

# The finite temperature QCD phase transition from domain wall fermions

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Extreme Computing and its Implications for the  
Nuclear Physics/Applied Mathematics/Computer  
Science Interface

Institute for Nuclear Theory  
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# Outline

1. QCD at Finite Temperature
2. Chiral Symmetry restoration and the anomalous  $U(1)_A$  symmetry
3. Domain Wall Fermions
4. Screening correlators and susceptibilities
5. Dirac spectrum



## The HotQCD collaboration

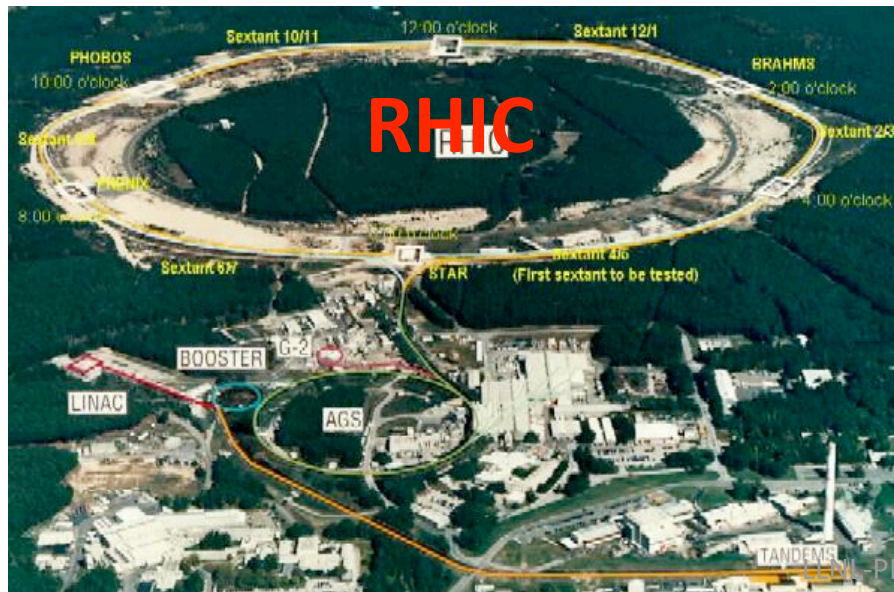
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# Hot QCD

- Matter of sufficient energy density existed in the first  $10^{-5}$  sec. after Big Bang.
- Interiors of neutron stars?
- Probed experimentally in heavy ion collisions.

RHIC: Au+Au collisions at 200 GeV/nucleon

LHC: Pb+Pb collisions at 2.76 TeV/nucleon



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# QCD

QCD Lagrangian:

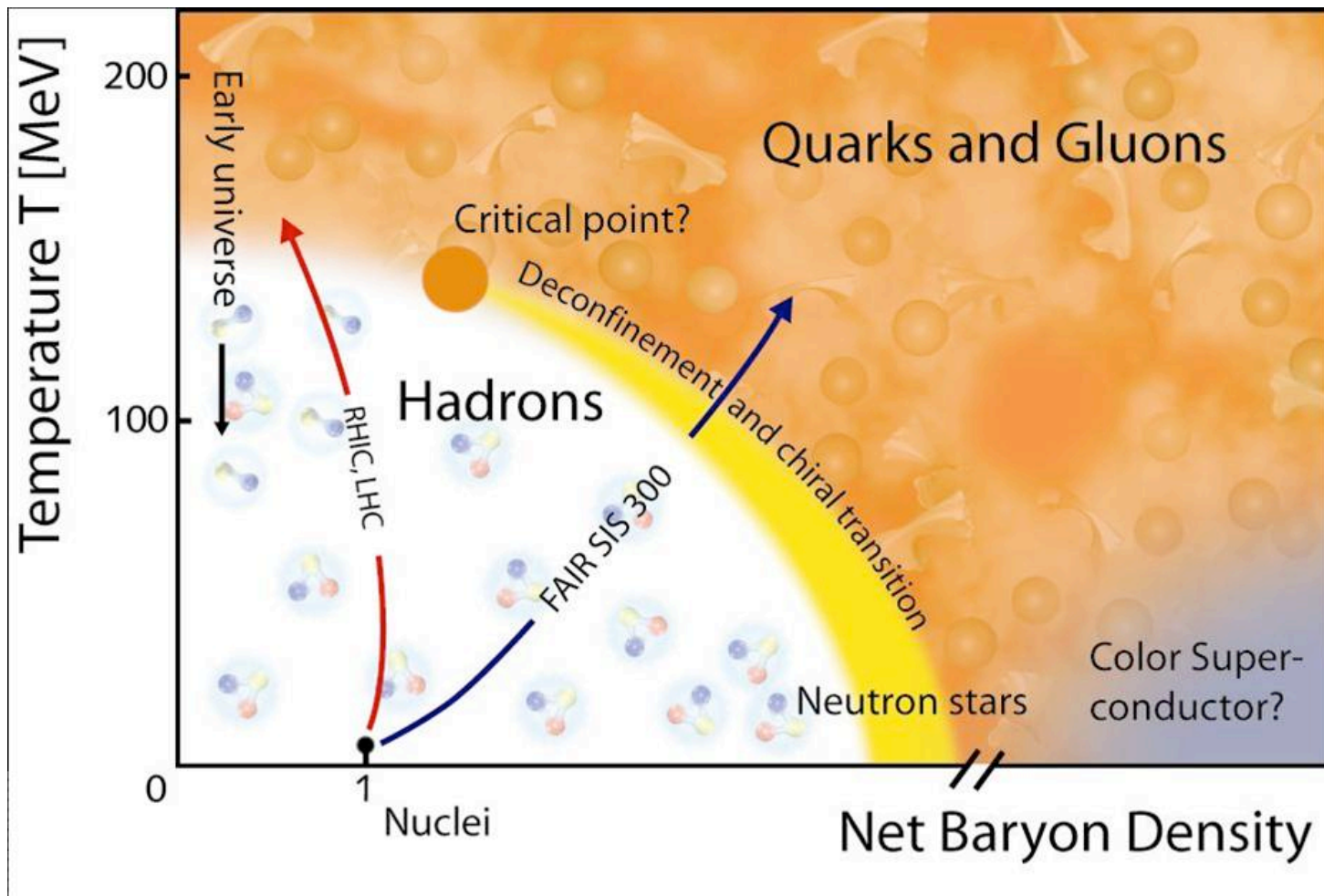
$$\mathcal{L}_{QCD} = \bar{\psi} (i\gamma^\mu \partial_\mu - m) \psi - g\bar{\psi} A_\mu^a T^a \psi - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu}$$
$$G_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - gf^{abc} A_\mu^b A_\nu^c$$

- Asymptotic Freedom: Weak coupling at high energies
- Strong coupling at low energies
- Confinement: Only color singlets
- Chiral symmetry: Classical  $SU(N_f)_L \times SU(N_f)_R \times U(1)_V \times U(1)_A$  symmetry
- Spontaneous  $\chi$ SB breaks  $SU(N_f)_L \times SU(N_f)_R \rightarrow SU(N_f)_V$
- Anomalous  $U(1)_A$  symmetry

# Finite Temperature QCD

- Hagedorn (1965) noticed that apparent exponential rise in density of hadronic states could imply a limiting temperature.
- In reality, hadrons are not point particles. At sufficiently high temperature  $T_c$ , thermal energy is sufficient to “melt” hadron states.
- Quark-gluon plasma (QGP)
- Deconfinement: Colored gluons, quarks are no longer bound in hadrons – free to propagate.
- Chiral symmetry restoration: Quarks propagate in QGP with current quark masses.
- Is the QGP truly a different phase? What is the nature of the phase transition?

# Phase Diagram



# Lattice QCD

- Normal field theoretic tools, i.e. perturbative expansion, does not work very well.
- Coupling is too strong for perturbation series to converge.
- In addition, at finite temperature, there is added infrared divergence that signals true non-perturbative behavior.
- Consider instead (Euclidean) path integral:

$$\int [D\bar{\psi}][D\psi][DA_\mu] \exp \left( - \int [\bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}] \right)$$

- Discretize on a 4-dimensional space-time lattice.
- $V = L^3 = (N_s a)^3$   $t = N_t a$
- $a$  is lattice spacing;  $a^{-1}$  sets UV cut-off scale in calculation.



# Lattice QCD at Finite Temperature

- Wish to calculate *thermal* expectation values:

$$\langle \mathcal{O} \rangle = \sum_n \langle n | \mathcal{O} e^{-H_{QCD}/T} | n \rangle$$

- Thermal partition function is just Euclidean path integral with  $T = 1/N_t a$  and (anti-)periodic BCs for (fermion) gauge fields.

$$Z = \int [\mathcal{D}A_\mu] \det(M) e^{-\int_0^{1/T} dt \int d^3x S_G(x,t)}$$

- Work at fixed  $N_t$ . Change temperature by varying the lattice spacing.

# Chiral Symmetry Restoration

- $SU(N_f)_L \times SU(N_f)_R$  spontaneously broken to  $SU(N_f)_V$
- Chiral condensate develops – analog of magnetization in Ising model.
- Spontaneous ordering of QCD vacuum
- For  $T > T_c$  chiral symmetry is restored – chiral condensate vanishes.
- Chiral condensate is an order parameter for chiral symmetry restoration.

# Banks-Casher

- Banks-Casher relation (1980):

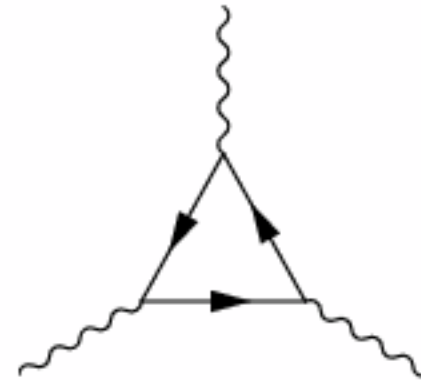
$$\begin{aligned}\langle \bar{q}q \rangle &= \lim_{m_q \rightarrow 0} \lim_{V \rightarrow \infty} \int d\lambda \rho(\lambda) \frac{-2m_q}{\lambda^2 + m_q^2} \\ &= -\pi \rho(\lambda = 0)\end{aligned}$$

- Remarkable result: Chiral condensate can be reconstructed using low-lying modes of the 4-d Dirac operator.
- Furthermore: Condensation of modes at  $\lambda=0$  in the chirally broken phase.
- Order of limits important: no  $\chi$ SB in finite volume.

# $U(1)_A$

- Classical symmetry of QCD Lagrangian.
- (Non-)conservation of flavor singlet axial current.
- Violated by Adler-Bell-Jackiw anomaly.

$$\partial_\mu J_5^\mu = \frac{g^2 N_f}{16\pi^2} \text{tr} \left( \tilde{F}_{\mu\nu} F^{\mu\nu} \right)$$
$$J_5^\mu = \bar{q} \gamma^\mu \gamma^5 q$$



# Gauge field topology

- RHS of anomaly equation corresponds to density of topological modes.

$$Q(x) = \frac{g^2}{16\pi} \text{tr} \left( \tilde{F}_{\mu\nu} F^{\mu\nu} \right)$$

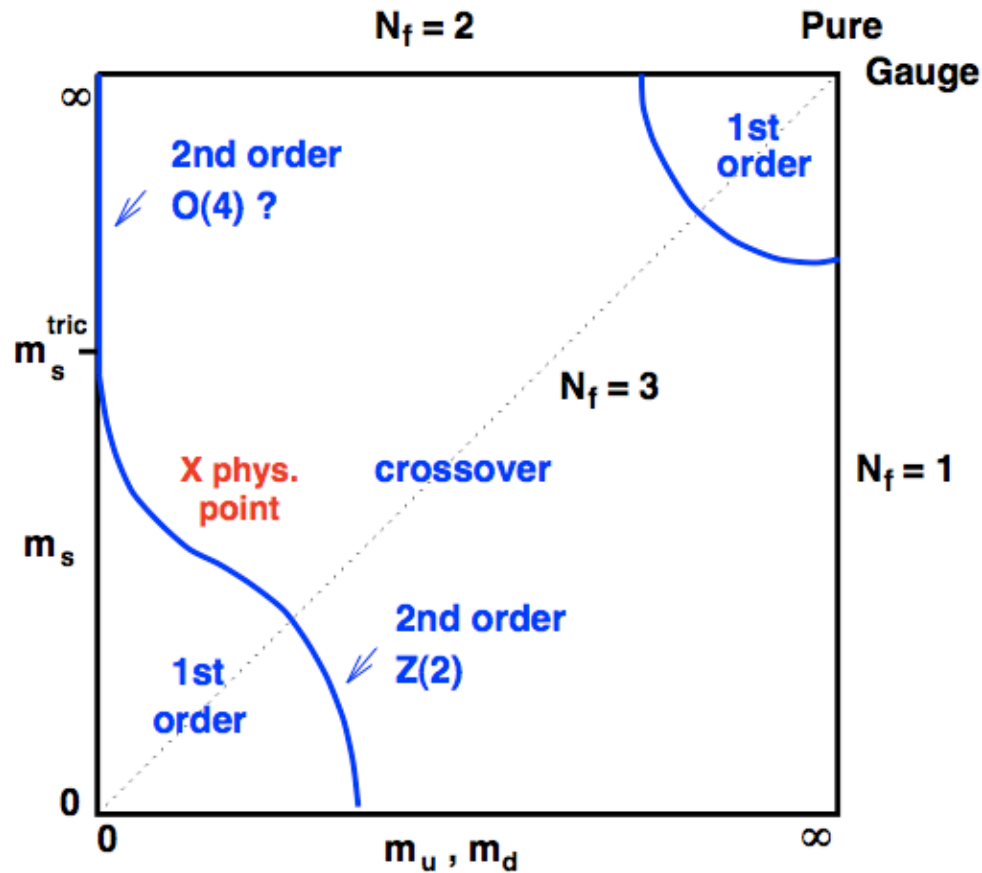
- Global topological charge – gauge field winding number
- Winding number equal to index of Dirac operator, *i.e.* difference between number of positive and negative chiral zero modes.

$$\nu = \int d^4x Q(x) = \text{index}(D) = n_+ - n_-$$

# $U(1)_A$ at finite temperature

- What happens to  $U(1)_A$  at finite temperature?
- Naively, ABJ anomaly independent of temperature.  $U(1)_A$  breaking at finite  $T$ ?
- $U(1)_A$  problem solved by ABJ anomaly *and* presence of non-trivial topology.
- At high temperature, configurations with non-zero topology may be sufficiently suppressed so that  $U(1)_A$  is *effectively* restored.

# Phase Diagram



- $N_f \geq 3$  expected to be first order
- $N_f = 2$  is second order
- 2+1f QCD with quarks at physical mass is likely crossover.
- $U(1)_A$  restoration at  $T_c$  may cause  $N_f = 2$  case to be first order.

# Literature Review

- Pisarski Wilczek (1984)
- LQCD calculations in mid-late 1990s (Columbia, MILC, Kogut+Sinclair+Lagae, Karsch *et. al.*, ...)
- Connection to low-lying Dirac modes: (Cohen, ...)
- Many calculations rely on staggered fermions – difficult because of reduced chiral symmetry at finite lattice spacing – need to be close to continuum...



# Domain Wall Fermions

- Chiral fermions on the lattice (Kaplan 1992).
- Left and right-handed chiral modes are bound to 4-d walls of 5-d theory.
- An exact chiral symmetry even at finite lattice spacing.

# Residual Mass

- Residual chiral symmetry breaking from finite  $L_s$ . Additive renormalization to quark masses.

$$m_{\text{res}}(L_s) = \frac{c_0}{L_s} + \frac{c_1}{L_s} \exp(-\alpha L_s)$$

- First term corresponds to localized lattice dislocations that mix states on the boundaries.
- Zero modes of 4-d Hermitian Wilson operator:

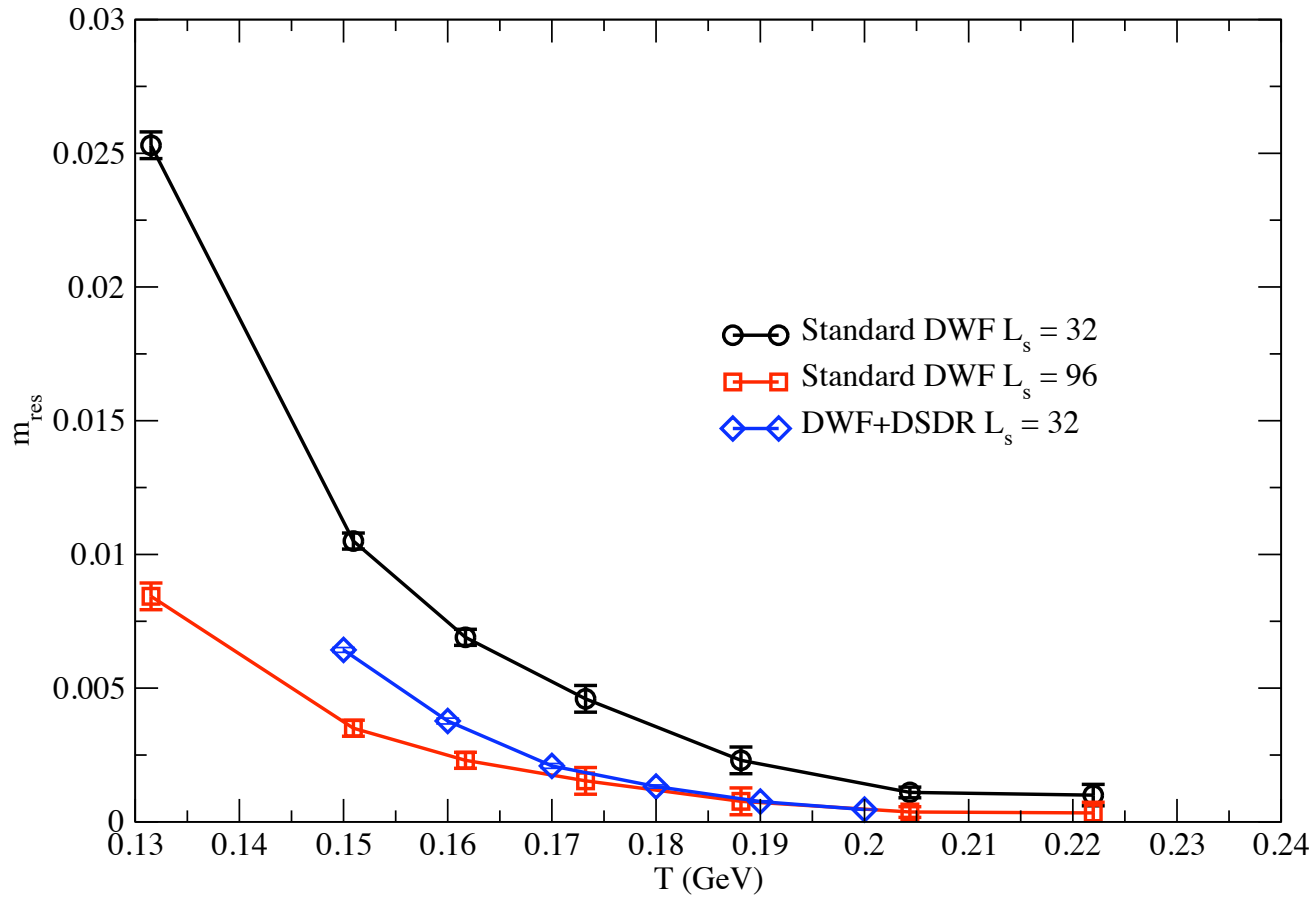
$$\gamma_5 D_W(-M_0)$$

# DSDR

- Dislocation Suppressing Determinant Ratio(DSDR).
- Introduce  $\det(D_W(-M_0))$  into fermion action (Vranas 2006, Fukaya *et. al.* 2006)
- Suppresses lattice dislocations that dominate  $m_{\text{res}}$  at coarse couplings.
- However, same modes responsible for topological change.
- Add extra weight factor:

$$\begin{aligned} \mathcal{W}(M_0, \epsilon_b, \epsilon_f) &= \frac{\det \left[ D_W^\dagger(-M_0 + 1\epsilon_b\gamma^5) D_W(-M_0 + 1\epsilon_b\gamma^5) \right]}{\det \left[ D_W^\dagger(-M_0 + 1\epsilon_f\gamma^5) D_W(-M_0 + 1\epsilon_f\gamma^5) \right]} \\ &= \frac{\det \left[ D_W^\dagger(-M_0) D_W(-M_0) + \epsilon_b^2 \right]}{\det \left[ D_W^\dagger(-M_0) D_W(-M_0) + \epsilon_f^2 \right]} \end{aligned}$$

# Residual Mass with DSDR



# Calculation Details

- $16^3 \times 8$  lattice volumes
- 7 temperature in the range  $T = 140 - 200$  MeV
- 3000-6000 HMC trajectories per temperature
- Temperatures fixed by zero-temperature calculations at three different bare couplings
- Adjust  $m_q$  so that  $m_\pi = 200$  MeV
- $m_s$  physical

# Screening Correlators

$$\begin{array}{ccc}
 \pi : \bar{\mathbf{q}} \gamma_5 \frac{\tau}{2} \mathbf{q} & \xleftrightarrow{\text{SU}(2)_L \times \text{SU}(2)_R} & \sigma : \bar{\mathbf{q}} \mathbf{q} \\
 \updownarrow \text{U}(1)_A & & \updownarrow \text{U}(1)_A \\
 \delta : \bar{\mathbf{q}} \frac{\tau}{2} \mathbf{q} & \xleftrightarrow{\text{SU}(2)_L \times \text{SU}(2)_R} & \eta' : \bar{\mathbf{q}} \gamma_5 \mathbf{q}
 \end{array}$$

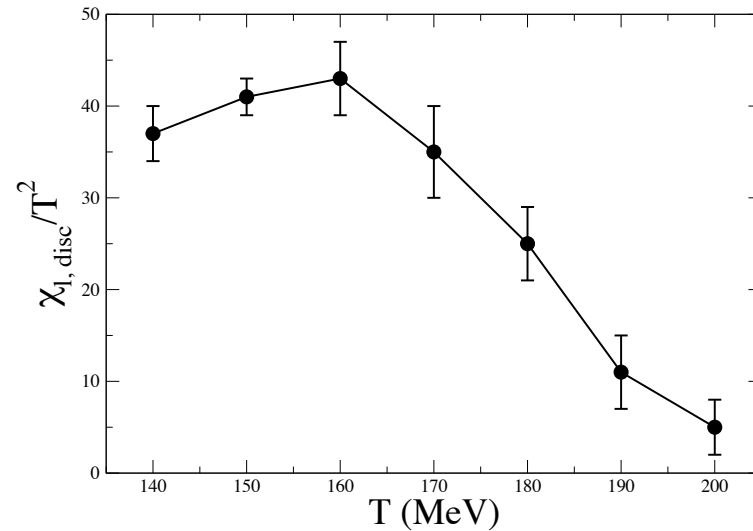
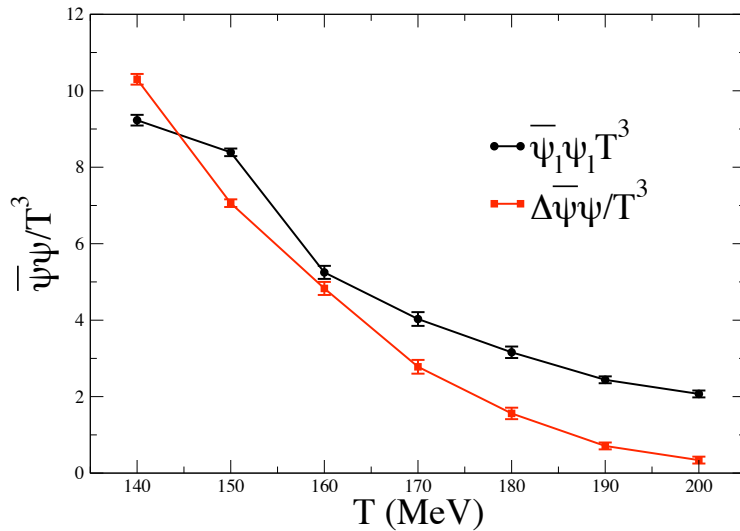
- Correlation functions in mesonic channels with propagation along spatial directions.
- Can be used to extract screening masses.
- Different channels related by chiral symmetry
- Can be used to examine  $\text{SU}(2)_L \times \text{SU}(2)_R$  or  $\text{U}(1)_A$  restoration in high temperature phase.

# Chiral Susceptibility and Chiral Condensate

$$\frac{\langle \bar{\psi}_q \psi_q \rangle}{T^3} = \frac{1}{VT^2} \frac{\partial \ln Z}{\partial m_q} = \frac{N_\tau^2}{N_\sigma^3} \langle \text{Tr} M_q^{-1} \rangle, \quad q = l, s.$$

$$\Delta_{l,s} = \langle \bar{\psi}_l \psi_l \rangle - m_l/m_s \langle \bar{\psi}_s \psi_s \rangle$$

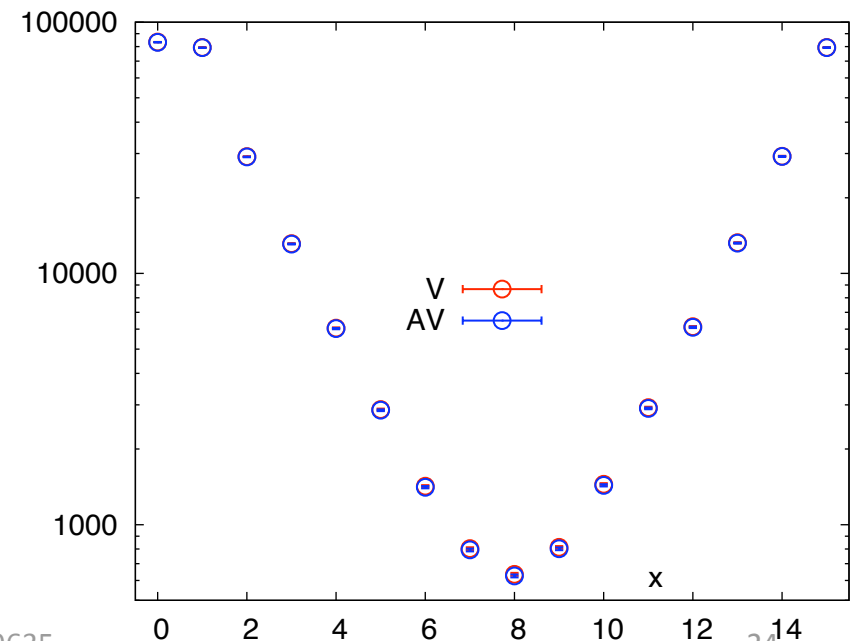
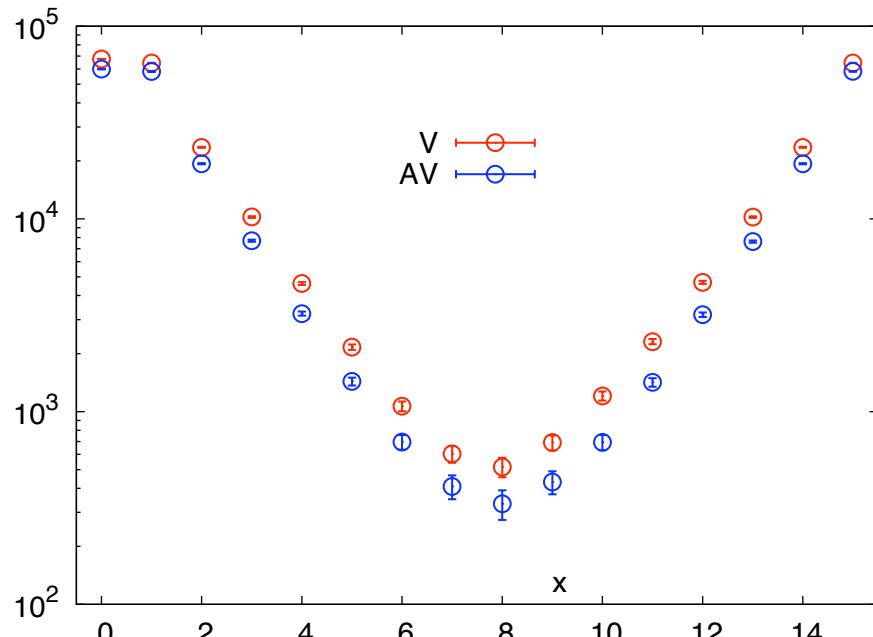
$$\chi_{l,disc} = \frac{1}{N_\sigma^3 N_\tau} \left\{ \langle (\text{Tr} M_l^{-1})^2 \rangle - \langle \text{Tr} M_l^{-1} \rangle^2 \right\}$$



# Vector/Axial Vector Correlators

Vector:  $\bar{q}\gamma^\mu q$

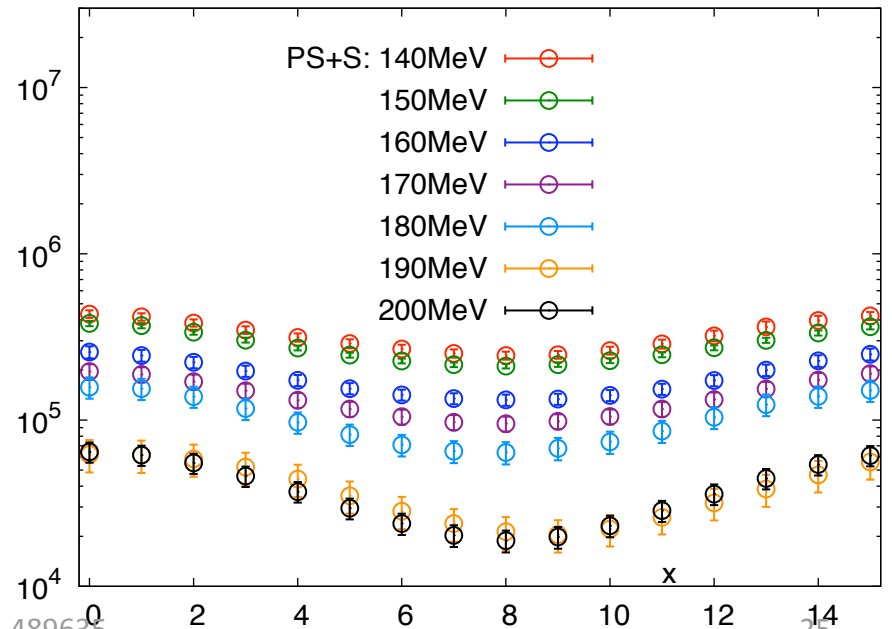
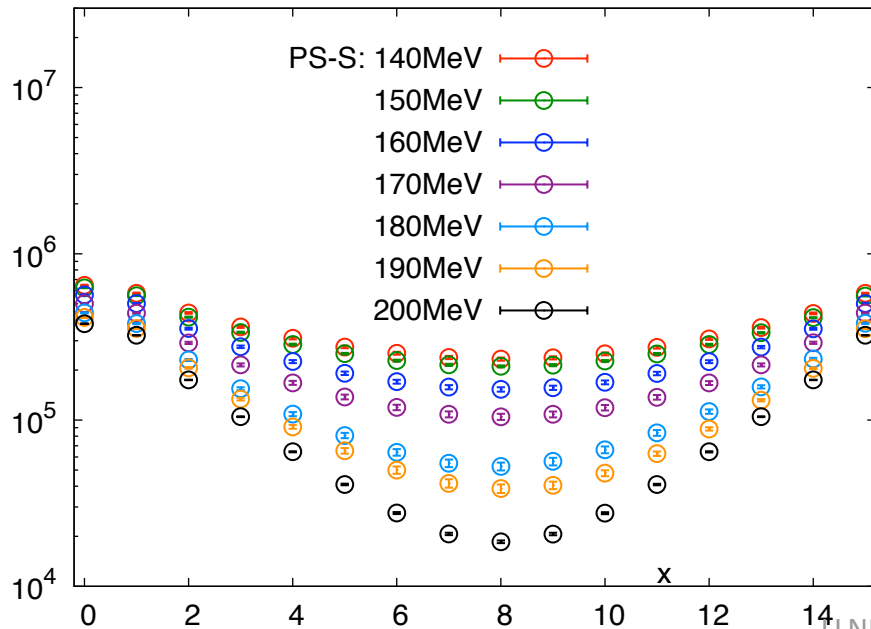
Axial Vector:  $\bar{q}\gamma^\mu\gamma^5 q$





# Scalar/Pseudoscalar Correlators

$$C_{SC(PS)}(x) = \langle \bar{u}_L d_R(x) \bar{d}_L u_R(0) + \bar{u}_L d_L(x) \bar{d}_L u_L(0) \rangle \pm \langle \bar{u}_L d_R(x) \bar{d}_R u_L(0) + \bar{u}_R d_L(x) \bar{d}_L u_R(0) \rangle.$$



# Susceptibilities

$$\frac{\chi_\sigma}{T^2} = \sum_{\vec{x}, \tau} G_\sigma(\tau, \vec{x}) = \frac{\chi_{l,con}}{T^2} + \frac{\chi_{l,disc}}{T^2}$$

$$\frac{\chi_\delta}{T^2} = \sum_{\vec{x}, \tau} G_\delta(\tau, \vec{x}) = \frac{\chi_{l,con}}{T^2}$$

$$\frac{\chi_\eta}{T^2} = \sum_{\vec{x}, \tau} G_\eta(\tau, \vec{x}) = \frac{\chi_{5,con}}{T^2} + \frac{\chi_{5,disc}}{T^2}$$

$$\frac{\chi_\pi}{T^2} = \sum_{\vec{x}, \tau} G_\delta(\tau, \vec{x}) = \frac{\chi_{5,con}}{T^2}$$

U(1)<sub>A</sub> restoration:

$$\Delta_{\pi-\delta} = \frac{\chi_\pi - \chi_\delta}{T^2}$$

$$= \frac{\chi_{5,conn} - \chi_{l,conn}}{T^2}$$

$$\lim_{m_q \rightarrow 0} \rightarrow \Delta_{\pi-\delta} = \frac{\chi_{l,disc}}{T^2} = \frac{\chi_{5,disc}}{T^2}$$

SU(2)<sub>L</sub> x SU(2)<sub>R</sub> restoration:

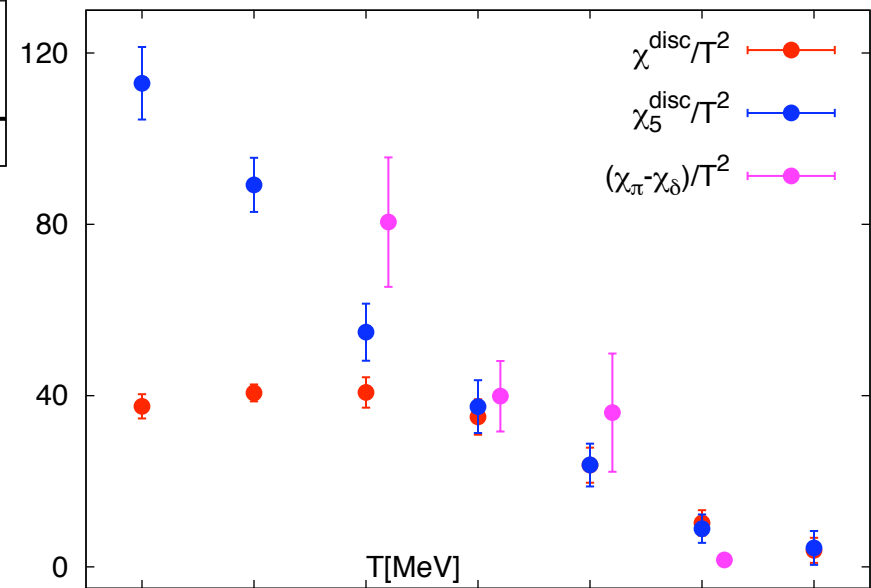
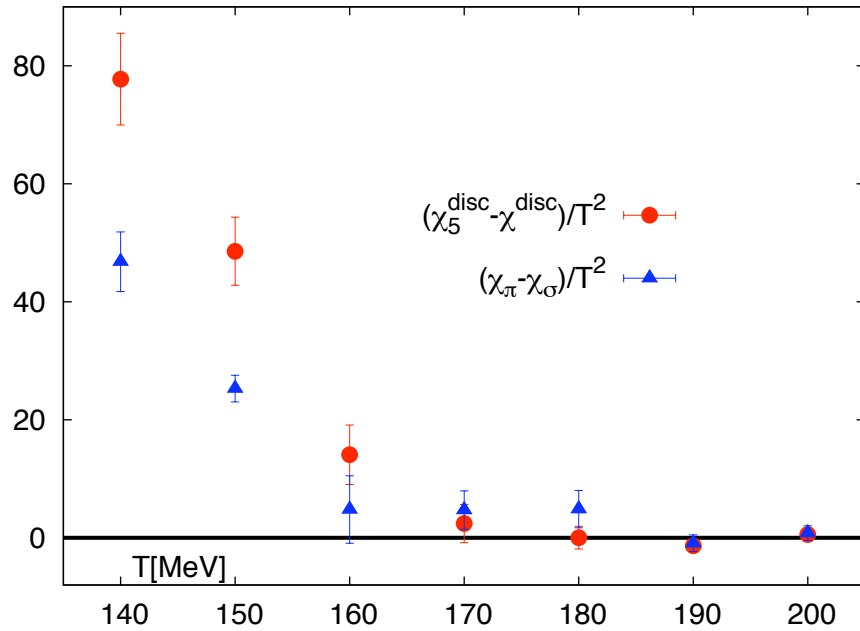
$$\chi_\pi = \chi_\sigma; \quad \chi_\eta = \chi_\delta$$

$$\Delta_{\pi-\sigma} = \frac{\chi_\pi - \chi_\sigma}{T^2} = \frac{\chi_{5,conn} - \chi_{l,disc} - \chi_{l,conn}}{T^2}$$

$$\Delta_{disc} = \frac{\chi_{5,disc} - \chi_{l,disc}}{T^2}$$

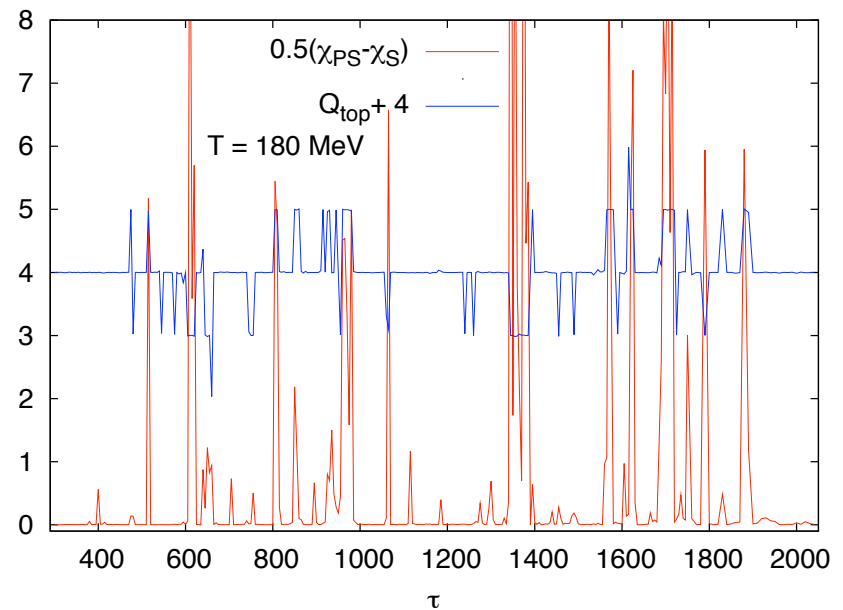
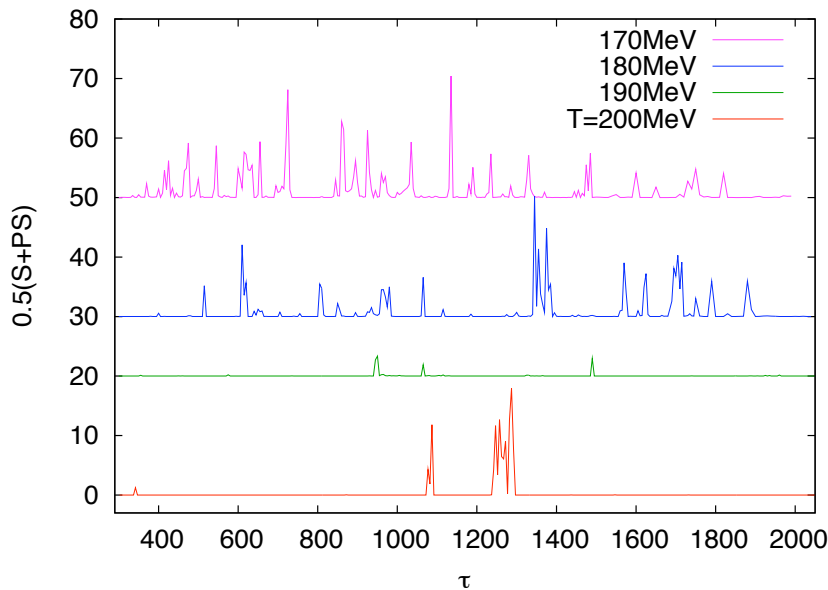
$$\lim_{m_q \rightarrow 0} \rightarrow \Delta_{\pi-\sigma} = \Delta_{disc} = 0$$

# Scalar/Pseudoscalar Susceptibilities



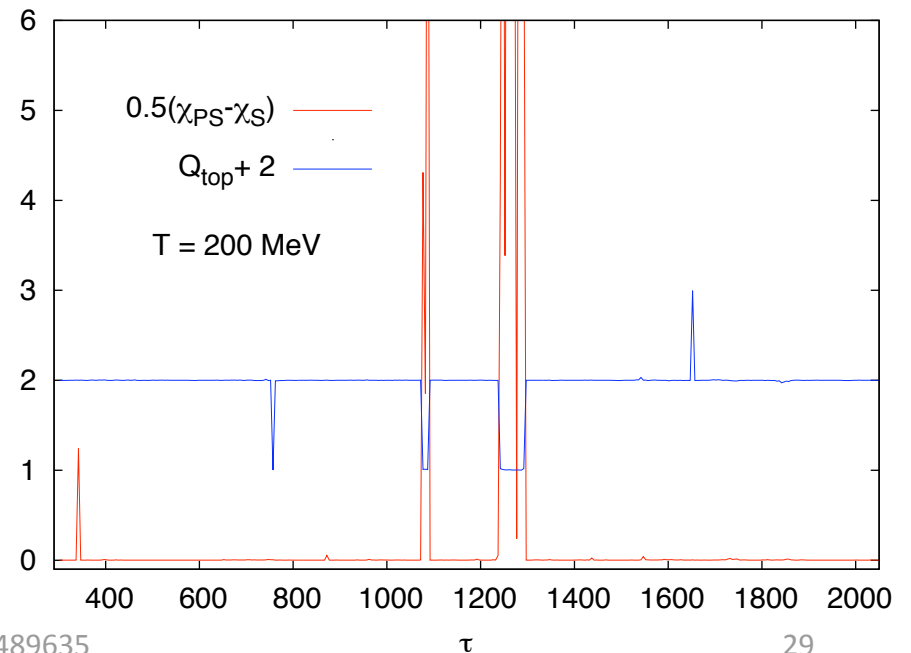
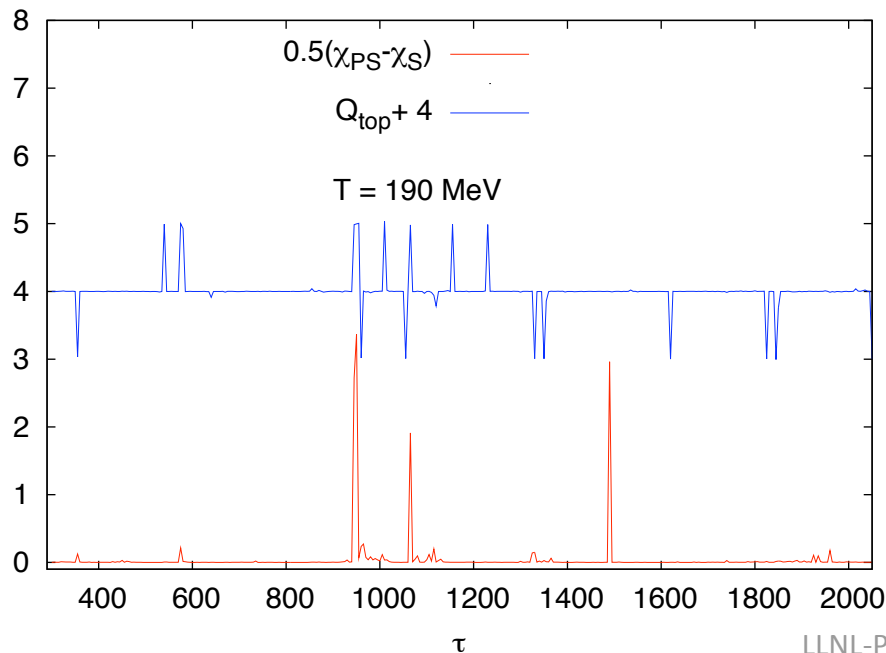
# Correlation to Topological Charge

- Contributions to  $U(1)_A$  breaking come seem to be highly correlated w/topological charge, *i.e.*  $U(1)_A$  breaking comes from objects with non-zero topology.



# Correlation to Topological Charge

- Topological susceptibility becomes smaller in the high temperature phase, *i.e.* object with non-zero topology are suppressed  $\rightarrow$  contributions to  $U(1)_A$  are smaller.



# Dirac Spectrum

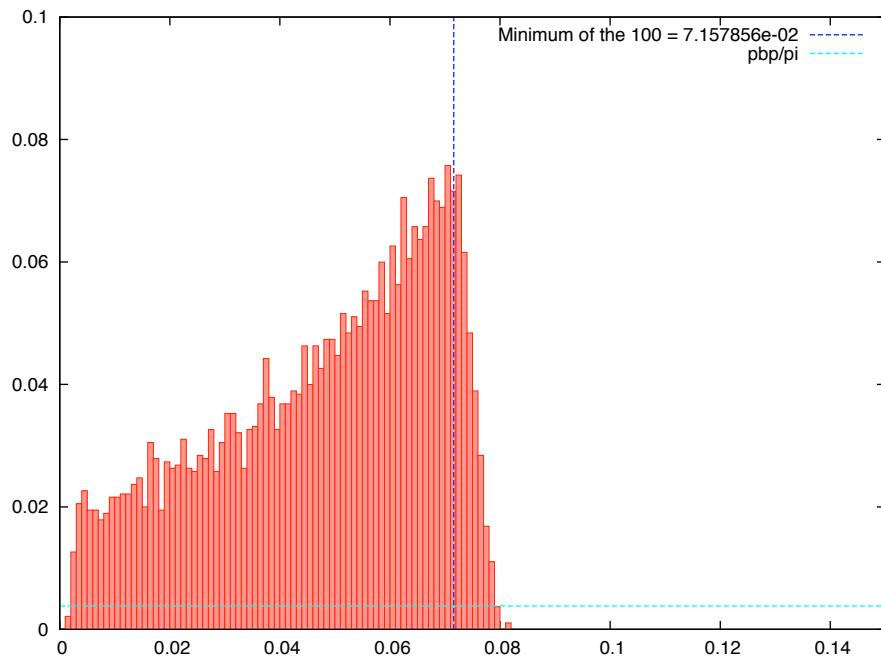
- Calculate low-lying eigenvalues of 5-D DWF operator.
- Lowest-lying modes correspond to 4-d modes bound to the wall.
- Connection between low modes of 5-d operator and 4-d low modes (needed for Casher-Banks) can be made via NPR.
- Modes with  $\lambda \sim m_q$  become zero modes relevant in the chiral limit.
- Can derive relation for  $\Delta_{\pi-\delta}$  in terms of  $\rho(\lambda)$  as well:

$$\Delta_{\pi-\delta} = \int d\lambda \rho(\lambda) \frac{4m_q^2}{(m_q^2 + \lambda^2)^2}$$

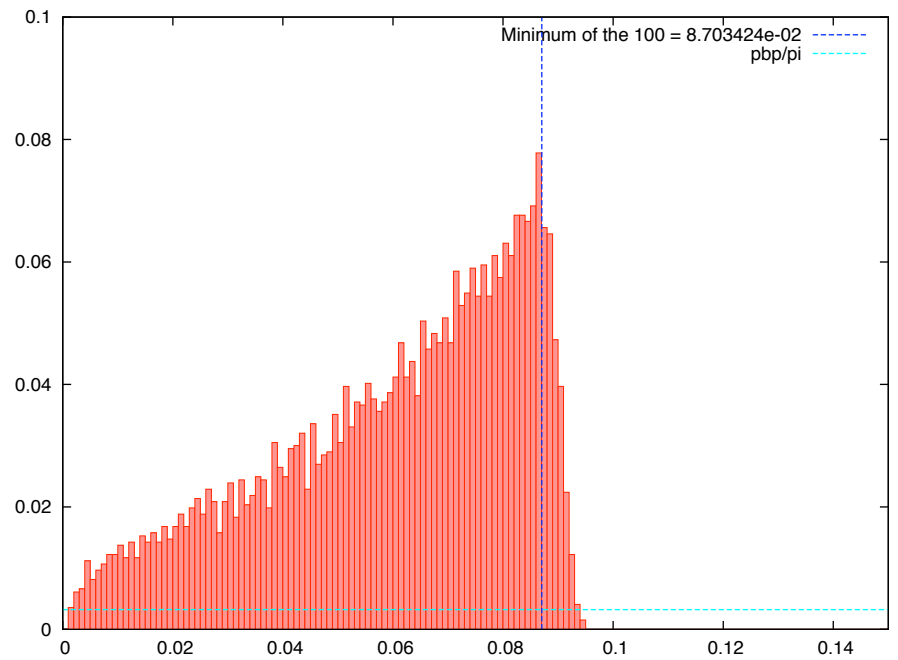
# Dirac Spectrum

Pileup of near-zero modes for  $T \leq T_c$

T = 150 MeV

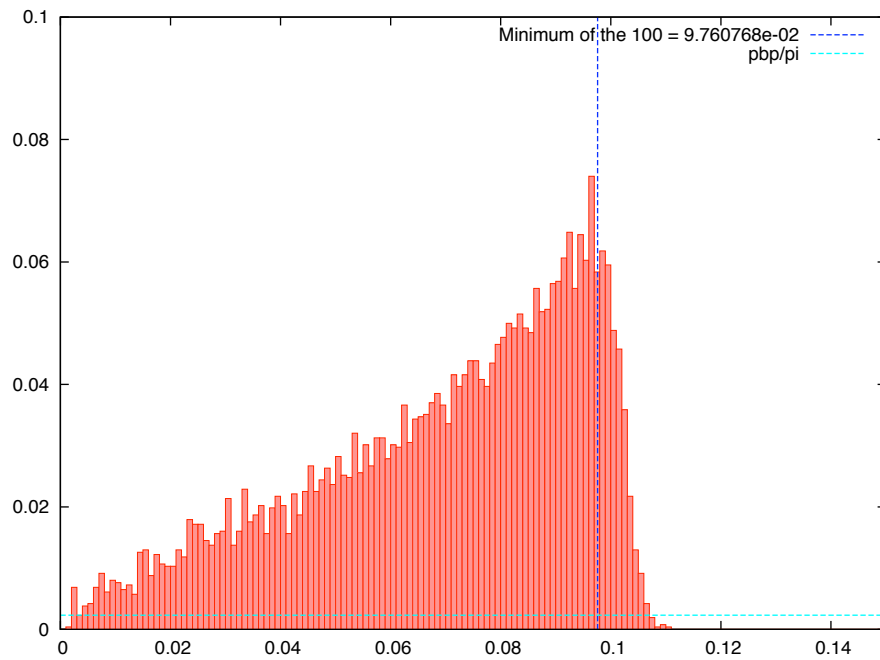


T = 160 MeV

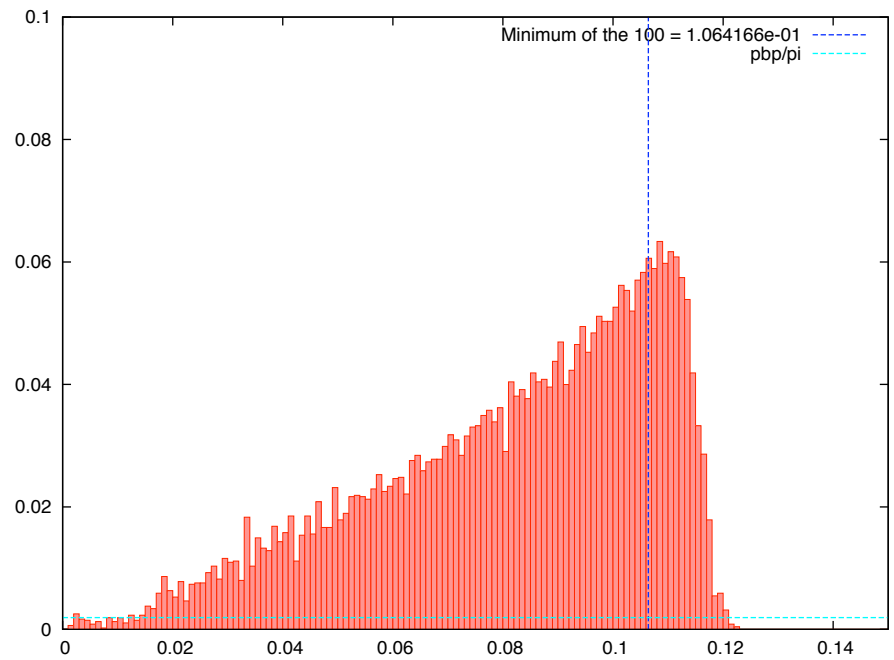


# Dirac Spectrum

T = 170 MeV



T = 180 MeV



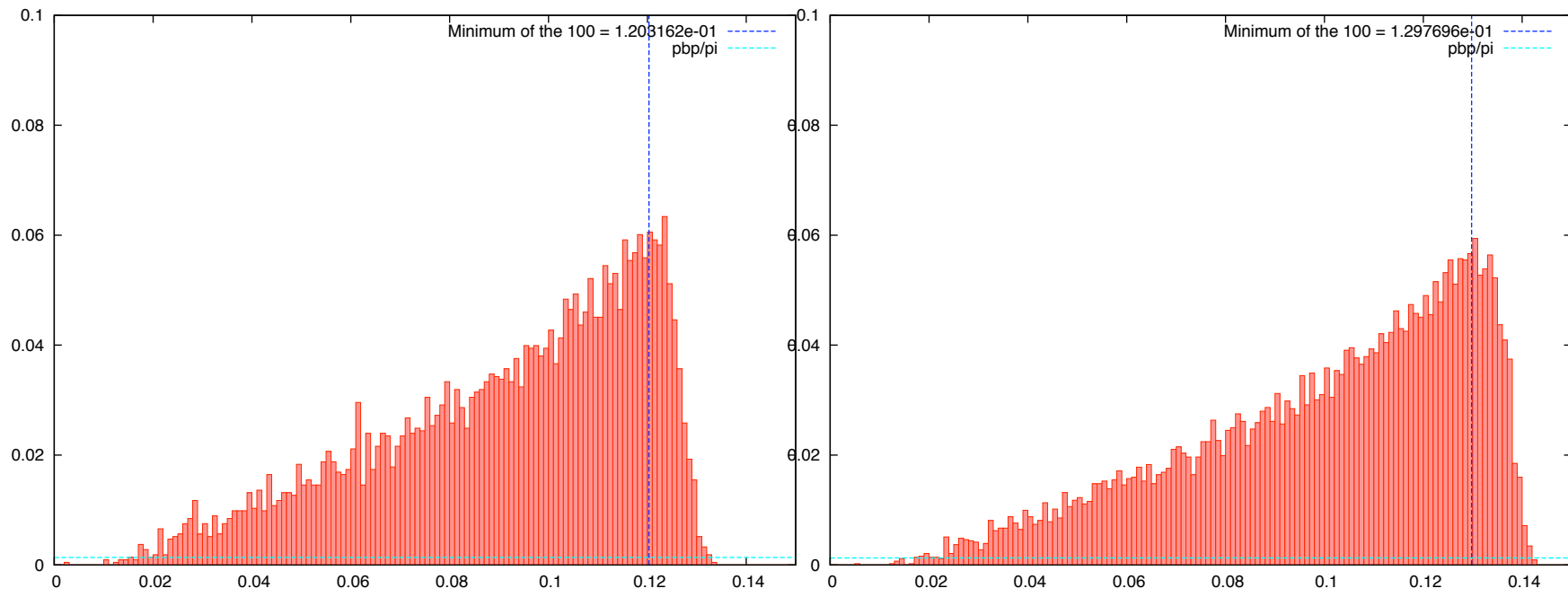


# Dirac Spectrum

Development of a gap near  $\lambda \approx 0$

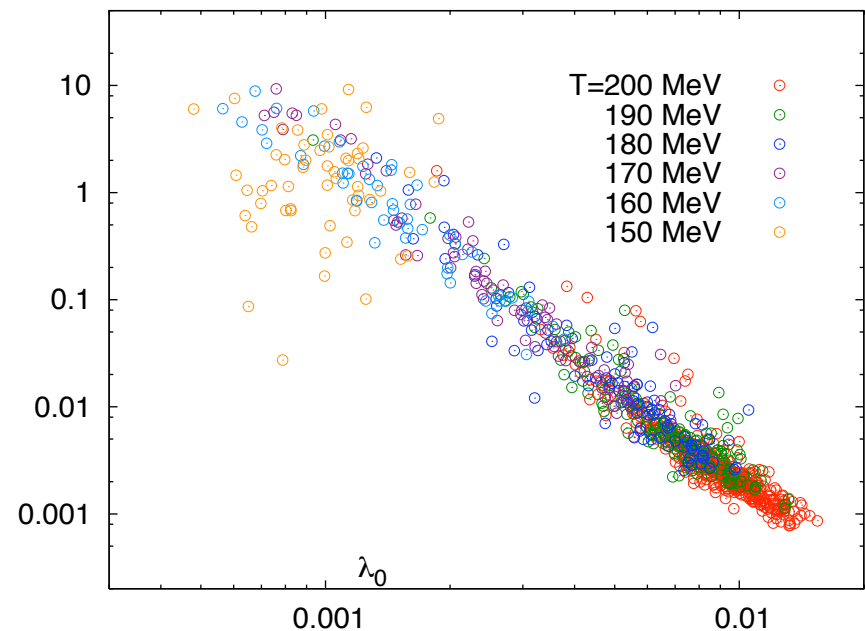
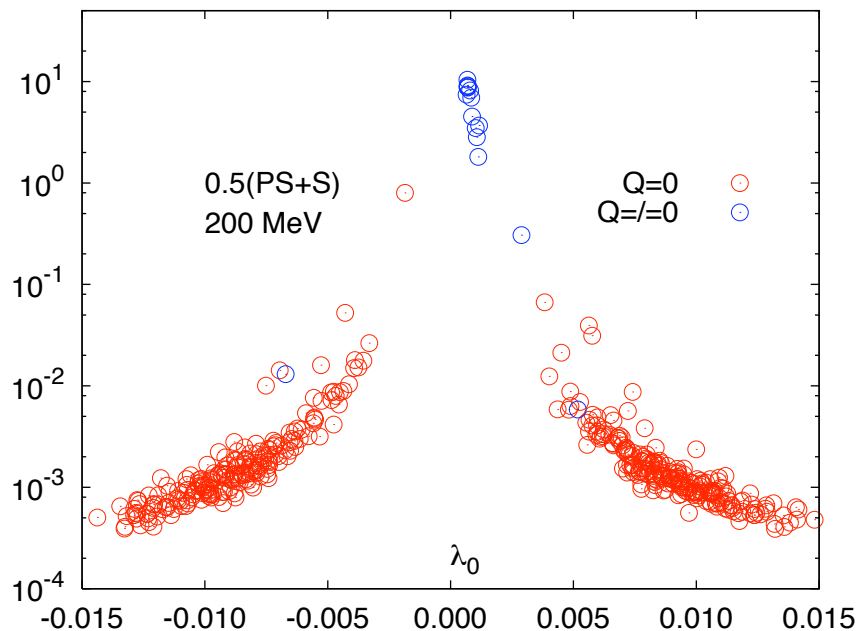
T = 190 MeV

T = 200 MeV



# Dirac Spectrum and $U(1)_A$

- Contributions to  $U(1)_A$  breaking come from configurations with small eigenvalues.
- Development of gap in eigenvalue spectrum: these contributions should disappear.



# Conclusions

- The restoration of  $SU(2)_L \times SU(2)_R$  has been heavily studied because of its direct relevance to heavy ion collisions.
- $T_c \approx 160 - 170$  MeV
- $U(1)_A$  for  $T \geq T_c$  less well understood.
- Calculation with chiral fermion formulation needed to clearly see connection between  $U(1)_A$  restoration, gauge field topology, low-lying eigenmodes of Dirac operator.
- $U(1)_A$  breaking terms in scalar/pseudoscalar correlators are still non-zero at  $T = T_c$
- However, development of gap in near-zero modes of eigenvalue spectrum suggest that  $U(1)_A$  may be restored in chiral limit.
- Larger volumes (ongoing), lighter mass?