Effects of low-lying eigenmodes in the epsilon regime of QCD

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Work in collaboration with H. Fukaya (YITP, Kyoto) and K. Ogawa (Sokendai, KEK)


Welcome to Tsukuba!

Goals of lattice QCD

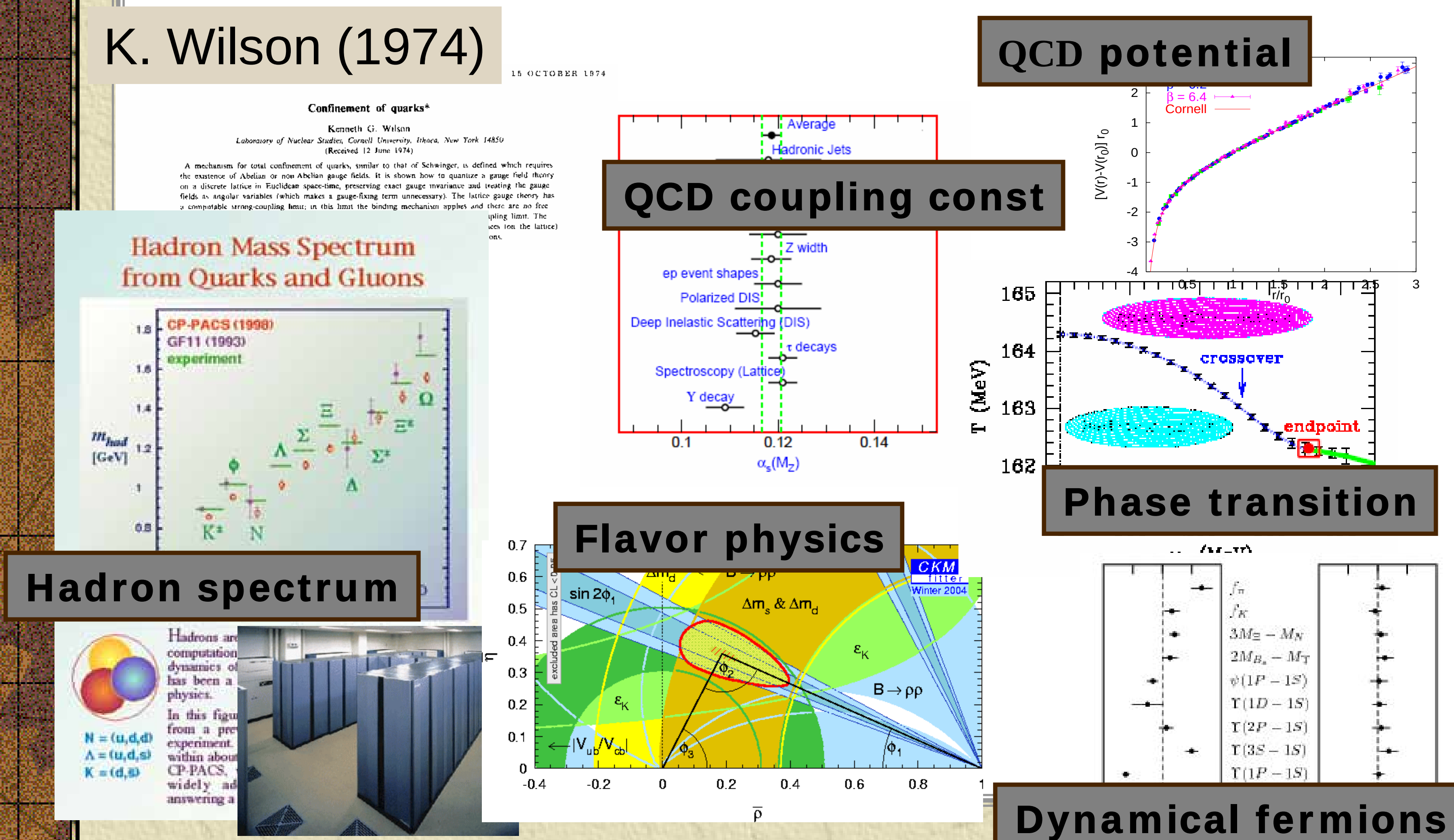
Understanding the dynamics of QCD

- Confinement
- Chiral symmetry breaking — pion as the Nambu-Goldston boson
- QCD in extreme conditions — finite temparature and density
- Hadron-hadron interactions; pentaquark etc.

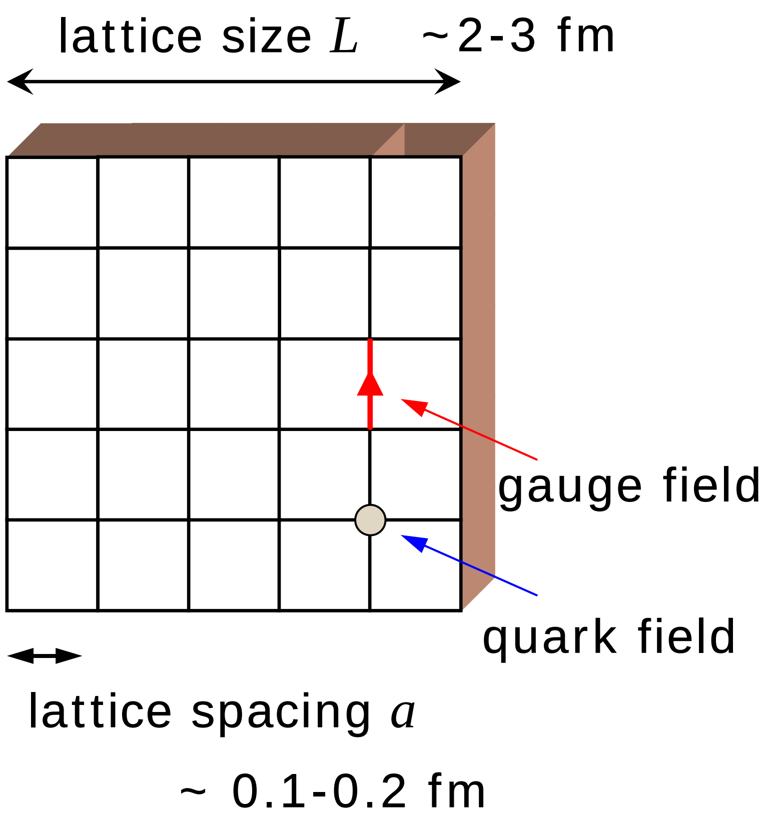
Precision calculation of hadron masses and matrix elements

- Test of QCD as the theory of strong interaction
- Determination of fundamental parameters
- Inputs to phenomenological analysis — kaon physics, B physics

30 years of lattice QCD



Lattice QCD



- Non-perturbative definition of QCD
- Monte Carlo simulation is possible.
- *"First principles"* calculation, but with approximations:
  - finite a
  - finite L
  - large m_q

  need extrapolations; source of systematic errors.

Dynamical fermions

Calculating the fermion determinant
= numerically very hard.

$$\int d\psi d\bar{\psi} e^{\int d^4x \bar{\psi}(\not{D}+m)\psi} = \det(\not{D}+m)$$

Quenched: neglect it
Unquenched: include it

<u>Common trick: pseudo-fermion</u>

$$|\det(\not{D}+m)|^2 = \int d\phi d\phi^\dagger e^{\int d^4x \phi^\dagger (\not{D}+m)^{-2}\phi}$$

— harder for smaller quark masses

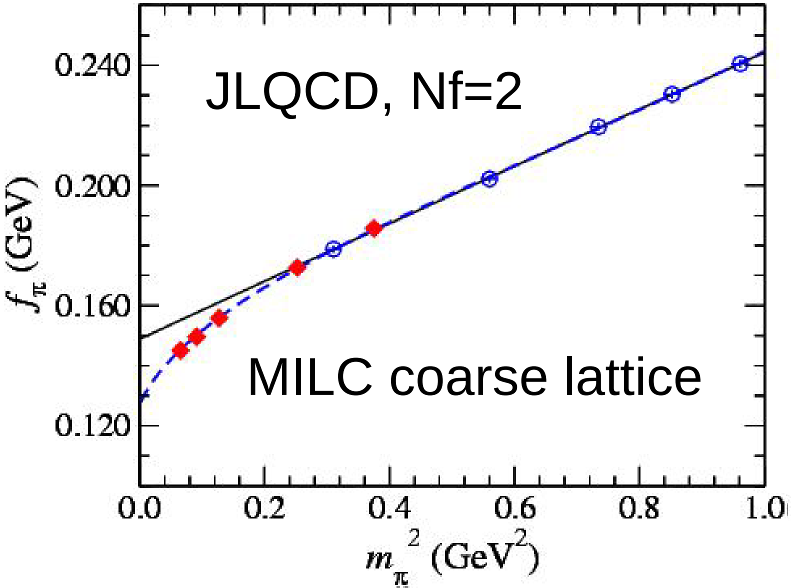
Problem of chiral "extrapolation"

- Chiral extrapolation is required to reach the physical up and down quark masses.
- Source of large systematic uncertainty.
- Computationally very hard in the dynamical fermion simulations, especially with the Wilson-type fermions

Chiral log

$$m_\pi^2 \ln m_\pi^2$$

with a fixed coefficient.



Note: ChPT

- Chiral perturbation theory
  - Gasser-Leutwyler in 80s
  - describes the dynamics of Nambu-Goldston pions
  - provides systematic expansion in p^2 and $m_\pi^{\,2}$

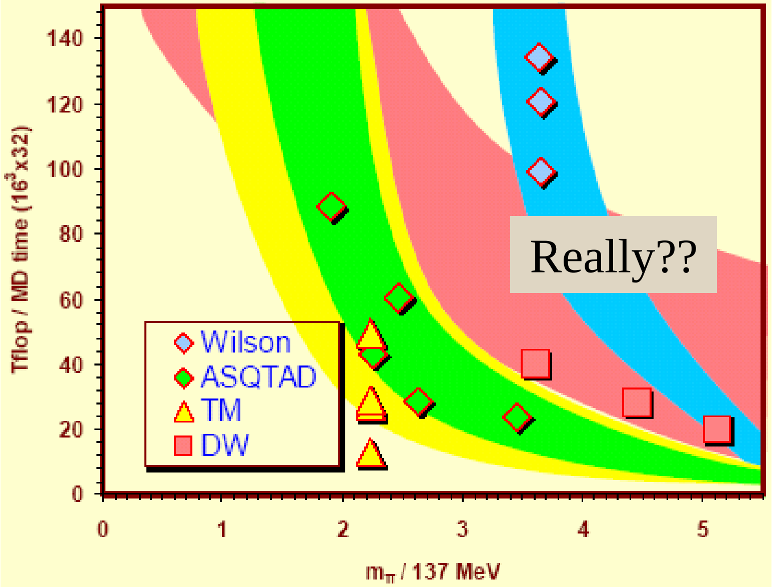
$$\mathcal{L} = \frac{F^2}{4}\mathrm{Tr}(\partial_\mu U \partial_\mu U^\dagger) - \frac{m\Sigma}{2}\mathrm{Tr}(e^{i\theta/N_f}U + e^{-i\theta/N_f}U^\dagger)$$

$$U(x) = \mathrm{e}^{i\sqrt{2}\xi(x)/F};\ \xi = \begin{pmatrix} \frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta_8 & \pi^+ & K^+ \\ \pi^- & -\frac{1}{\sqrt{2}}\pi^0 + \frac{1}{\sqrt{6}}\eta_8 & K^0 \\ K^- & \bar{K}^0 & -\frac{2}{\sqrt{6}}\eta_8 \end{pmatrix}$$

How hard?

- Computer time grows as $1/m_q^3$
- No guarantee that κ_c is really reached with the Wilson fermion = first order phase transition
- Exceptional trajectory $\Delta H \gg 1$ is often observed.

Kennedy@Lattice 2004



Advantage of fermion formulations having well-defined chiral limit.

Jumping to the chiral limit

- Hope is to extract physical quantities without chiral extrapolation — possible?
- The advantage of the Ginsparg-Wilson fermions would become more apparent.
- Interesting to see if they really work near the chiral limit.
- Effects of dynamical fermions.

An immediate problem

- Price one has to pay = finite volume effect.
- On a L=1.5 fm lattice physical pion gives $m_{\pi}L\sim 1$; pion Compton wave-length is 2π times the lattice size. For smaller quark masses it is even longer.

Such region is known as the epsilon regime of QCD.

QCD in the epsilon regime

Chiral Lagrangian

$$\mathcal{L} = \frac{F^2}{4}\mathrm{Tr}(\partial_\mu U \partial_\mu U^\dagger) - \frac{m\Sigma}{2}\mathrm{Tr}(e^{i\theta/N_f}U + e^{-i\theta/N_f}U^\dagger)$$

When $m \to 0$ ($m_\pi L<1$), fluctuation of the zero momentum mode becomes important.

$$U(x) = U_0\,\mathrm{e}^{i\sqrt{2}\xi(x)/F}$$

and integrate over U_0.

Expansion in terms of

$$\frac{m_\pi}{\Lambda} \sim \frac{p^2}{\Lambda^2} \sim \frac{1}{L^2F^2} \sim \varepsilon^2$$

Gasser-Leutwyler (1987)

ε -expansion: systematic analytical calculation is possible.

Analytic predictions

Leutwyler-Smilga (1992)

- Quark mass dependence of the QCD partition function
- Topological susceptibility
- Sum rules for the eigenvalues of the Dirac operator

Verbaarschot-Zahed, Akemann, Damgaard, … (1993~)

- Eigenvalue distribution of the Dirac operator from the Random Matrix Theory

Damgaard et al. (2002~)

- Correlation functions in the epsilon regime

Can test the lattice simulation using these known relations; determine the fundamental parameters: F, $\boldsymbol{\Sigma}$, LECs

Outline of this talk

1. Brief review of the Leutwyler-Smilga's predictions
2. Ginsparg-Wilson fermions
3. Lattice setup
4. Truncated Determinant Approximation for Nf=1
5. Numerical results for the partition function, etc.
6. Correlation functions

1. Brief review of the Leutwyler-Smilga's predictions

Partition function for N_f=1

- No Nambu-Goldstone mode in the Nf=1 case.
- Freeze the momentum fluctuation in the ε regime

$$Z = \exp[\Sigma V \,\mathrm{Re}(me^{i\theta})]$$

Partition function for each topological sector:

$$Z_\nu / Z = I_\nu(m\Sigma V)\exp(-m\Sigma V)$$

Topological susceptibility:

$$\left\langle \nu^2 \right\rangle = \sum_\nu \nu^2 Z_\nu / Z \to m\Sigma V \;(m \to 0)$$

Partition function for $N_f \geq 2$

$$\mathcal{L} = \frac{F^2}{4}\mathrm{Tr}(\partial_\mu U \partial_\mu U^\dagger) - \frac{m\Sigma}{2}\mathrm{Tr}(e^{i\theta/N_f}U + e^{-i\theta/N_f}U^\dagger)$$

- Degenerate vacua

$$Z = \int_{SU(N_f)} d\mu(U_0) \exp[\Sigma V \,\mathrm{Re}(e^{i\theta/N_f}\ \mathrm{tr}(mU_0^\dagger))]$$

- At Nf=2,

$$Z_\nu = I_\nu^2(m\Sigma V) - I_{\nu+1}(m\Sigma V) I_{\nu-1}(m\Sigma V)$$

for any fixed topology.

Sum rules for eigenvalues

- Derivative of Z_ν w.r.t. m

$$\int [dG] e^{-S_G} m^\nu \prod_n{}' (\lambda_n^2 + m^2) = m^\nu \left\langle \prod_n{}' (1 + \frac{m}{\lambda_n^2}) \right\rangle_\nu$$

Then, for each topological sector,

$$\left\langle \sum_n{}' \frac{1}{(\lambda_n \Sigma V)^2} \right\rangle_\nu = \frac{1}{4(\nu + N_f)}$$

LHS is UV divergent, but only affects 1/V corrections.

$\sum_n{}' \approx \frac{N_c}{4\pi} V \int \lambda^3 d\lambda$ gives 1/V contribution.

Smilga, in "Handbook of QCD"

"*The main interest here is not so much to "confirm" these exact theoretical results by computer, but, rather, to test lattice methods. This was a challenge for lattice people…*"

2. Ginsparg-Wilson fermions

Chiral symmetry on the lattice

- Chiral symmetry — invariance under the chiral transformation

$$\delta\psi = i\alpha\gamma_5\psi;\ \delta\bar{\psi} = i\alpha\bar{\psi}\gamma_5$$

- Nielsen-Ninomiya theorem (1981) = no lattice Dirac operator to satisfy
  - Right continuum limit
  - No doublers
  - Locality
  - Chiral symmetry $D\gamma_5 + \gamma_5 D = 0$

natural, because we need axial U(1) anomaly

Ginsparg-Wilson relation

- Introduce a modified chiral transformation by Luscher (1998)

$$\delta\psi = i\alpha\gamma_5\left[1-\frac{1}{2}aD\right]\psi;\ \delta\bar{\psi} = i\alpha\bar{\psi}\left[1-\frac{1}{2}aD\right]\gamma_5$$

- Invariant if *D* satisfies the Ginsparg-Wilson relation (1982).

$$D\gamma_5 + \gamma_5 D = aD\gamma_5 D$$

Exact chiral symmetry is realized at finite *a*.

Consistent with anomaly

- Fermion measure is not invariant under the modified chiral transformation.

$$\prod_n d\psi_n d\bar{\psi}_n \to J^{-2}\prod_n d\psi_n d\bar{\psi}_n;\ \ln J = i\alpha\int d^4x \sum_k \bar{u}_k(x)\gamma_5 u_k(x)$$

- Eigenvectors of the Dirac operator

$$Du_k(x) = \lambda_k u_k(x);\ D\gamma_5 u_k(x) = \lambda_k^* \gamma_5 u_k(x)$$

- The trace of γ_5 vanishes unless there are zero modes λ_k=0, which appears from topologically non-trivial gauge configurations.

$$\int d^4x \sum_k \bar{u}_k(x)\gamma_5 u_k(x) = n_R - n_L = q = \frac{1}{16\pi^2}\int d^4x \,\mathrm{Tr}\, F_{\mu\nu}\tilde{F}_{\mu\nu}$$

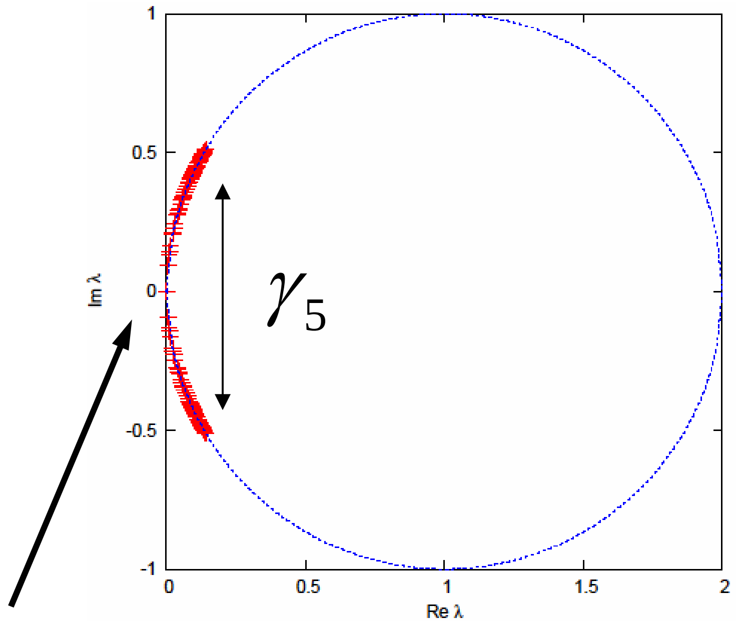
Atiyah-Singer index theorem

Eigenvalues for GW fermion

- Using

$$D\gamma_5 + \gamma_5 D = aD\gamma_5 D$$
$$D^\dagger = \gamma_5 D \gamma_5$$

  one can show that the eigenvalues lie on a circle.
- In the continuum limit they lie on the imaginary axis.

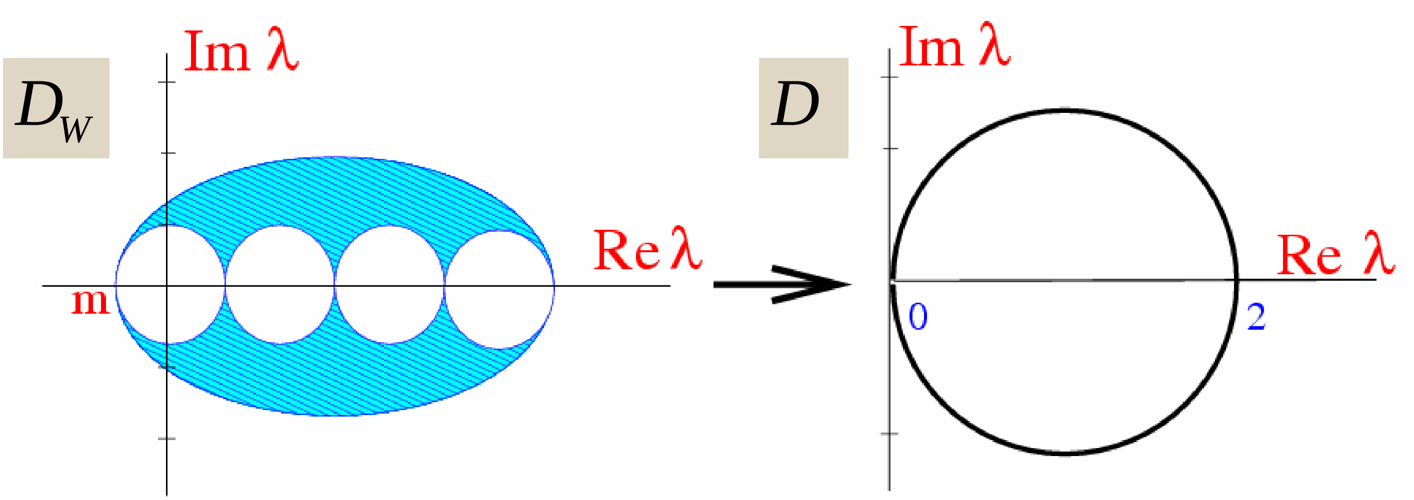


Zero modes

Neuberger Dirac operator

- Overlap Dirac operator — Neuberger (1998)

$$D = \frac{1}{a}\left[1 - \frac{A}{\sqrt{A^\dagger A}}\right];\ A = 1 - aD_W$$



Drawing stolen from M. Creutz's write-up

3. Lattice setup: implementation of the overlap Dirac operator

Lattice setup

- β =5.85, 10^4 lattice
- a = 0.123 fm (or 1/a = 1.6 GeV)
- $V = (1.23\ \text{fm})^4$

- $M_\pi L = 1$ at m = 7 MeV
- $m\Sigma V = 1$ at m = 42 MeV
- 168, 290, 149 quenched configurations for $|\nu|$=0, 1, 2

Overlap Dirac operator

- Overlap Dirac operator

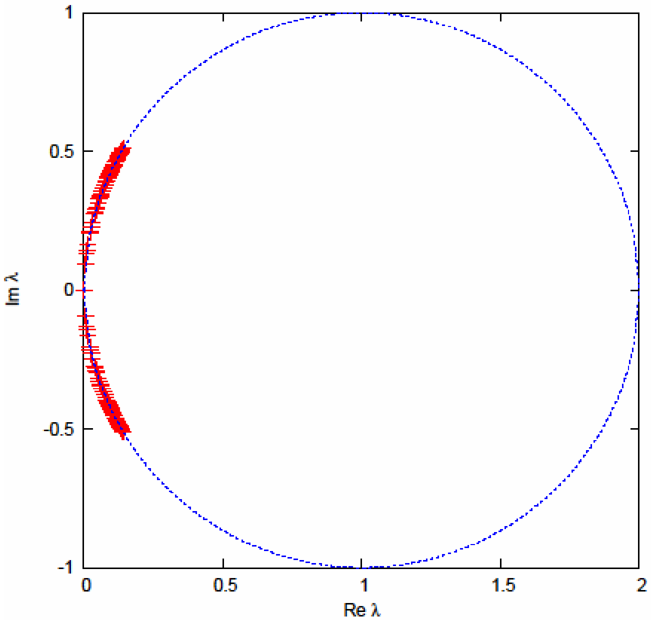
$$D = \frac{1+s}{a}\left[1+\gamma_5 \,\mathrm{sgn}(H_W)\right]$$

- For sgn(H_W), 14 lowest eigenmodes of H_W is treated exactly; the rest is approximated using the Chebyshev polynomial (order 100-200) to satisfy the accuracy 10^{-10}
- On an Itanium 2 (1.3 GHz, 3MB) workstation one multiplication of *D* takes about 10 sec.

Eigenvalues & eigenvectors

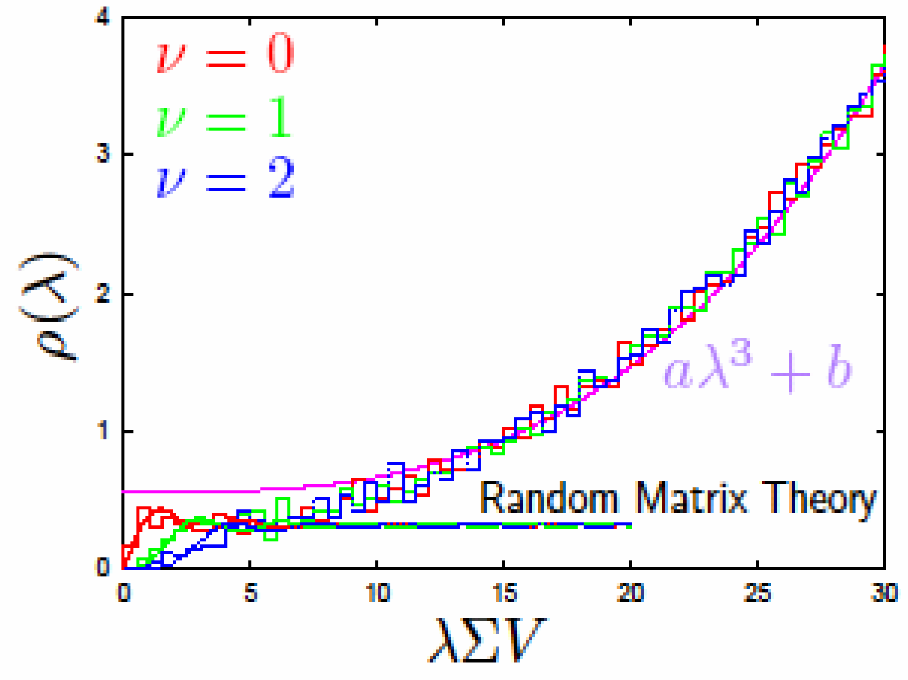
- For each gauge config, 50 lowest eigenvalues and their eigenvectors are calculated using the ARPACK (implicitly restarted Arnoldi method).
- They appear as pairs (λ_i, λ_i*); calculate

$$\frac{1+\gamma_5}{2} D \frac{1+\gamma_5}{2} = \mathrm{Re}(\lambda)$$



- Topological charge is determined by counting the number of zero modes.

Eigenvalue distribution



Away from the chiral regime, it is consistent with a free quark form

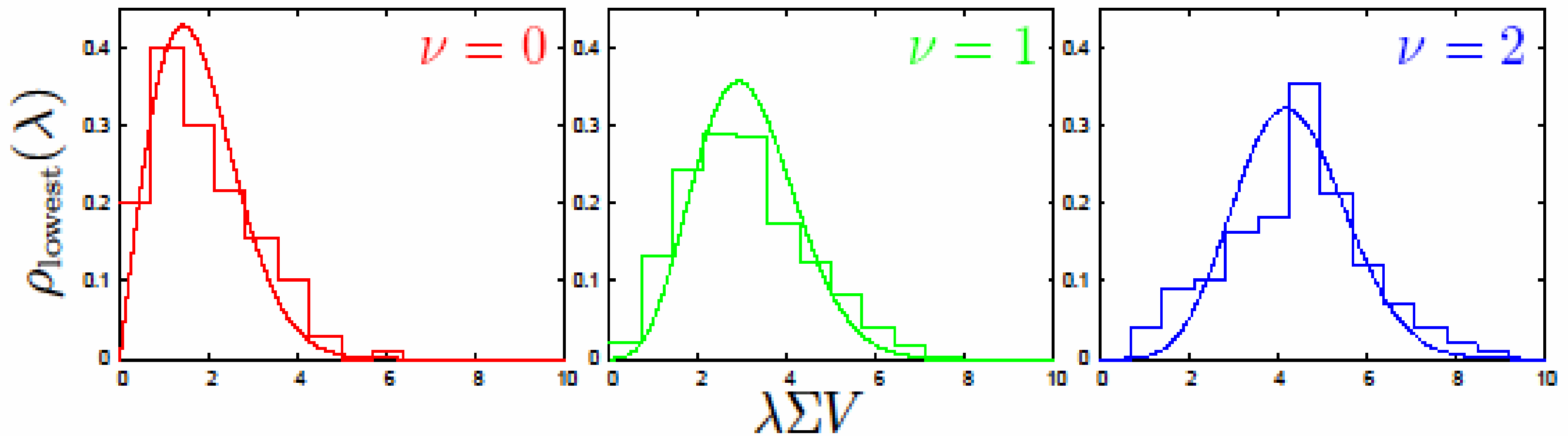
$$\sim \lambda^3$$

independent of topology

Near the chiral limit, the distribution becomes sensitive to the topological charge; described well with the Random Matrix Theory.

Comparison with RMT

Distribution of the lowest lying mode:



Lines are from RMT (Nishigaki, Damgaard, Wettig (1998))

Similar lattice observations by
Edwards, Heller, Kiskis, Narayanan (1999); Hasenfratz et al. (2002); Bietenholz, Jansen, Shcheredin (2003); Giusti, Luscher, Weisz, Wittig (2003); Galletly et al. (2003)

Note: Random Matrix Theory

- Randomly distributed eigenvalues obey a partition function

$$Z_{\nu,N_f} = \int DW \det^{N_f}\begin{pmatrix} m & iW \\ iW^\dagger & m \end{pmatrix} e^{-N_f/2\mathrm{Tr}\,\nu(W^\dagger W)}$$

nxm matrix with $\boldsymbol{\nu}=m-n$ and $N=n+m$

- Corresponds to the chiral lagrangian in the epsilon regime in the limit of $N\to\infty$.
- The lowest lying eigenvalue distributes as

$$P^{\nu=0}(z) \propto z e^{-z^2/4},\ P^{\nu=1}(z) \propto z I_2(z) e^{-z^2/4},\ \ldots;\ z = m\Sigma V$$

4. Truncated determinant approximation for N_f=1

Fermion determinant

$$\det(D+m)=\prod_i\left(\left|\lambda_i\right|^2+m^2\right)$$

- The low-lying eigenmodes should be most relevant to the low energy physics.
- Higher modes reflect short distance physics, sensitive to the lattice artifact.

- Reweighting the quenched config with a truncated determinant

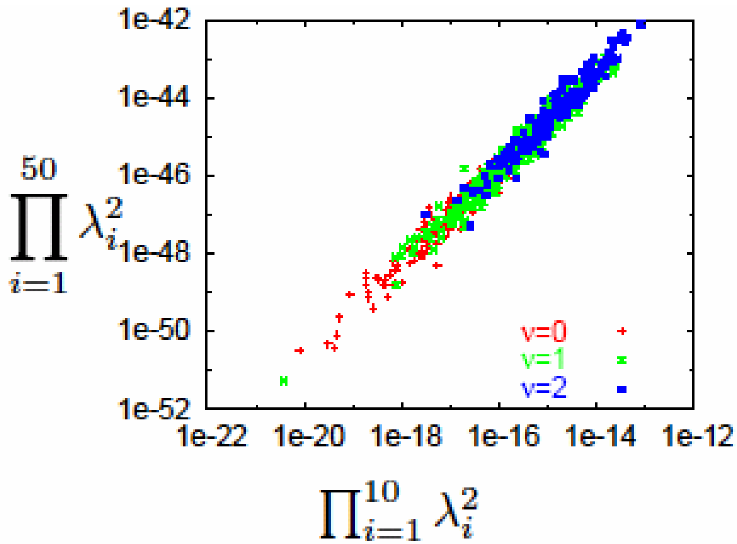
$$\prod_{i=1}^{N_{\max}}\left(\left|\lambda_i\right|^2+m^2\right)$$

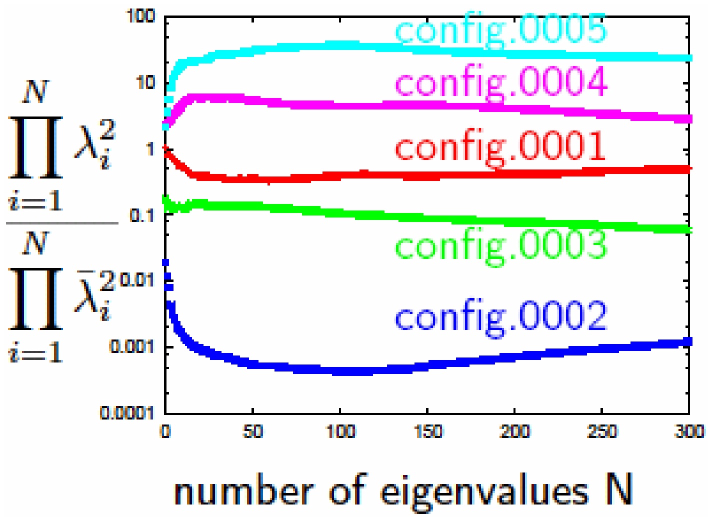
- Duncan, Eichten, Thacker (1998)
  - Treat the low-lying mode exactly in Monte Carlo
  - Higher mode could be included by an effective gauge action or multiboson.

How effective?

Here we just neglect the effects of higher modes.

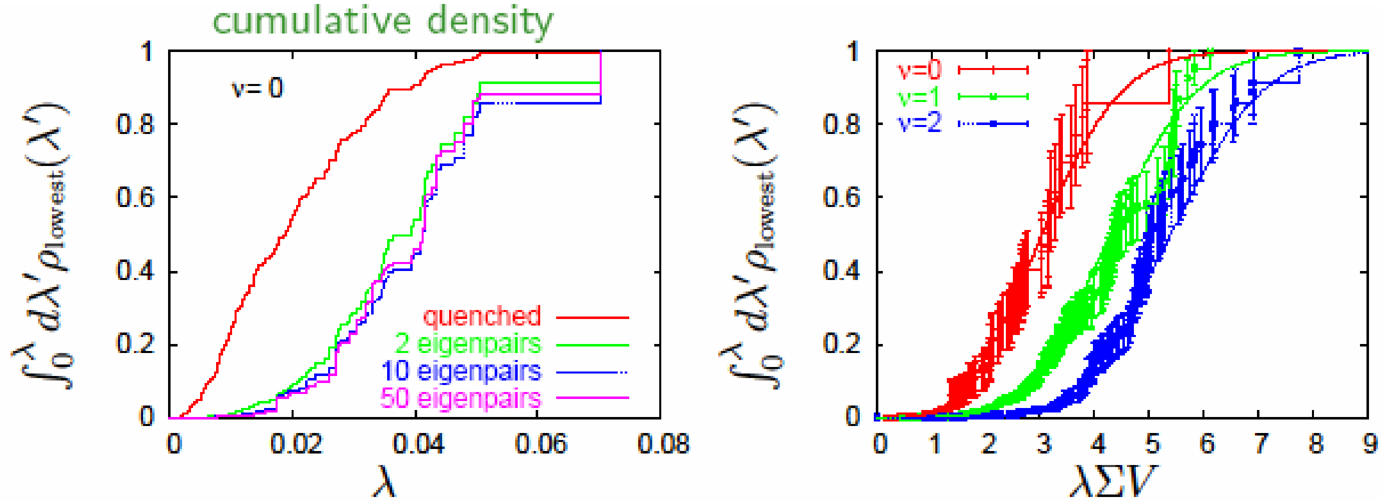
- Their effect is approximately constant, and independent of topology.
- Can be checked for each observable by varying N_{max}.





Effect on the eigenvalue distribution

Cumulative density of the first eigenvalue:

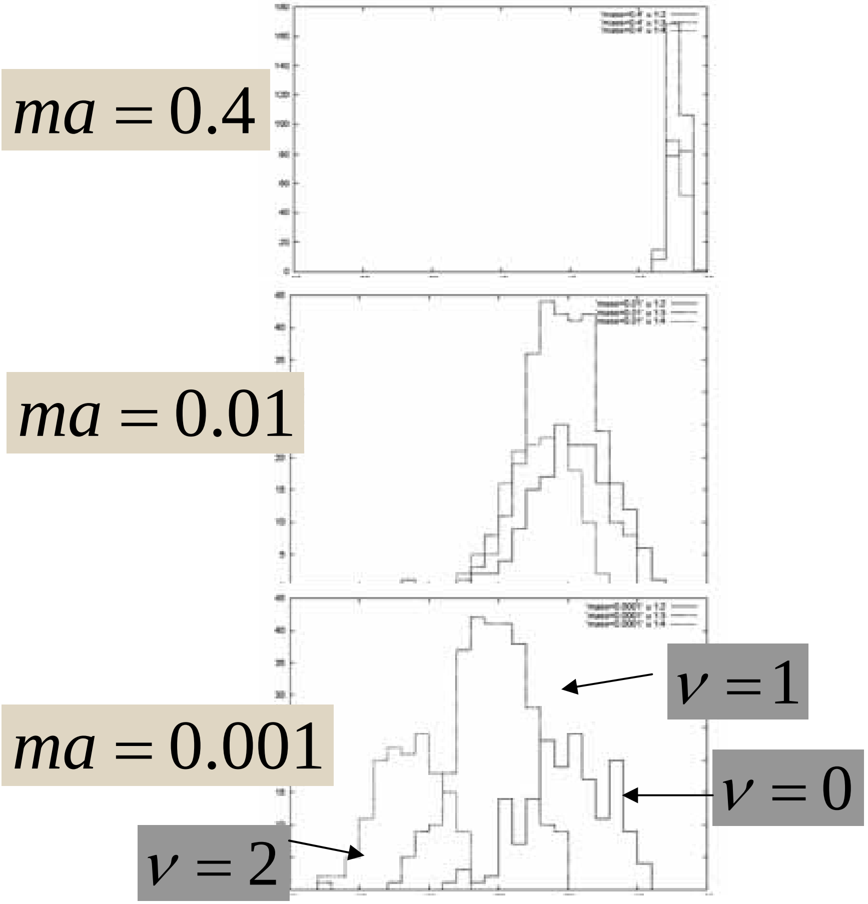


Curves are expectations of RMT.

Disadvantages

- NOT exact

  It may be possible to make it exact: Borici – UV suppressed fermion.
- Effective number of statistical samples is substantially smaller.



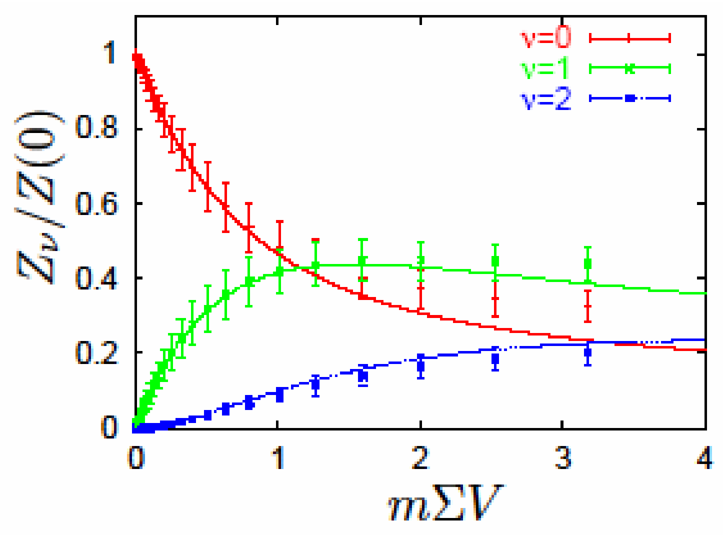
$$\log_{10} \prod_{i=0}^{N_{\max}} \left(\lambda_i^2 + m^2 \right)$$

5. Numerical results for the partition function, etc.

QCD partition function

- For N_f=1, the QCD partition function is expected to behave as

$$Z_\nu / Z = I_\nu(m\Sigma V)\exp(-m\Sigma V)$$



- Good agreemenet below

$$m\Sigma V \simeq 2$$

- A fit yields

$$\Sigma = (243\,\mathrm{MeV})^3$$

Topological susceptibility

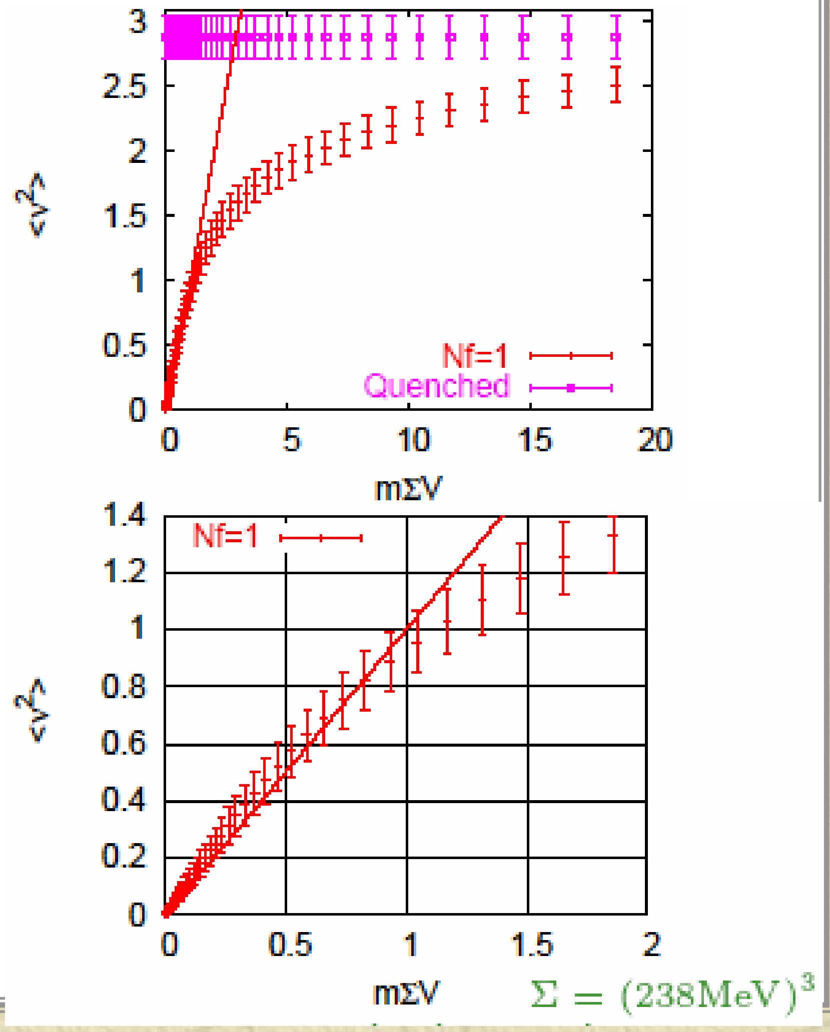
- Topological susceptibility should behave as

$$\left\langle \nu^2 \right\rangle = \frac{1}{N_f} m\Sigma V$$

- Well reproduced with

$$\Sigma = (238\,\mathrm{MeV})^3$$

Earlier study by Kovacs (2001)

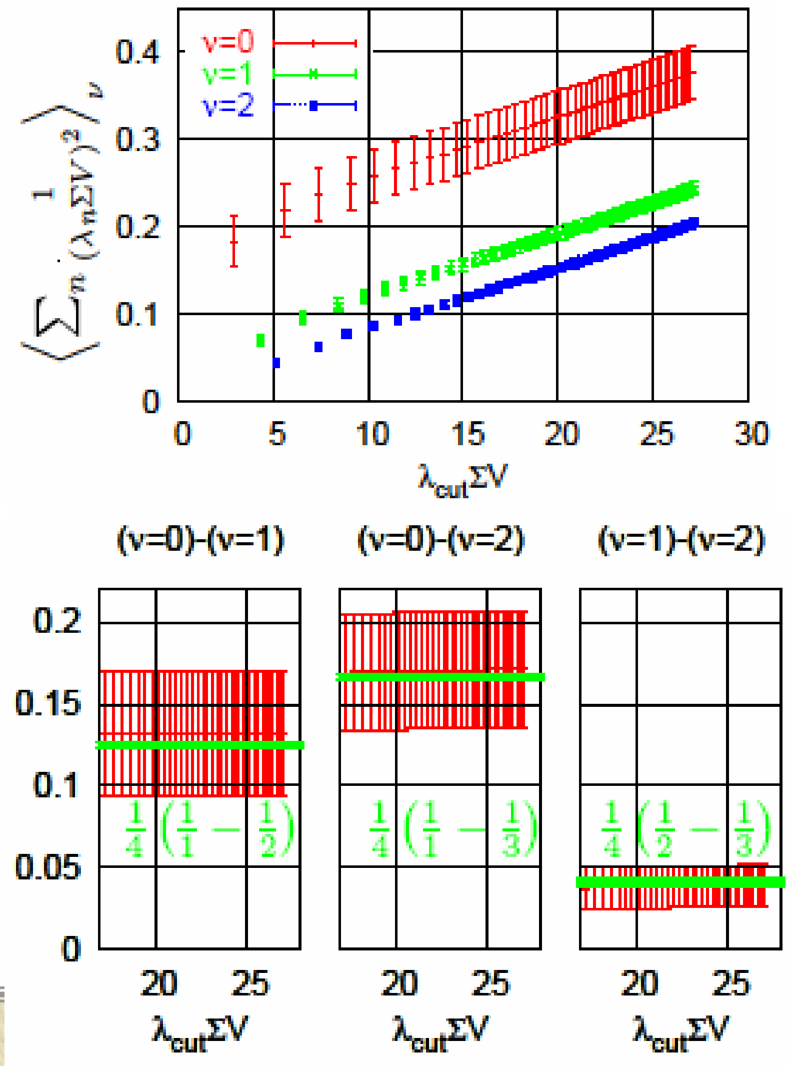


Leutwyler-Smilga sum rule

$$\left\langle \sum_n{}' \frac{1}{(\lambda_n \Sigma V)^2} \right\rangle_\nu = \frac{1}{4(\nu+1)}$$

- LHS is quadratically divergent; need UV cutoff and careful study of volume dependence.
- Consider differences among different topological sectors.

$$\Sigma = (236\,\mathrm{MeV})^3$$



6. Correlation functions

Correlators in the epsilon regime

- Once the properties of the vacuum is confirmed, the interest would be in the excitations.
- ChPT analysis of meson correlation functions:
  - Damgaard et al. (2002, 2003)
  - Giusti et al. (2003, 2004); Hernandez-Laine (2003)
  - First numerical study: Giusti et al. (2004); Bietenholz et al. (2004)
- Possibility to determine the parameters in ChPT: F_π, Σ, LOCs w/o chiral extrapolation.

An example

In the quenched ChPT,

$$\left\langle P^1(t)P^1(0)\right\rangle = L^3 C_P^1 - \frac{\Sigma^2}{2F^2}\left[-\frac{m_0^2 T^3}{N_c} c_+ h_2(\tau) + \left(\frac{\alpha}{N_c} c_+ - b_+\right) T h_1(\tau)\right]$$

$$c_+ = 2\left(I_\nu(\mu)K_\nu(\mu) - I_{\nu+1}(\mu)K_{\nu-1}(\mu) - \frac{\nu}{\mu^2}\right), \quad b_+ = 2\left(1 + \frac{\nu^2}{\mu^2}\right)$$

$$h_2(\tau) = \frac{1}{24}\left[\tau^2(\tau-1)^2 - \frac{1}{30}\right], \quad h_1(\tau) = \frac{1}{2}\left[\left(\tau - \frac{1}{2}\right)^2 - \frac{1}{12}\right], \quad \tau = \frac{t}{T}$$

- Divergence in the massless limit $\mu \equiv m\Sigma V \to 0$
- Strong dependence on the toplogical charge
- Allows to determine F, α, m_0^2, in principle

Lattice measurement

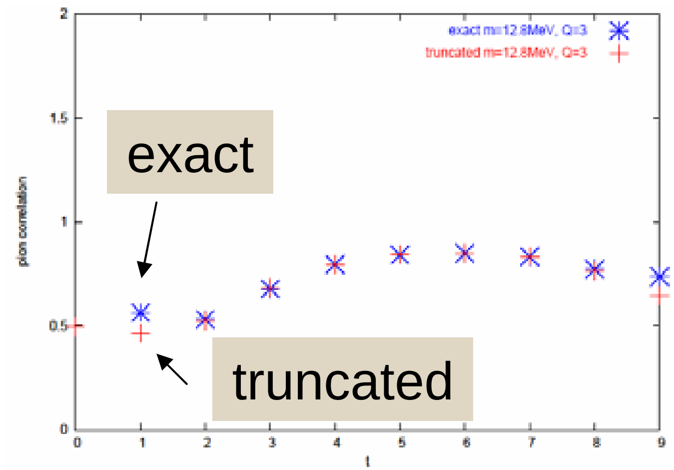
- Very hard to solve the quark propagator near the massless limit.
- Construction using the eigenvectors

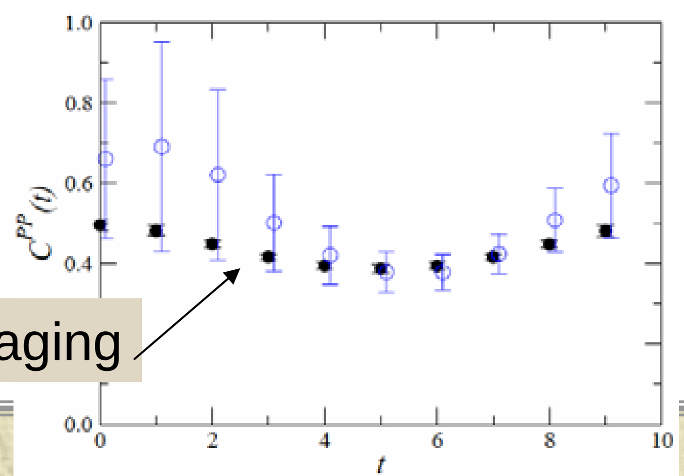
$$\langle q(x)\overline{q}(0)\rangle = \sum_i \frac{u_i(x)\overline{u}_i(0)}{m+\lambda_i}, \quad Du_i(x) = \lambda_i u_i(x).$$

  saturates the PP correlator with the 50 eigenmodes to 99.5%. Only below ma=0.008 and for $\nu \neq 0$.
- For moderate mass values, the preconditioning with the known eigenvectors works well as noticed by Giusti, Hoelbling, Luscher, Wittig (2003).

More about techniques

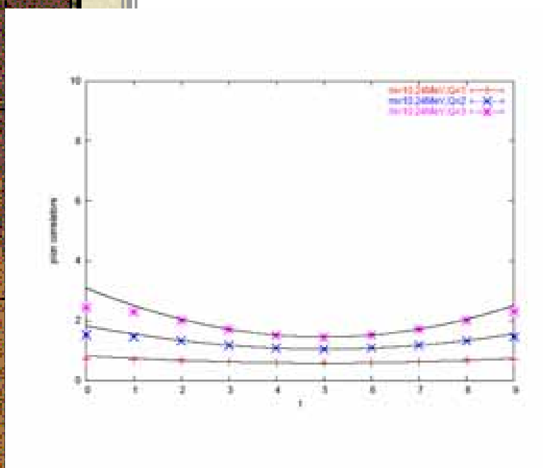
- Low-mode saturation
  - as discussed in the previous page
- Low-mode averaging
  - Source point can be freely chosen without extra cost for inversion.
  - By averaging over lattice points, one can get much better statistics.
  - Also proposed by Giusti et al. (2004)



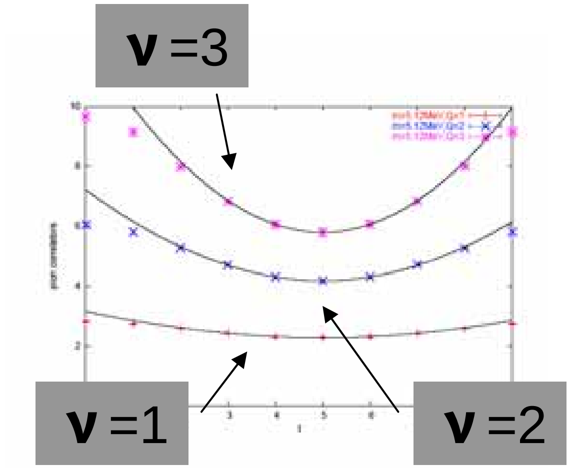


A preliminary result

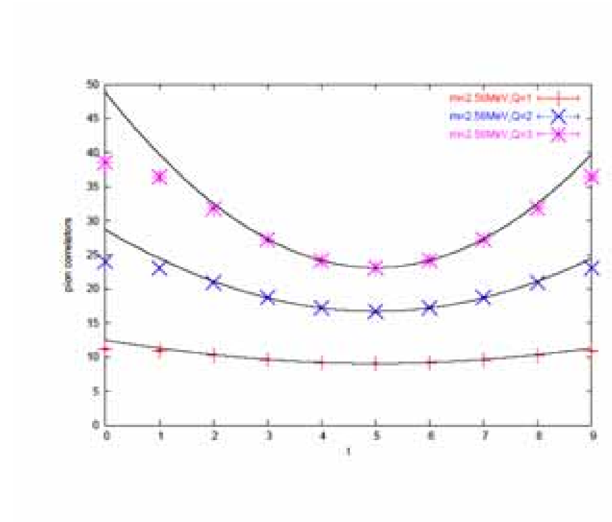
"pion correlator"



m = 10 MeV



m = 5 MeV



m = 2.5 MeV

Expected behavior:

$$\sim \frac{\nu^2}{(m\Sigma V)^2}\left(\frac{t}{T}-\frac{1}{2}\right)^2$$

A fit yields

$$\Sigma \simeq (300\ \mathrm{MeV})^3, \quad F \simeq 110\,\mathrm{MeV}$$

at Nf=0. m_0=600 MeV is assumed.

Summary and Discussions

Issues…

- *To make the calculations exact, one must include the effects of higher modes. Is it feasible?*
  - Include them using the multi-boson-like algorithms. Highly non-local…
  - Consider the truncated version as a new definition of the GW Dirac operator. Locality is okay --- Borici.

Truncated determinant algorithm

Duncan, Eichten, Thacker (1998)

- Separate the fermion determinant as

$$\det H = (\det H)_{\text{low } \lambda} \cdot (\det H)_{\text{high } \lambda}$$

- Explicitly calculate the “low” eigenvalues.
- “high” eigenmodes are approximated by polynomial.

$$\det H^2 = \lim_{n\to\infty} [\det P_n(H^2)]^{-1} = \lim_{n\to\infty} \prod_{k=1}^{n} \det[(H-\mu_k)^2 + \nu_k^2]^{-1}$$

$$P_n(z) = \mathrm{const} \prod_{k=1}^{n} (z - z_k) \xrightarrow[n\to\infty]{} 1/z; \quad \sqrt{z} = \mu + i\nu$$

- Then, introduce pseudo-fermions for each k (multi-boson).

UV suppressed fermions

Borici (2002)

- Define the lattice Dirac operator such that the UV modes are suppressed in the determinant.

$$D = \frac{\mu}{a}\gamma_5 \tanh \frac{aH_W}{\mu}; \quad H_W = \gamma_5 D_W$$

- Eigenvalues become independent of gauge configurations above μ .
- Locality is okay: analytic, 2π periodic in the momentum space.
- Alternative way to regularize the fermion field.

More issues…

- *As volume increases, the calculation of the eigenvalues/eigenvectors becomes much harder. What to do?*
  - Eigenvalue distributes more densely ~V; calculation cost ~ V^2. Certainly much more difficult. Maybe one could treat the lowest few eigenmodes exactly and the rest with some other algorithms…

Summary

- Using the overlap Dirac operator, the theoretical predictions in the epsilon regime are reproduced. They are related to the properties of the QCD vacuum.
- The reweighting with the truncated determinant works reasonably well.
- Application is broader: it is also possible to probe the low energy physics through the correlation functions.


Enjoy your stay!