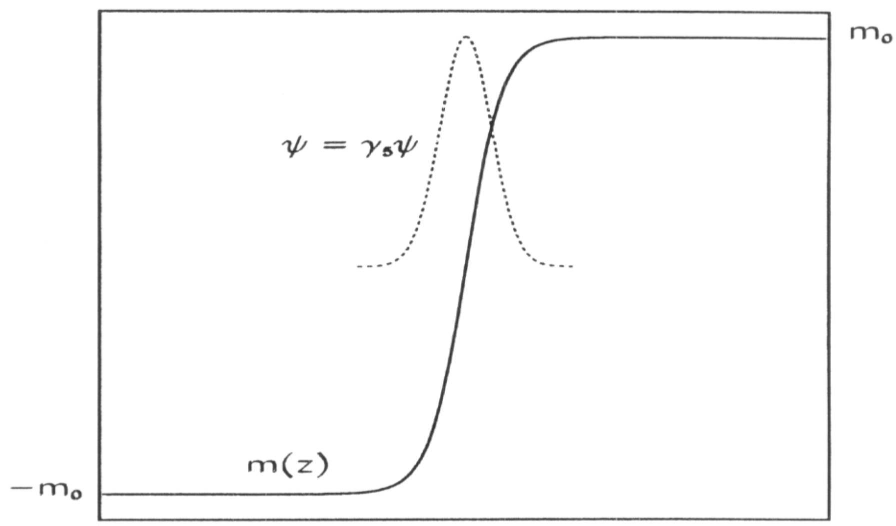
Lüscher

Two very different and apparently disconnected avenues lead to operators satisfying the GW relation:

- **Domain-wall in 5 dimensions**

An infinite domain-wall (DW) in 5D leads naturally to chiral fermions in 4D

Rubakov, Shaposhnikov
Callan, Harvey



On the lattice the DW construction a , a_s, N_s :

Kaplan, Shamir
Narayanan, Neuberger

$N_s \to \infty$ at finite a and a_s , we expect a lattice "chiral" fermion $\to$ satisfies GW relation !

Defining $A \equiv m_0 - D_W$

$$a_s \mathcal{D}\Psi = -P_L \Psi(s + a_s) - P_R \Psi(s - a_s) + (1 - a_s A)\Psi(s)$$

4D effective action of the light boundary fields:

$$aD_{N_s} = 1 - \gamma_5 \frac{(1+\bar{Q})^{N_s} - (1-\bar{Q})^{N_s}}{(1+\bar{Q})^{N_s} + (1-\bar{Q})^{N_s}}$$

with $\bar{Q} \equiv \gamma_5 \frac{a_s A}{2 - a_s A}$

Neuberger

Kikukawa, Noguchi

Borici

In the limit $N_s \to \infty$:

$$aD_{N_s} \to 1 - \gamma_5 \mathrm{sign}(\bar{\mathrm{Q}})$$

$$\{D_{N_s}, \gamma_5\} - D_{N_s} \gamma_5 D_{N_s} \to 0$$

$$N_s \to \infty$$

If furthermore $a_s \to 0$ we obtain the overlap operator:

$$\lim_{a_s \to 0} \lim_{N_s \to \infty} aD_{N_s} \to 1 - \gamma_5 \mathrm{sign}(\mathrm{Q})$$

$Q = \gamma_5 A$ [redacted]

Neuberger

- **Fixed-Point Dirac operator**

Hasenfratz, Niedermayer

RG blocking procedure from the continuum

$$e^{-\bar{\psi}D'\psi} = \int \mathcal{D}\phi\mathcal{D}\bar{\phi}\exp\left\{-(\bar{\psi}-\bar{\phi})R(\psi-\phi)-\bar{\phi}D\phi\right\}$$

R is generically not chirally symmetric (e.g. proportional to unit matrix)

$$\boxed{\gamma_5 D' + D'\gamma_5 = 2D'\gamma_5 R^{-1} D'}$$

$$D^{FP} = D' = D$$

Must be constructed iteratively

Why χ-symmetry at finite a ?

Renormalization: operator classification and mixing is enormously simplified by the exact chiral symmetry

$$\Psi_{R,L} = \hat{P}_{\pm}\Psi \qquad \bar{\Psi}_{L,R} = \bar{\Psi}P_{\pm}$$

with $P_{\pm} \equiv (1 \pm \gamma_5)/2$ and $\hat{P}_{\pm} \equiv (1 \pm \gamma_5(1 - aD))/2$

$$\bar{\Psi}D\Psi = \bar{\Psi}_L D\Psi_L + \bar{\Psi}_R D\Psi_R,$$

There is an exact $SU(N_f)_L \times SU(N_f)_R$ symmetry:

$$\Psi_L \to V_L\Psi_L \qquad \Psi_R \to V_R\Psi_R \quad V_{L,R} \in SU(N_f)_{L,R}$$

Adding quark masses: $\bar{\Psi}_L m\Psi_R + \bar{\Psi}_R m^{\dagger}\Psi_L$

Spurion analysis: mixing possible between operators with the same transformation properties under

$$\Psi_L \to V_L\Psi_L \qquad \Psi_R \to V_R\Psi_R \qquad m \to V_L m V_R^{\dagger}$$

- A conserved axial current and no additive mass renormalization

- $Z_P = Z_S = Z_m^{-1}$

Hasenfratz

- d $= 6$ operators relevant for $\Delta I = 1/2$, ϵ'/ϵ mix as in the continuum

  Perturbative calculations of renormalization constants

DW: Aoki, *et al* Overlap: Capitani, Giusti

Improvement: $O(a)$ (almost) automatic

The exact chiral symmetry forbids

- operators of d $= 5$ in the action

- operators of d $= 4$ with the symmetries of quark bilinears

Capitani *et al*

Regime of light quark masses

QCD partition function dominated by the nearly massless pions at low energies:

- $M_\pi L \gg 1 \rightarrow$ requires very large volumes
- $M_\pi L \leq 1 \rightarrow$ large finite volume effects

Finite volume effects can be precisely predicted by chiral perturbation theory (χPT), including the effects of topological zero modes !!

$$p \ll 4\pi F_\pi$$

$$\boxed{\mathcal{L} = \frac{F_\pi^2}{4}\,\mathrm{tr}\left\{\partial_\mu U^\dagger \partial_\mu U\right\} - \frac{\Sigma}{2}\,\mathrm{tr}\left\{\mathcal{M} e^{i\theta/N_f} U^\dagger + \mathrm{cc}\right\} + \ldots}$$

Gasser, Leutwyler

Usual χPT or p-expansion:

$$M_\pi L \geq 1 \rightarrow M_\pi \sim p \sim 1/L \ll 4\,\pi F_\pi$$

$$U = \exp(i\sqrt{2}\,\xi/F_\pi) = 1 + i\sqrt{2}\,\xi/F_\pi + \ldots$$

"Unusual" χPT or ϵ-expansion:

$$M_\pi L \leq 1 \rightarrow M_\pi \sim p^2 = O(\epsilon^2)$$

The zero mode of the pion becomes non perturbative signalling the restoration of chiral symmetry in finite volume.

Defining $U = U_o \, e^{i\,\xi(x)}$

$$\mathcal{Z} = \int_{SU\,(N_f)} dU_o \int d\xi \;\; e^{-\mathcal{L}(U_o,\xi)}$$

Gasser, Leutwyler

In the quenched theory:

Morel, Sharpe, Bernard, Golterman

Damgaard et al

$$\mathcal{Z} = \int_{Gl(N_f|N_f)} dU_o \int d\xi \;\; e^{-\mathcal{L}(U_o,\xi)}$$

Analytic expressions can be found in sectors of fixed topology both in the full and quenched theories:

$$\mathcal{Z}_\nu = \int \frac{d\theta}{2\pi} \, e^{-i\nu\theta} \; \mathcal{Z}(\theta)$$

Examples

- Quark condensate: $z \equiv m\Sigma V$

  Full:

$$\frac{\Sigma_\nu(m,V)}{\Sigma} = \frac{\partial}{\partial m} log(\det_{ij} I_{i-j+\nu}(m\Sigma V))$$
$$\simeq \frac{|\nu|}{z} + \frac{z}{2(N_f+|\nu|)} + O(z^2)$$

Gasser, Leutwyler

Leutwyler, Smilga

  Quenched:

$$\frac{\Sigma_\nu(m,V)}{\Sigma} = z(I_\nu(z)K_\nu(z) + I_{\nu+1}(z)K_{\nu-1}(z)) + \frac{\nu}{z}$$
$$\simeq \frac{|\nu|}{z} + \frac{z}{2|\nu|} + O(z^2) \quad |\nu| \geq 1$$

Damgaard, Osborn, Toublan, Verbaarschot

- Correlators of quark bilinears $\langle PP \rangle$, $\langle SS \rangle$

  Full

Hansen

Hansen, Leutwyler

  Quenched

→ Damgaard,Diamantini,H.,Jansen

(Q)chpt predicts precisely the dependence on m and V including the effect of zero modes: it is essential that the Dirac operator has exact zero modes

Implementations of GW fermions

Overlap: $D_{ov} = 1 - A/\sqrt{A^\dagger A} \quad A \equiv m_0 - D_W$

(or $D_{ov} = 1 - \gamma_5 Q/\sqrt{Q^2} = 1 - \gamma_5 \mathrm{sign}(\mathrm{Q}), \quad \mathrm{Q} \equiv \gamma_5 \mathrm{A}$)

Approximations of $\mathrm{sign}(\mathrm{Q})$ **or** $1/\sqrt{Q^2}$

A1 Polynomial approximation of $1/\sqrt{Q^2}$: e.g. Chebyshev

H.,Jansen,Lellouch

Bunk

A2 Rational approximations or partial fractions: optimal rational approximation, polar formula

$$\mathrm{sign}(Q) = lim_{N\to\infty} Q(c_0 + \sum_{k=1}^{N} \frac{c_k}{Q^2+q_k})$$

Inversion uses a multimass solver CG

Neuberger

Edwards,Heller, Narayanan

A3 Lanczos: $(Q^2)^{+1/2} x = y$ from $Q^2 x = y$

Borici

A4 Rational approximation as 5D operator

Narayanan, Neuberger

Cost increase with respect to Wilson: number of Q matrix$\times$vector multiplications (MVs):

- Polynomial approximations $\sim$ 2 N

- Rational approximations: $\sim$ 2 # CG in one inversion of $Q^2 + q_k,\ q_k \geq 0$ (uses multimass solver)

Convergence is bounded by an exponential in both cases:

$$||D_N - D_{ov}|| < e^{-2\sqrt{\epsilon}n}$$

$$\epsilon \equiv \lambda_{min}(Q^2)/\lambda_{max}(Q^2)$$

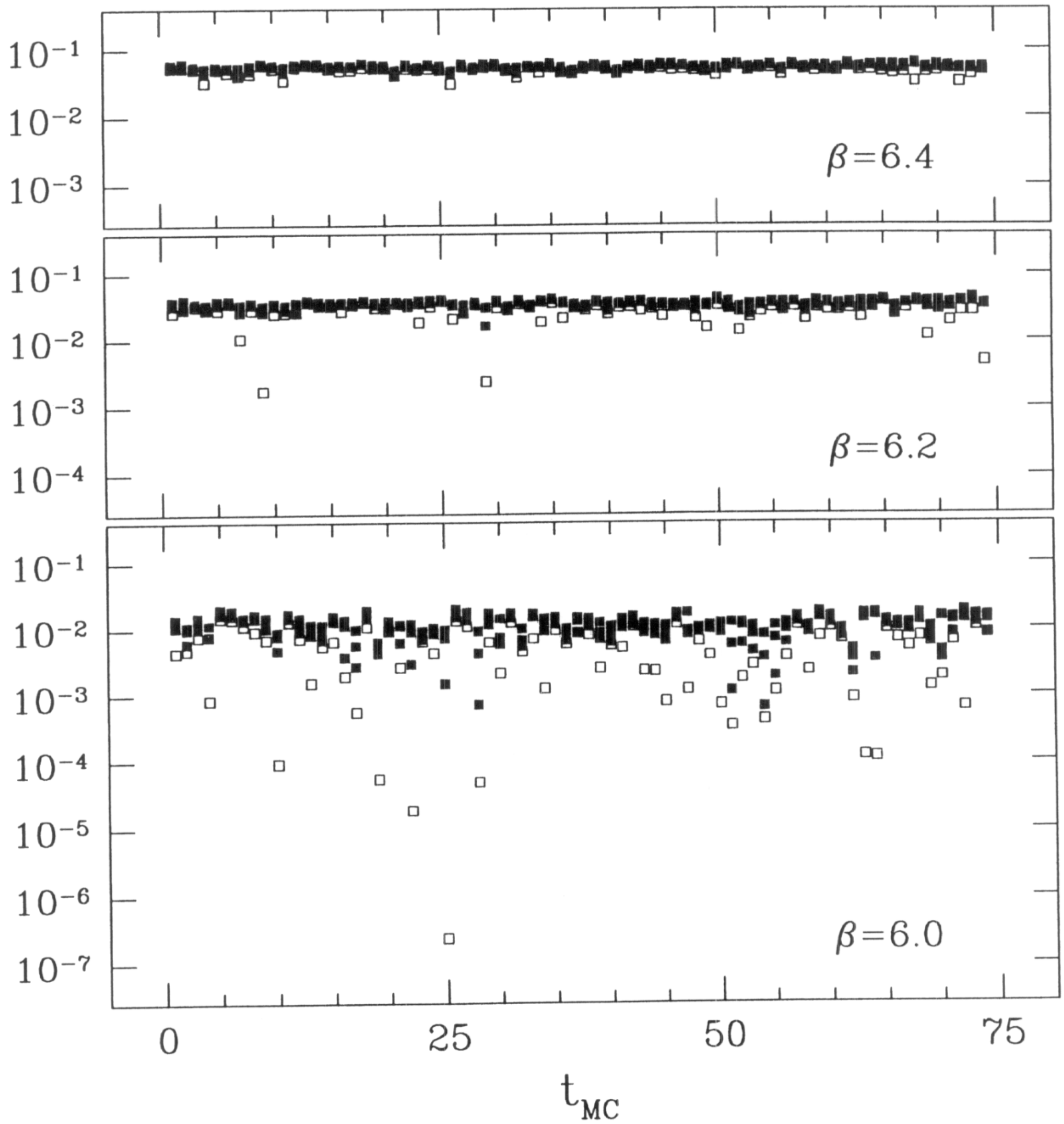
with A1: n = N   A2: n = # CG

Eg: $\beta = 6.0\ V = 16^3 * 32,\ 10^{-6}$ accuracy

Method	MVs
Rational(Remez 14)	$\sim 2 \times 150$
Chebyshev	$\sim 2 \times 200$

But vector updates in multimass-solver are costly!

The asymptotic convergence of the different approximations of the sign(Q) or $1/\sqrt{Q^2}$ is controlled by the small eigenvalues of Q^2:



DW

At finite N_s the DW gives a rational approximation to the sign function:

$$aD_{N_s} = 1 - \gamma_5 \frac{(1+\bar{Q})^{N_s} - (1-\bar{Q})^{N_s}}{(1+\bar{Q})^{N_s} + (1-\bar{Q})^{N_s}} \simeq 1 - \gamma_5 \mathrm{sign}(\bar{Q})$$

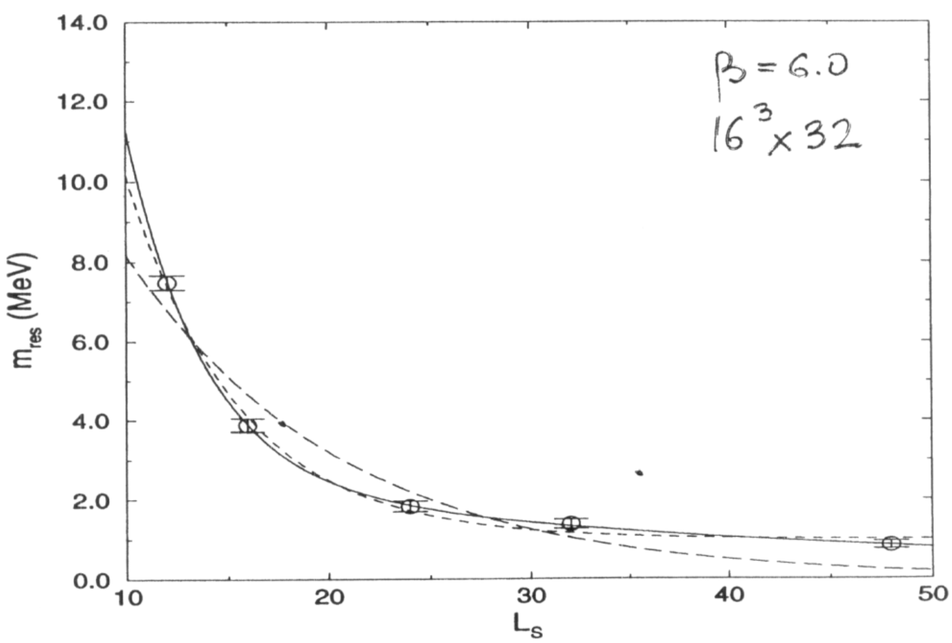
with $\bar{Q} \equiv \gamma_5 \frac{a_s A}{2 - a_s A}$

Convergence is exponential in N_s with rate $\omega \simeq 2\sqrt{\lambda_{\min}(\bar{Q}^2)}$:

$$||\mathrm{sign}(\bar{Q}) - \frac{(1+\bar{Q})^{N_s} - (1-\bar{Q})^{N_s}}{(1+\bar{Q})^{N_s} + (1-\bar{Q})^{N_s}}|| < e^{-N_s \omega}$$

Residual mass measures violation of GW symmetry:

$$m_{res} \equiv \frac{\sum_{\vec{x}} \langle \delta S(x) P_5(0) \rangle}{\sum_{\vec{x}} \langle P_5(x) P_5(0) \rangle} |_{m=0} \quad t \to \infty$$



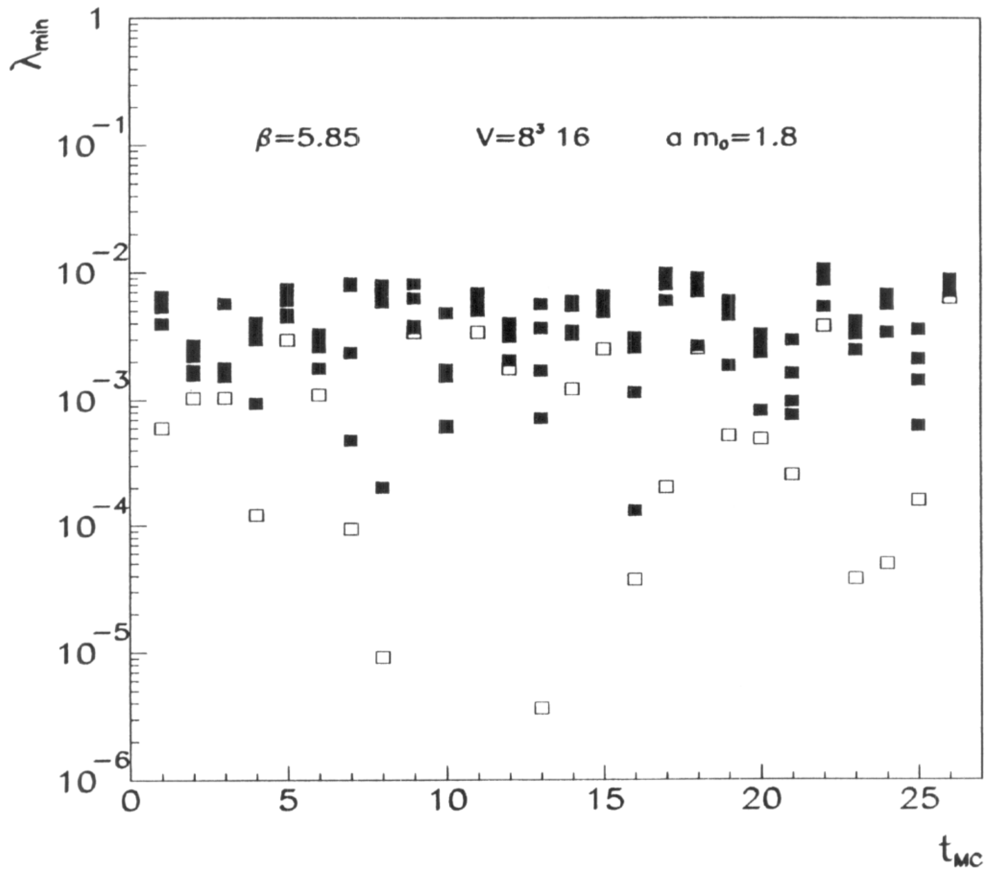
Blum et a

→ Taniguchi

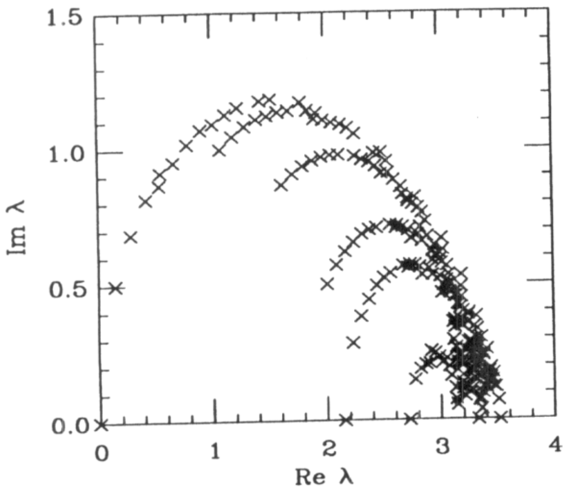
The smallest eigenvalues of $\bar{Q}^2$ can be obtained by minimizing the Ritz functional

$$\frac{\langle\Phi|a_s^2 A^\dagger A|\Phi\rangle}{\langle\Phi|(2-a_s A^\dagger)(2-a_s A)|\Phi\rangle}$$

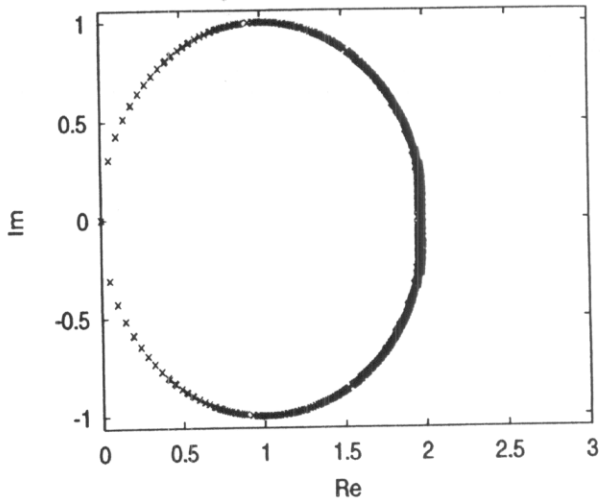
H., Jansen, Lüscher



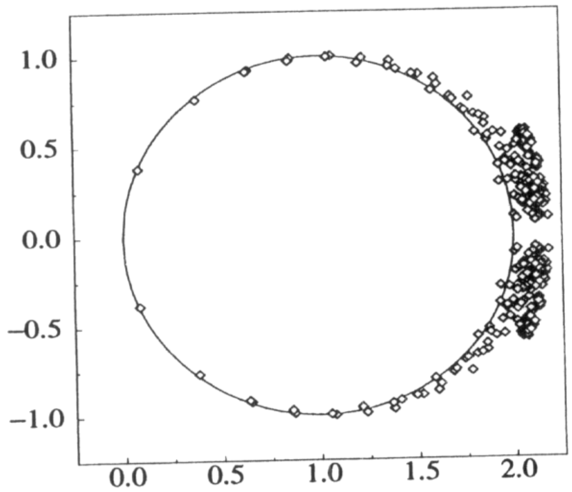
FP operator: a truncation is necessary $\longrightarrow$ Dirac operator with allowed hypercubic couplings which approximates as much as possible the FP operator or simply the GW relation



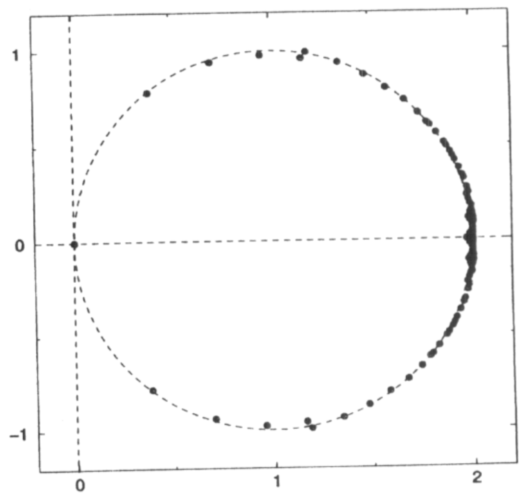
DeGrand GW1 $\times 6.5$



Bietenholz *et al* FP1 $\times 20$



Gattringer, Hip, Lang GW2 $\times 24$



Hasenfratz *et al* FP2 $\times 20$

New elements: fat links inGW1, FP1, FP2, amplification factor for the links FP1 , clover term all

E.g. FP2 increase in cost a factor ~~40~~ 20 and the GW symmetr is satisfied to $O(10^{-2})$ at $a = 0.13$ fm in $V = 8^4$

Improvements

The difficulty comes from the slow convergence of the different approximations of the sign(Q) or $1/\sqrt{Q^2}$ which is controlled by the small eigenvalues of Q^2:

$$\text{cost} \sim \frac{1}{\sqrt{\lambda_{\min}(Q^2)}}$$

A better convergence can be achieved if:

1. A small eigenspace of $O(10)$ very small eigenvalues is treated exactly

2. The gap is increased

   – by improving the gauge action
   – by improving A

3. Algorithmic improvement

Locality is also related to the size of the gap !

H., Jansen, Lüscher

Improvement 1: isolated eigenvalues can be cheaply treated exactly

Overlap: for those few eigenvalues $\lambda_i, i = 1, .., p$ of Q^2, such that $\lambda_i \ll$ gap with eigenvectors $|\Psi_i\rangle$

$$(A^\dagger A)^{-1/2} = P_n(A^\dagger A - \sum_i^p \lambda_i |\Psi_i\rangle\langle\Psi_i|) + \sum_i^p \lambda_i^{-1/2} |\Psi_i\rangle\langle\Psi_i$$

Exponential convergence with rate:

$$2\sqrt{\epsilon} = 2\sqrt{\lambda_{p+1}/\lambda_{max}} \gg 2\sqrt{\lambda_1/\lambda_{max}}$$

DW: a 5D operator such that the corresponding effective 4D action is $\tilde{D}_{N_s} = D_{N_s} + \Delta$:

$$aD_{N_s} = 1 - \gamma_5 \sum_i \frac{(1+\mu_i)^{N_s} - (1-\mu_i)^{N_s}}{(1+\mu_i)^{N_s} + (1-\mu_i)^{N_s}} |\Psi_i\rangle\langle\Psi_i|$$

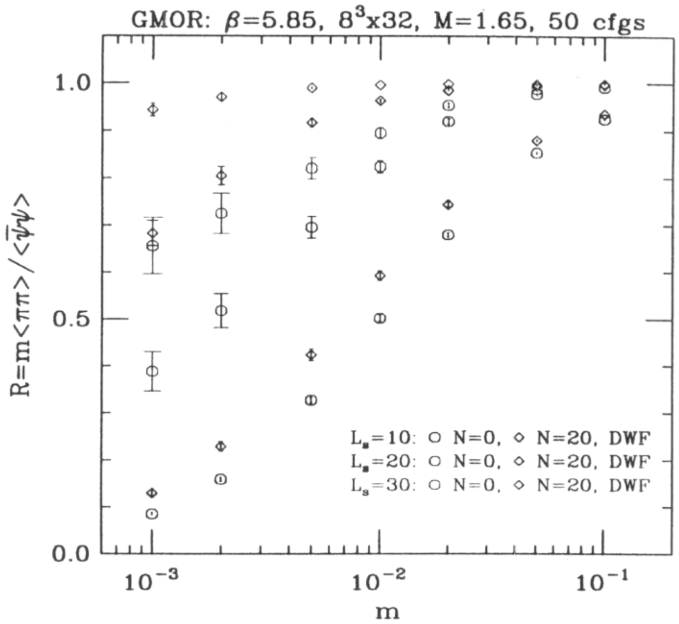
$$\Delta \equiv -\gamma_5 \sum_{i=1}^p (\epsilon(\mu_i) - \frac{(1+\mu_i)^{N_s} - (1-\mu_i)^{N_s}}{(1+\mu_i)^{N_s} + (1-\mu_i)^{N_s}}) |\Psi_i\rangle\langle\Psi_i|$$

$$\bar{Q}|\Psi_i\rangle = \mu_i|\Psi_i\rangle$$

Exponential convergence with lowest rate: $2|\mu_{p+1}| \gg 2|\mu_1|$

There is not a unique way of constructing such 5D operator

Method 1: Modification of the unimproved operator by extra boundary terms which depend on Δ



Edwards, Heller

Method 2: $A \to \hat{A}$ such that

$$\hat{\bar{Q}} \equiv a_s \hat{A}(2 - a_s \hat{A})^{-1} = \bar{Q} + \sum_{i=1}^{p} (\text{sign}(\mu_{\rm i}) - \mu_{\rm i}) |\Psi_{\rm i}\rangle\langle\Psi_{\rm i}|$$

H., Jansen, Lüscher

Condition number of the resulting 5D operators can depend on the method.

Improvement 2.1: Increasing the gap by improving the gauge action

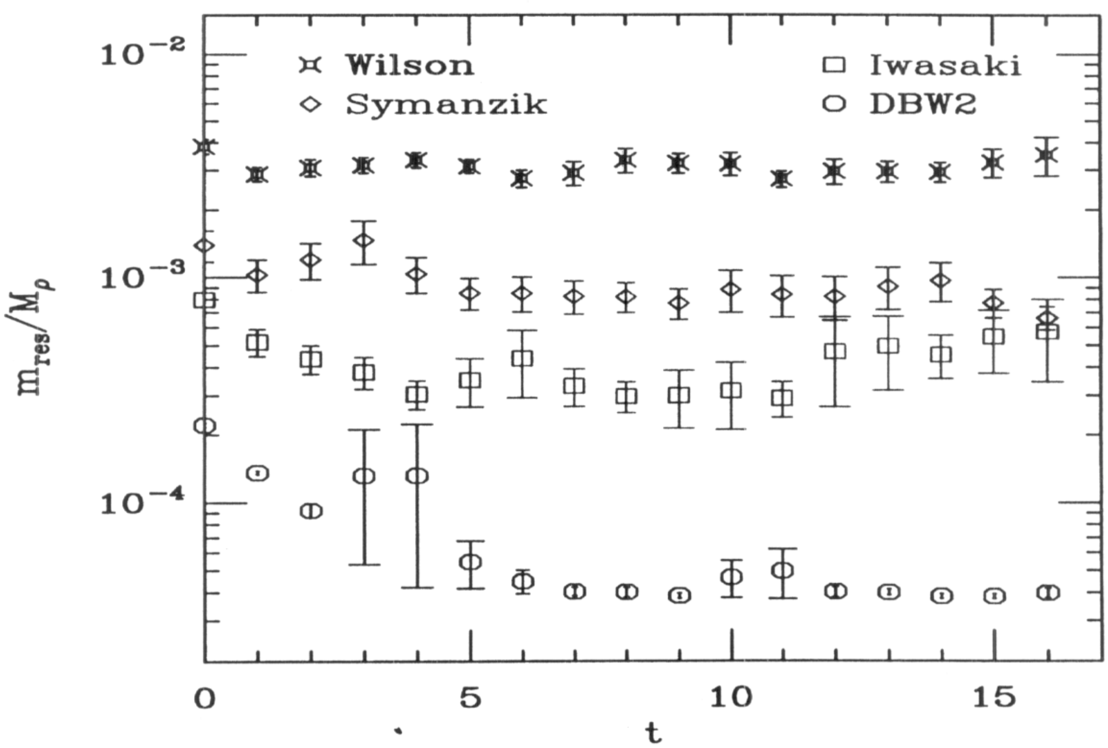
CP-PACS Coll.

This is a in principle cheap solution!

- Symanzik action (one loop and tadpole improved)
- RG improved: Iwasaki's, DBW2(QCD-Taro):

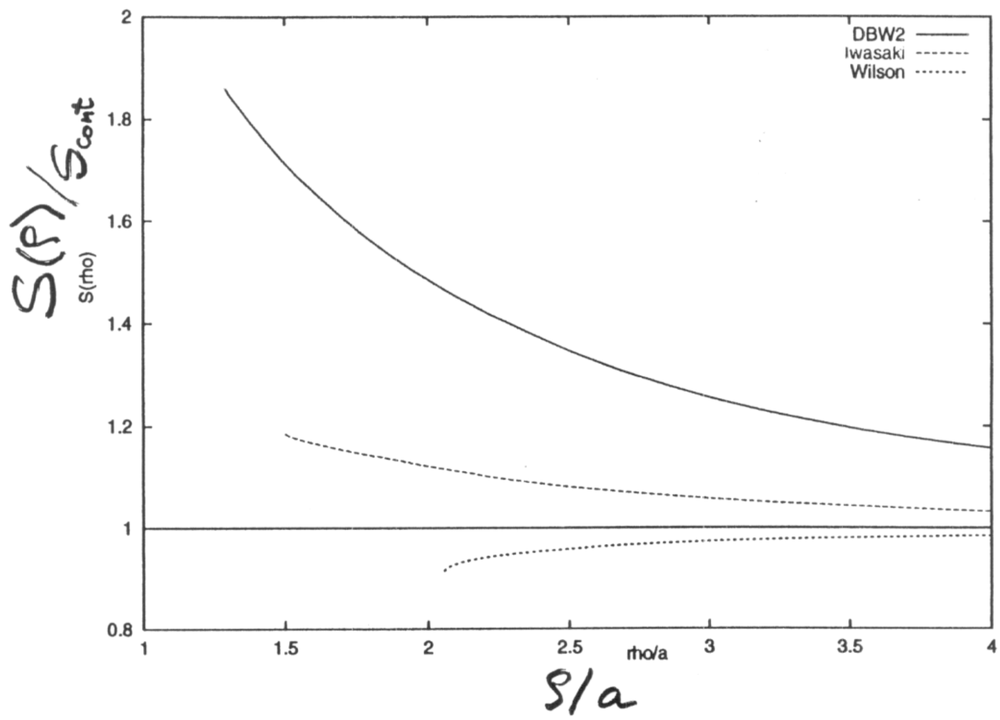
$$S_G = \left(\frac{\beta}{3}\right)\left(\sum_{x;\mu<\nu}(1-8C_1)P_{\mu\nu} + C_1 \sum_{x;\mu\neq\nu} R_{\mu\nu}\right)$$

$$C_1 = -0.331(\mathrm{IW}), -1.4068(\mathrm{DBW2})$$

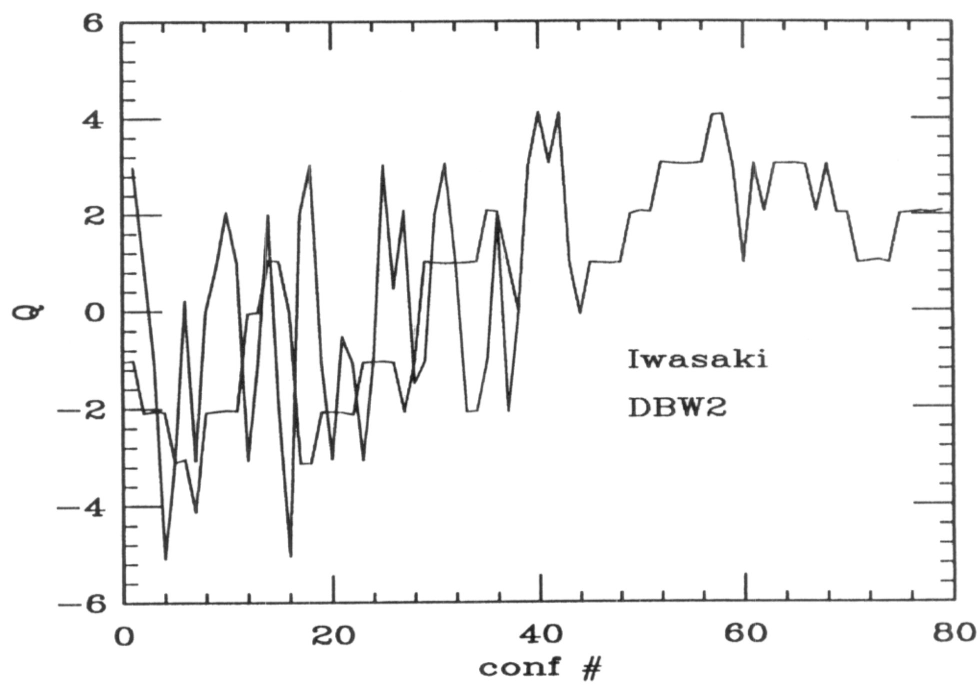


→ RBC, Orgiros

The DBW2 strongly supresses small (and not so small!) instantons and dislocations:



Garcia-Perez



→ RBC, Orgiro

See also talks:

Y. Aoki, S. Sasaki

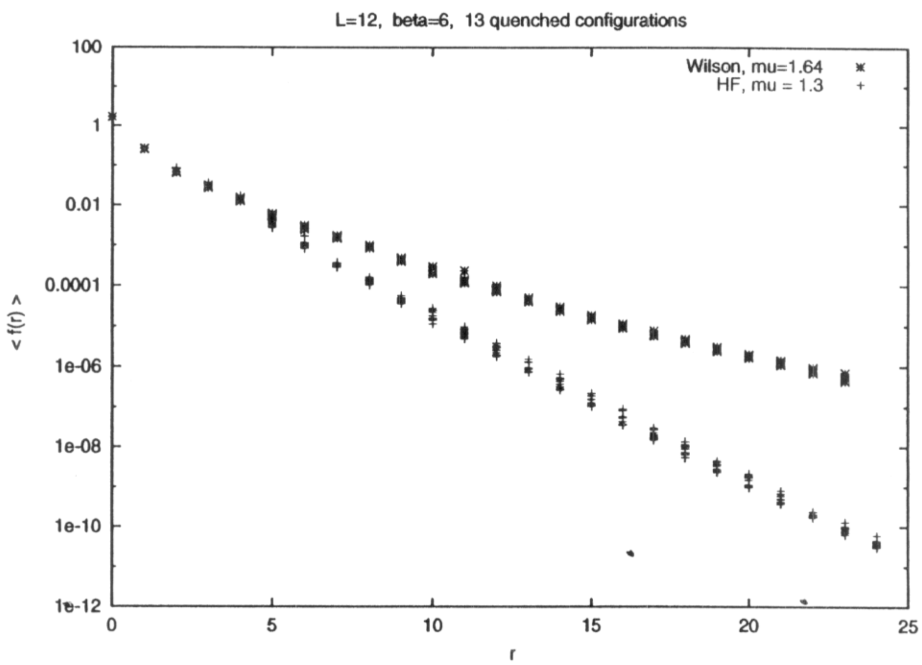
Improvement 2.2: "overlapping" a Dirac operator which approximately satisfies GW (e.g. FP)

Bietenholz

$$\{D', \gamma_5\} = D'\gamma_5 D' \rightarrow D' = 1 - A'/\sqrt{A'^{\dagger}A'}, \quad A' \equiv 1 - D'$$

Action	Overhead	Cost overlap
GW1	$\sim$6.5	$\sim 1/5$
GW2	$\sim$24	$\sim 1/2$
FP1	$\sim$20	$\sim 1/5$
FP2	$\sim$20	$\sim 1/20$

The gain in the convergence does not quite compensate the overhead, but the locality should be improved (but fattenning!) and also scaling in the case of the truncated FP



Bietenholz *et al*

Improvement 3: Algorithms

Rational approximations of $\mathrm{sign}(Q)$:

The vector updates play a very significant role for a large number of poles!

→ van den Eshof *et al*

- Using a better rational approximation of $\sqrt{Q^2}^{-1}$:

  Zolotarev theorem:

$$Min\{||1-\sqrt{x}f(x)||_\infty^{[\lambda_{\min},\lambda_{\max}]}\} \rightarrow f(x) = D\frac{\prod_{l=1}^{k-1}(x+c_{2l})}{\prod_{l=1}^{k}(x+c_{2l-1})}$$

$$c_l = \frac{\mathrm{sn}^2(lK/2k;\kappa)}{1-\mathrm{sn}^2(lK/2k;\kappa)}, \quad l = 1,,,,2k-1 \quad \kappa = \sqrt{1-\lambda_{min}/\lambda_{max}}$$

  \# poles for accuracy 1%

$\sqrt{\lambda_{max}/\lambda_{min}}$	Polar	Remez	Zolotarev
200	19	7	5
1000	42	12	6
100000	>500	?	10

- Remove converged systems from multimass-solver: 20%

$\beta = 6.0, V = 16^4$

confs	1	2	3	4	5
$\lambda_{\text{min}} 10^3$	0.455	1.39	1.17	2.23	3.02
λ_{max}	2.42	2.42	2.42	2.42	2.42
poles Neub.	143	82	89	65	56
poles Zolo.	21	18	19	17	16
Chebyshev					
MVs	9501	3501	4001	2301	2201
time/s	655	247	278	160	154
Lanczos/PFE					
MVs	2281	1969	1953	1853	1769
time/s	150	131	129	124	118
PFE/CG Neuberger					
MVs	?	985	977	929	887
time/s	?	340	362	274	215
PFE/CG Zolotarev					
MVs	1141	985	977	927	885
time/s	154	125	125	116	102
PFE/CG Zolotarev + removing					
MVs	1205	1033	1033	971	927
time/s	122	93	97	87	79

But not projection out of the smallest eigenvalues $\rightarrow$ needs more study

$\rightarrow$ van den Eshof *et al*

Inversion of D_{ov}

→ Wenger

- Inexact CG : adapt the precision of the $\mathrm{sign}(\mathrm{Q}^2)$ to match the stage of the CG search. This is easy with polynomial but not rational approximations

- Reduce the two nested CG of a rational approximated overlap to a single 5D CG

Neuberger

Search for the better conditioned 5D operators by exploiting equivalence classes of continued fractions

Physics results

DW fermions are running ahead towards the solution of legendary problems, overlap fermions are just starting

Quenched simulations:

- Hadron spectrum
- Low energy constants $(\Sigma, f_{\pi,K})$ and quark masses
- Matrix elements: $\Delta I = 1/2$, ϵ'/ϵ with DW!!

$\longrightarrow$ Martinelli

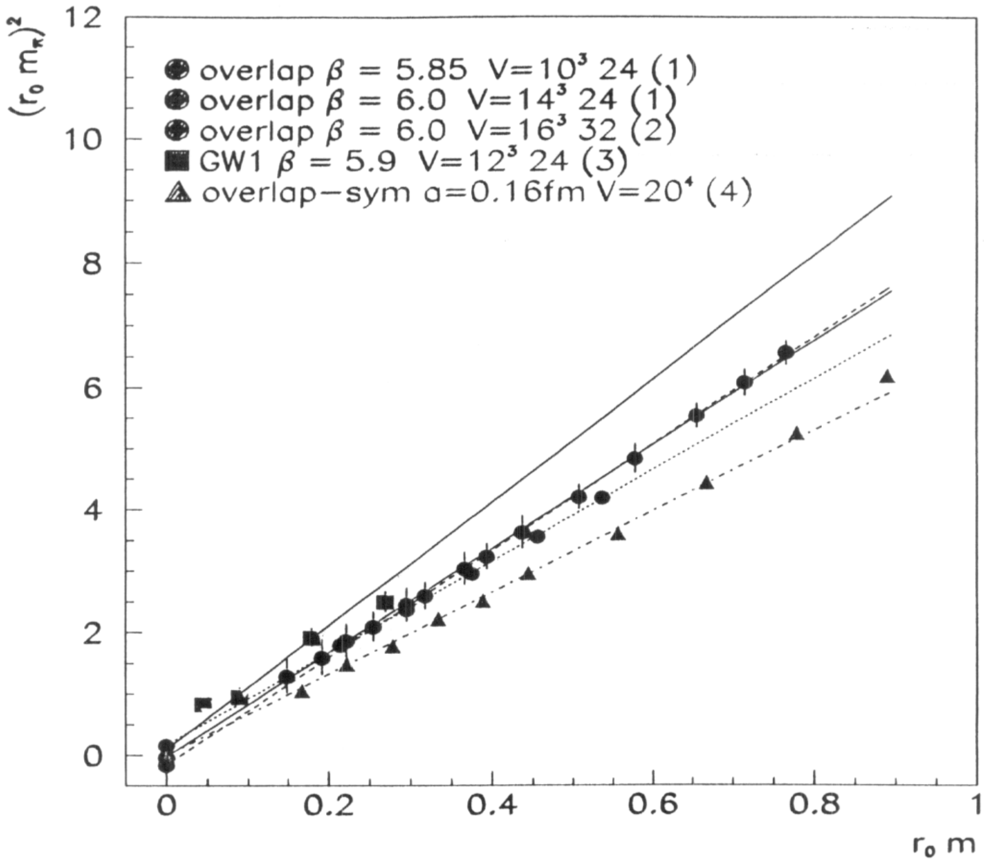
- Topology and QCD vacuum

$\longrightarrow$ Edwards

Unquenched simulations with DW fermions: QCD thermodynamics

$\longrightarrow$ Christ

m_π^2 versus m



(1) H., Jansen, Lellouch, Wittig

(2) Giusti, Hoebling, Rebbi

(3) DeGrand

(4) Dong *et al*

(5) Hasenfratz *et al*

As expected, good control over chiral symmetry!

See also talks:

L. Giusti, C. Hoebling, T. Joerg, S. Dong

Quark condensate

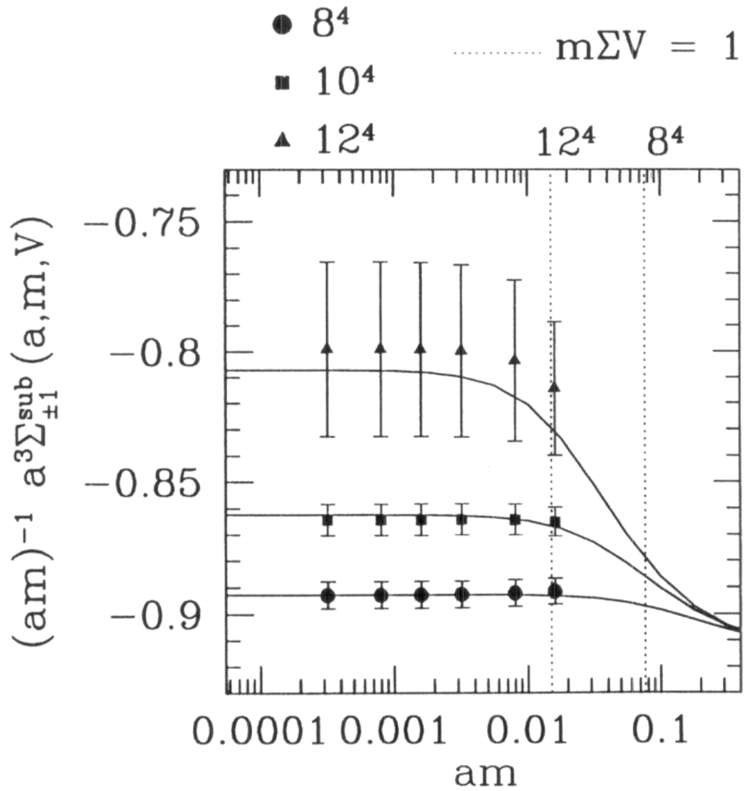
Low energy theorems at infinite V

$$\frac{\Sigma}{F^2} = \frac{1}{4}\lim_{m\to 0}\frac{m_\pi^2}{m} \qquad \frac{\Sigma}{F} = \frac{1}{2}\lim_{m\to 0}|\langle 0|P|\pi\rangle|$$

At finite volume: $m_\pi L \gg 1, \quad m_\pi/F_\pi \ll 1$

If $m_\pi L \ll 1$ (ϵ regime): finite–size scaling

$$\langle \bar{q}q\rangle_{\nu=\pm1}(m,V) \quad \to \quad C\frac{m}{a^2} + \frac{1}{mV} + \frac{1}{2}\,m\Sigma^2 V + \mathcal{O}(m^2)$$



H., Jansen, Lellouch

Damgaard et al

DeGrand

$\to$ Hasenfratz *et al*

Renormalization factors: $Z_S = Z_P = Z_m^{-1}$

Are known in perturbation theory for DW and the standard overlap

Aoki *et al*, Alexandrou *et al*, Giusti &Capitani,

New non-perturbative determinations:

- RI/MOM scheme for DW and overlap — Blum *et al*

  Giusti, Hoelbling, Rebbi

- Matching to continuum Wilson

$$Z_S^{-1}(g_0) = Z_M(g_0) = U_M \cdot \frac{1}{r_0 m}|_{(r_0 m_P)^2 = x_{ref}}$$

$$U_M \equiv lim_{g_0' \to 0}\{Z_M^w(g_0') \times (r_0 m_w)(g_0')\}|_{(r_0 m_P)^2} = x_{ref}$$

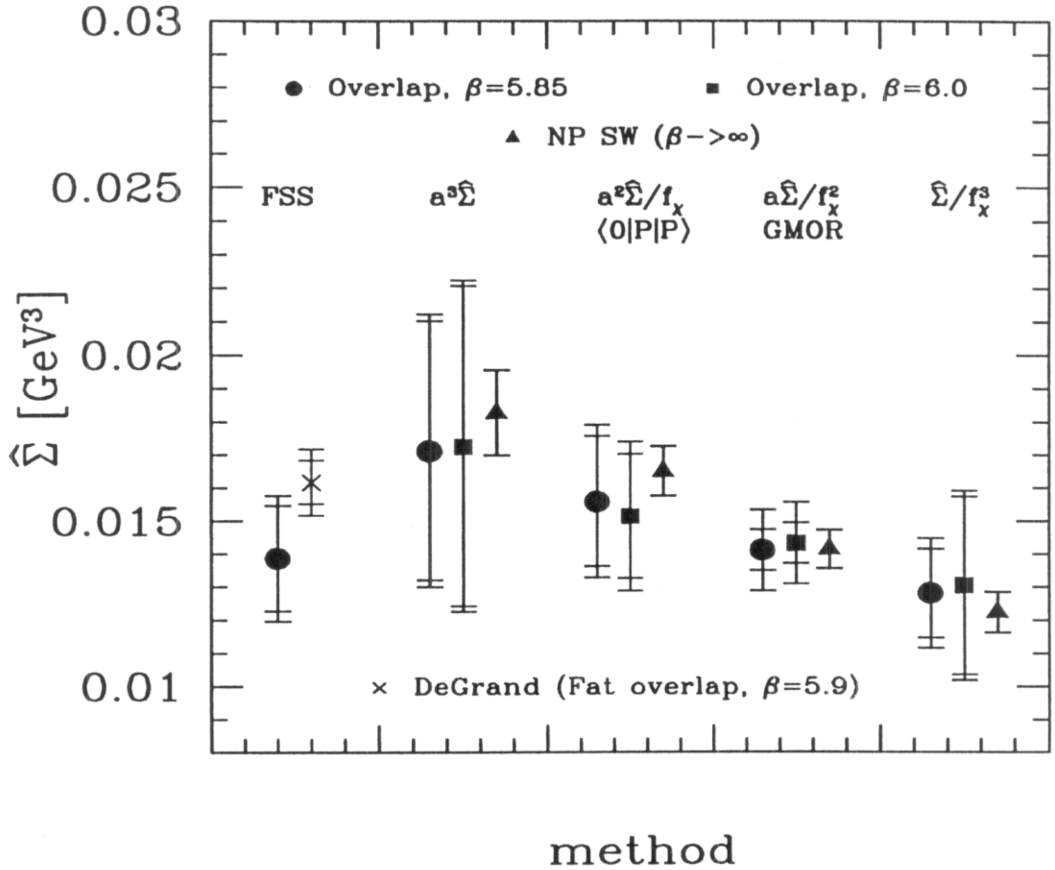
H., Jansen, Lellouch, Wittig

Degrand

Dong, *et al*

Method	PTh	PThmf	RI/MOM	Wilson
$Z_S^{ov}(\beta = 5.85)$	1.12	1.26	-	1.44(11)
$Z_S^{ov}(\beta = 6.0)$	1.14	1.31	1.41(6)	1.43(11)

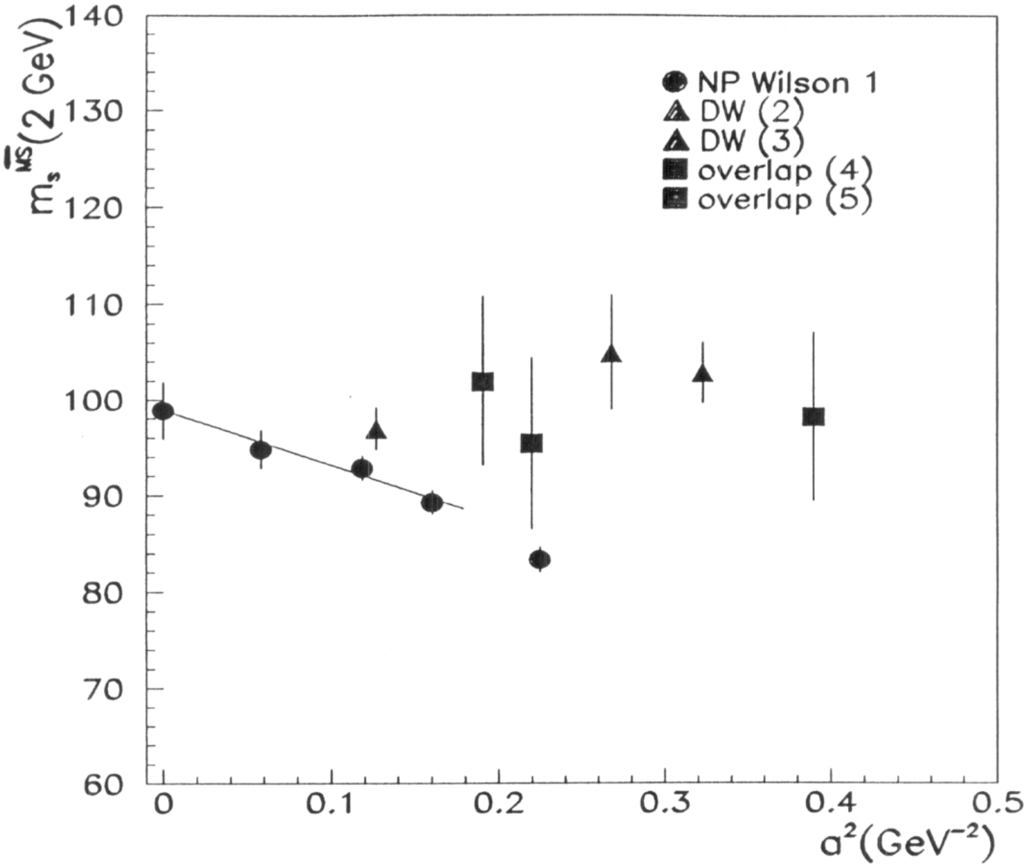
Condensate in quenched QCD



→ H, Jansen, Lellouch, Wittig

- Good agreement between finite-size scaling condensate and other methods
- Small discretization errors from overlap fermions
- Large systematic error due to chiral extrapolation or quenching effects

Quark masses



(1) Garden *et al*

(2) Blum *et al*

(3) Ali Khan it et al

(4) Giusti, Hoebling, Rebbi

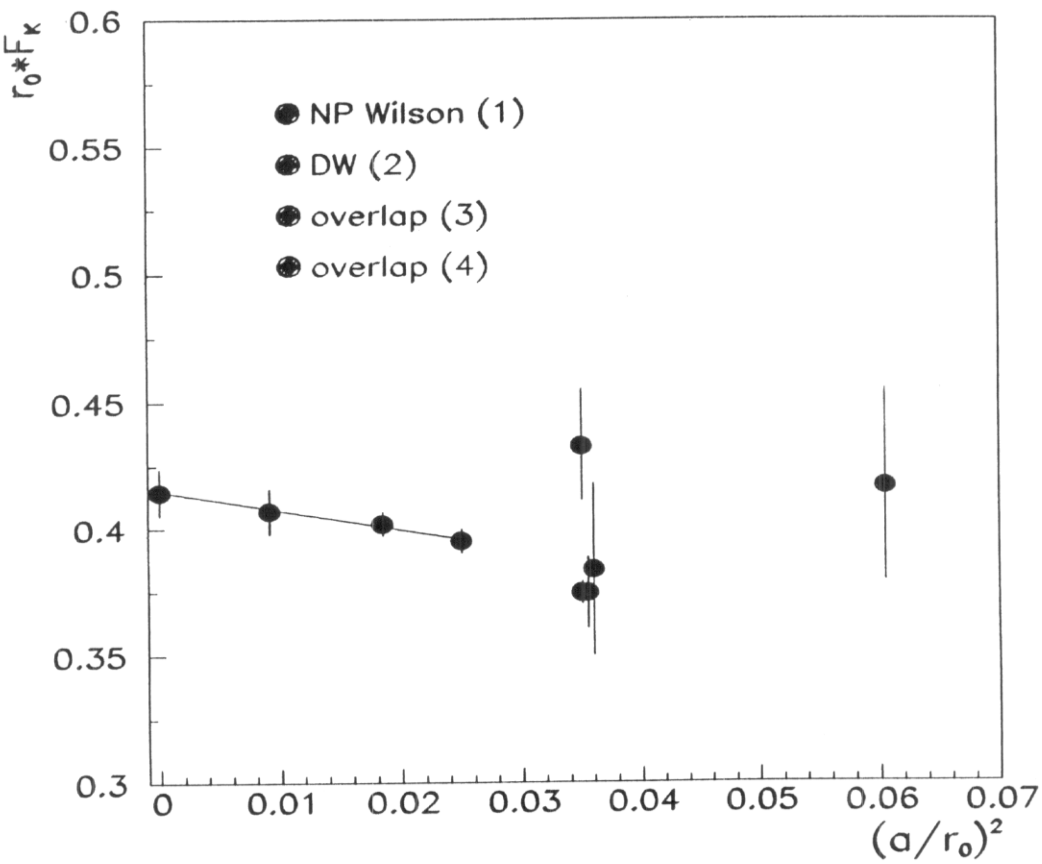
(5) H., Jansen, Lellouch, Wittig

Small $O(a^2)$ discretization errors!

Decay constants: f_K, f_π

Can be extracted without renormalization in regularizations that preserve chiral symmetry:

$$f_K = \lim_{M_{PS}^2 \to m_K^2} \frac{2m}{M_{PS}^2} |\langle O|P|PS\rangle|$$



(1) Garden *et al*

(2) Blum *et al*

(3) Giusti, Hoebling, Rebbi

(4) H., Jansen, Lellouch, Wittig

Conclusions

- Having an exact chiral symmetry at finite a in lattice QCD permits the exploration of the regime of light quark masses and might turn out to be essential in solving long standing problems like $\Delta I = 1/2$ or even ϵ'/ϵ
- It is possible to maintain an exact chiral symmetry, but it is very costly: $O(100)\times$ Wilson fermions
- Several ideas to improve the situation: improving the gauge action, the fermion action, the algorithm have not yet resulted in a significant cost improvement in logarithmic terms
- Several quenched simulations have been performed showing that these actions do not have large discretization errors $O(a)^2$ and can reach a regime of quark masses which is forbidden with Wilson fermions