Chiral Symmetry and Residual Mass in Lattice QCD with Domain-Wall Fermions

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"New Horizons for Lattice Computations with Chiral Fermions"
Brookhaven National Laboratory, USA
May 14-18, 2012

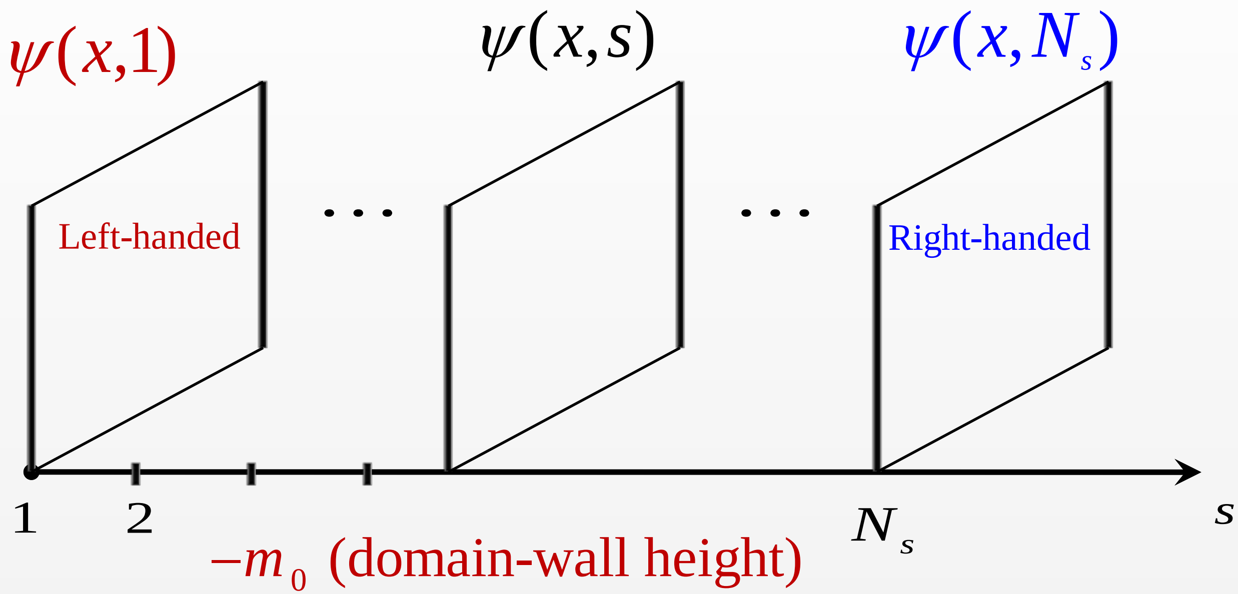
Outline

- Introduction
- Axial Ward Idenity in Lattice QCD with ODWF
- Generating Functional for n-point Green's Function
- A New Formula for the Residual Mass
- An Upper Bound for the Residual Mass
- Concluding Remarks

Reference:

Yu-Chih Chen, TWC, "Chiral Symmetry and Residual Mass in Lattice QCD with Optimal Domain-Wall Fermion", in preparation

Domain-Wall Fermions [Kaplan, 1992]



D_{dwf} is a local op. with the nearest neighbor coupling along $\hat{s}$

$$\int [d\bar{\psi}][d\psi] \exp\left(-\bar{\Psi} D_{\text{dwf}} \Psi\right) = \det D_c \qquad D_c = \frac{1+\gamma_5 S}{1-\gamma_5 S}$$

$$N_s \to \infty, \quad S \to \frac{H}{\sqrt{H^2}}, \qquad D_c \gamma_5 + \gamma_5 D_c = 0, \text{ Exact Chiral Sym.}$$

At finite N_s, S is not equal to the optimal rational approx.

Optimal Rational Approximation for Square Root

For the inverse square root function, the optimal rational approx. was obtained by Zolotarev in 1877.

$$\frac{1}{\sqrt{x}}, \quad x \in [1, b]$$

$$R_Z^{(n-1,n)}(x) = \frac{2\Lambda}{1+\Lambda}\frac{1}{M}\frac{\prod_{l=1}^{n-1}\left(1+x/C_{2l}\right)}{\prod_{l=1}^{n}\left(1+x/C_{2l-1}\right)}$$

$$R_Z^{(n,n)}(x) = \frac{2\lambda}{1+\lambda}\frac{1}{m}\frac{\prod_{l=1}^{n}\left(1+x/c_{2l}\right)}{\prod_{l=1}^{n}\left(1+x/c_{2l-1}\right)}$$

where $\lambda, \Lambda, m, M, C_{2l}, C_{2l-1}, c_{2l}, c_{2l-1}$

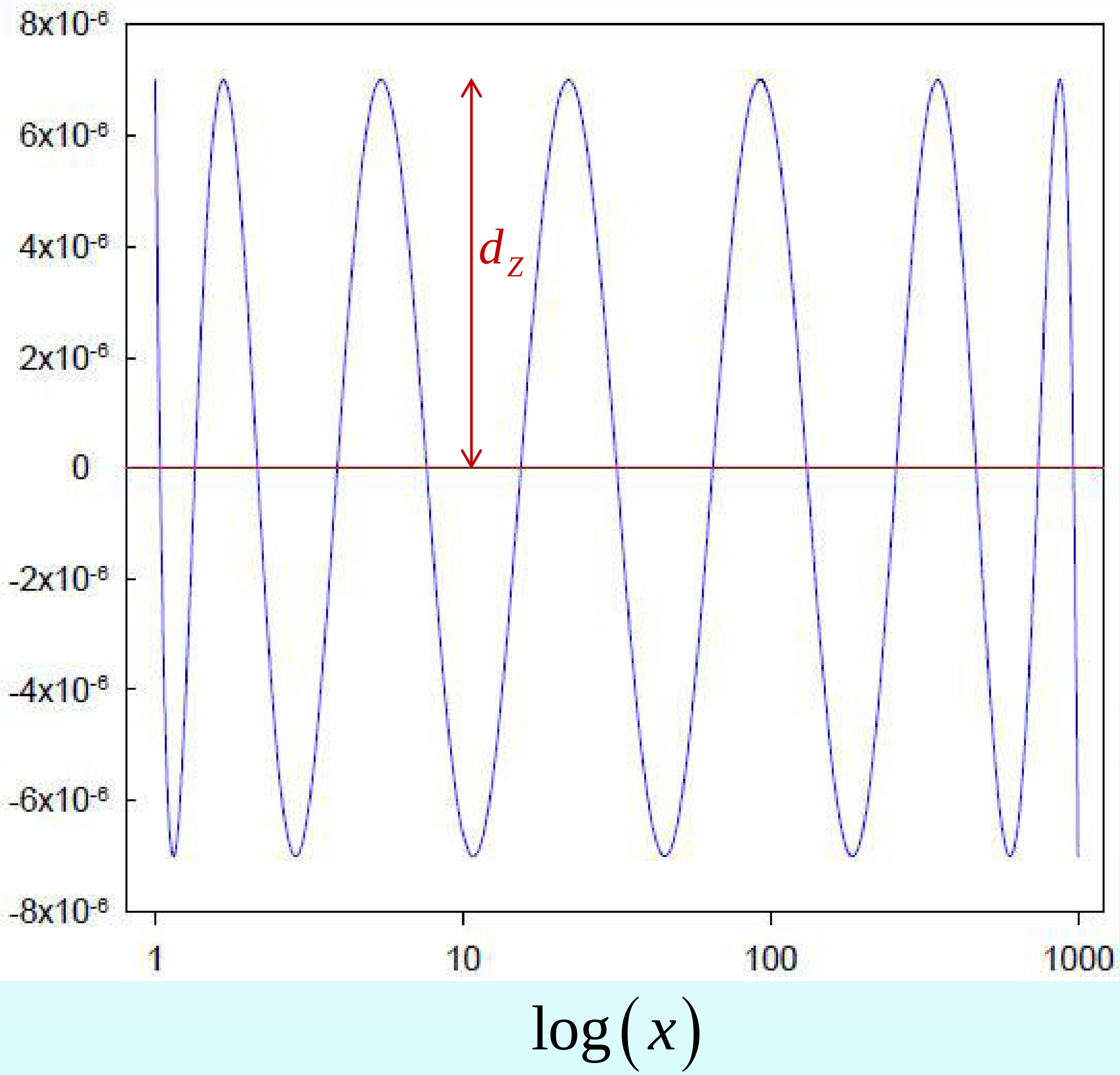
are expressed in terms of the

Jacobian Elliptic functions.

Yegor **I**vanovich **Zolotarev**
(1847 –1878)

Salient Feature of Optimal Rational Approximation

$$1-\sqrt{x}R_Z^{(n,m)}(x)$$



Has $(n+m+2)$ alternate change of sign in $[x_{\min}, x_{\max}]$, and attains its max. and min. (all with equal magnitude)

In the figure, $n = m = 6$ it has 14 alternate change of sign in [1,1000]

Optimal Domain-Wall Fermion

[TWC, Phys. Rev. Lett. 90 (2003) 071601]

$$A_{\text{odwf}} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\psi}_{x,s} \left[\left(I + \rho_s D_w \right)_{x,x'} \delta_{s,s'} - \left(I - \sigma_s D_w \right)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1} \right) \right] \psi_{x',s'}$$

$$\equiv \bar{\Psi} D_{\text{odwf}} \Psi$$

$$D_w = \sum_{\mu=1}^{4} \gamma_\mu t_\mu + W - m_0, \qquad m_0 \in (0,2)$$

$$t_\mu(x,x') = \frac{1}{2} \left[U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

$$W(x,x') = \sum_{\mu=1}^{4} \frac{1}{2} \left[2\delta_{x,x'} - U_\mu(x) \delta_{x',x+\mu} - U_\mu^\dagger(x') \delta_{x',x-\mu} \right]$$

with boundary conditions

$$P_+ \psi(x,0) = -r m_q P_+ \psi(x, N_s), \qquad m_q\text{: bare quark mass}$$

$$P_- \psi(x, N_s + 1) = -r m_q P_- \psi(x,1), \qquad P_\pm = \frac{1}{2}(1 \pm \gamma_5)$$

Optimal Domain-Wall Fermion (cont.)

The action for Pauli-Villars fields is similar to $A_{\rm odwf}$

$$A_{PV} = \sum_{s,s'=1}^{N_s} \sum_{x,x'} \bar{\phi}_{x,s} \left[\left(I + \rho_s D_w \right)_{x,x'} \delta_{s,s'} - \left(I - \sigma_s D_w \right)_{x,x'} \left(P_- \delta_{s',s+1} + P_+ \delta_{s',s-1} \right) \right] \phi_{x',s'}$$

but with boundary conditions: $P_+ \phi(x,0) = -P_+ \phi(x, N_s),$

$$P_- \phi(x, N_s + 1) = -P_- \phi(x,1)$$

- In the original formulation of ODWF, $\rho_s = \sigma_s = \omega_s$

$$\omega_s = \frac{1}{\lambda_{\min}} \sqrt{1 - \kappa'^2 sn^2(v_s; \kappa')}, \quad s = 1, \cdots, N_s$$

where $sn(v_s;\kappa')$ is the Jacobian elliptic function with argument v_s and modulus $\kappa' = \sqrt{1 - \lambda_{\min}^2 / \lambda_{\max}^2}$,
$\lambda_{\min}^2$ and $\lambda_{\max}^2$ are lower and upper bounds of the eigenvalues of H_w^2

Optimal Domain-Wall Fermion (cont.)

$$\int [d\bar{\psi}][d\psi]\left[d\bar{\phi}\right][d\phi]\exp\left(-A_{\text{odwf}} - A_{\text{PV}}\right) = \det D(m_q)$$

The effective 4D Dirac operator

$$D(m_q) = m_q + \left(m_0 - m_q/2\right)\left[1 + \gamma_5 S_{opt}\left(H_w\right)\right]$$

$$S_{opt}\left(H_w\right) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1 - \omega_s H_w}{1 + \omega_s H_w}$$

$$= \begin{cases} H_w R_Z^{(n-1,n)}\left(H_w^2\right), & N_s = 2n \\ H_w R_Z^{(n,n)}\left(H_w^2\right), & N_s = 2n+1 \end{cases}$$

Zolotarev optimal rational approximation for $\dfrac{1}{\sqrt{H_w^2}}$

Optimal Domain-Wall Fermion (cont.)

- For $\rho_s = c\omega_s + d,\ \sigma_s = c\omega_s - d, \quad c, d$ (constants)

  The effective 4D Dirac operator becomes

$$D(m_q) = m_q + \left(m_0(1 - d m_0) - \frac{m_q}{2} \right) \left[1 + \gamma_5 S_{opt}(H) \right], \quad H = \frac{cH_w}{1 + d\gamma_5 H_w}$$

$$S_{opt}(H) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s}, \quad T_s = \frac{1 - \omega_s H}{1 + \omega_s H}$$

only $d = 0$ is good for the projection of low-modes of $D(0)$

$$= \begin{cases} H R_Z^{(n-1,n)}(H^2), & N_s = 2n \\ H R_Z^{(n,n)}(H^2), & N_s = 2n+1 \end{cases}$$

Optimal Domain-Wall Fermion (cont.)

➢ For the special case $\rho_s = 1,\ \sigma_s = 0$

It reduces to the conventional DWF which does not have the optimal chiral symmetry.

$$D(m_q) = m_q + \left(\frac{m_0}{2}(2-m_0) - \frac{m_q}{2} \right) \left[1 + \gamma_5 S_{\text{polar}}(H) \right], \quad H = \frac{H_w}{2+\gamma_5 H_w}$$

$$S_{\text{polar}}(H) = \frac{1-T^{N_s}}{1+T^{N_s}}, \qquad T = \frac{1-H}{1+H}$$

$$b_l = \sec^2\left[\frac{\pi}{N_s}\left(l - \frac{1}{2} \right) \right]$$

$$d_l = \tan^2\left[\frac{\pi}{N_s}\left(l - \frac{1}{2} \right) \right]$$

$$= \begin{cases} H\left(\dfrac{2}{N_s} \displaystyle\sum_{l=1}^{n} \frac{b_l}{H^2 + d_l} \right), & N_s = 2n \\ H\left(\dfrac{1}{N_s} + \dfrac{2}{N_s} \displaystyle\sum_{l=1}^{n} \frac{b_l}{H^2 + d_l} \right), & N_s = 2n+1 \end{cases}$$

Polar approximation

Axial Ward Idenity in Lattice QCD with ODWF

$$\mathcal{A}_f = \sum_{s,s'=0}^{N_s+3} \sum_{x,x'} \bar{\psi}_s(x) \{ (\rho_s D_w + \mathbb{1})_{x,x'} \delta_{s,s'} + (\sigma_s D_w - \mathbb{1})_{x,x'} (P_- \delta_{s',s+1} + P_+ \delta_{s',s-1}) \} \psi_{s'}(x').$$

with boundary conditions

$$P_+ \psi(x,-1) = -r m_q P_+ \psi(x, N_s+3),$$

$$P_- \psi(x, N_s+4) = -r m_q P_- \psi(x, 0),$$

Transparent layers:

[TWC, hep-lat/0303008]

$$\rho_0 = \rho_{N_s+3} = \sigma_0 = \sigma_{N_s+3} = 0$$

$$\rho_n = \rho_{n+1} = \sigma_n = \sigma_{n+1} = 0 \qquad n = [N_s/2]$$

The quark fields are defined in terms of the boundary modes

$$q(x) = \sqrt{r} \left[P_- \psi_0(x) + P_+ \psi_{N_s+3}(x) \right],$$

$$\bar{q}(x) = \sqrt{r} \left[\bar{\psi}_0(x) P_+ + \bar{\psi}_{N_s+3}(x) P_- \right].$$

Axial Ward Idenity (cont.)

Now we consider N_f flavors of quarks with degenerate mass m_q, and the infinitesimal flavor non-singlet transformation

$$\delta \psi_s(x) = i\theta_s(x)\lambda^a \psi_s(x)$$

$$\delta \bar{\psi}_s(x) = -i\theta_s(x)\lambda^a \bar{\psi}_s(x)$$

$$\theta_s(x) = \begin{cases} \theta(x), & 0 \le s \le n, \quad n \equiv \left[\frac{N_s}{2}\right], \\ -\theta(x), & n+1 \le s \le N_s + 3. \end{cases}$$

Here λ^a is one of the flavor group generators in the fundamental representation

$$\delta \sum_{s=0}^{N_s+3} \sum_{x,y} \rho_s \left[\bar{\psi}_s(x)\lambda^a D_w(x,y)\psi_s(y)\right] = \sum_x i\theta(x) \sum_\mu \Delta_\mu \hat{j}^a_\mu(x)$$

$$\delta \sum_{s=0}^{N_s+3} [-\bar{\psi}_s(x)\lambda^a P_- \psi_{s+1}(x) - \bar{\psi}_s(x)\lambda^a P_+ \psi_{s-1}(x)] = -\sum_x 2i\theta(x)[J^a_5(x,n) + m_q \bar{q}(x)\lambda^a \gamma_5 q(x)]$$

$$\delta \sum_{s=0}^{N_s+3} \sum_{x,y} \sigma_s \{\bar{\psi}_s(x)\lambda^a D_w(x,y)[P_- \psi_{s+1}(y) + P_+ \psi_{s-1}(y)]\} = \sum_x i\theta(x) \sum_\mu \Delta_\mu \hat{k}^a_\mu(x)$$

Axial Ward Idenity (cont.)

$$J_5^a(x,n) = -\bar{\psi}_n(x)\lambda^a P_- \psi_{n+1}(x) + \bar{\psi}_{n+1}(x)\lambda^a P_+ \psi_n(x)$$

$$\hat{j}_\mu^a(x) \equiv \sum_{s=1}^{N_s+2} \text{sign}\left(n - s + \frac{1}{2}\right) j_\mu^a(x,s)$$

$$j_\mu^a(x,s) = \frac{\rho_s}{2}\left[\bar{\psi}_s(x)\lambda^a(1-\gamma_\mu)U_\mu(x)\psi_s(x+\mu) - \bar{\psi}_s(x+\mu)\lambda^a(1+\gamma_\mu)U_\mu^\dagger(x)\psi_s(x)\right]$$

$$\hat{k}_\mu^a(x) \equiv \hat{k}_\mu^{a+}(x) + \hat{k}_\mu^{a-}(x),$$

$$\hat{k}_\mu^{a\pm}(x) \equiv \sum_{s=1}^{N_s+2} \text{sign}\left(n - s + \frac{1}{2}\right) k_\mu^{a\pm}(x,s)$$

$$k_\mu^{a\pm}(x,s) = \frac{\sigma_s}{2}\left[\bar{\psi}_s(x)\lambda^a(1-\gamma_\mu)U_\mu(x)P_\pm\psi_{s\mp1}(x+\mu) - \bar{\psi}_s(x+\mu)\lambda^a(1+\gamma_\mu)U_\mu^\dagger(x)P_\pm\psi_{s\mp1}(x)\right]$$

$$J_\mu^a(x) \equiv \hat{k}_\mu^a(x) + \hat{j}_\mu^a(x)$$

$$\Delta_\mu f(x,s) \equiv f(x,s) - f(x-\mu,s)$$

Axial Ward Idenity (cont.)

For any observable $\mathcal{O}$, $\delta^a \langle \mathcal{O} \rangle = 0$, which gives the axial Ward identity

$$\Delta_\mu \langle J_\mu^a(x) \mathcal{O}(y) \rangle = 2m_q \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle + 2\langle J_5^a(x,n) \mathcal{O}(y) \rangle + i \langle \delta^a \mathcal{O}(y) \rangle$$

As $N_s \to \infty$, the anomalous term $\langle J_5^a(x,n) \mathcal{O}(y) \rangle$ vanishes if $\mathcal{O}(y)$ only involves the quark fields [Furman & Shamir, 1995]

After summing over all sites x

$$-i \sum_x \langle \delta^a \mathcal{O}(y) \rangle = 2m_q \sum_x \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle + 2 \sum_x \langle J_5^a(x,n) \mathcal{O}(y) \rangle$$

Thus, the effect of chiral symmetry breaking due to finite N_s can be regarded as an additive mass to the bare quark mass m_q, the so-called residual mass

$$m_{res}[\mathcal{O}(y)] = \frac{\sum_x \langle J_5^a(x,n) \mathcal{O}(y) \rangle}{\sum_x \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle}$$

dependent on O, and y

Axial Ward Idenity (cont.)

Summing over all sites y in the AWI gives the global residual mass

$$M_{res}[\mathcal{O}] = \frac{\sum_{x,y} \langle J_5^a(x,n) \mathcal{O}(y) \rangle}{\sum_{x,y} \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \mathcal{O}(y) \rangle}$$

For $\mathcal{O}(y) = \bar{q}(y) \lambda^b \gamma_5 q(y)$ pseudoscalar

$$m_{res}(y) = \frac{\sum_{x} \langle J_5^a(x,n) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}{\sum_{x} \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}$$ local

$$M_{res} = \frac{\sum_{x,y} \langle J_5^a(x,n) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}{\sum_{x,y} \langle \bar{q}(x) \lambda^a \gamma_5 q(x) \bar{q}(y) \lambda^b \gamma_5 q(y) \rangle}$$ global

which are usually used as a measure of the chiral symmetry breaking due to finite N_s

Generating Functional for n-point Green's Function

Use the transformation

$$\eta_s = (P_-\delta_{s',s} + P_+\delta_{s',s-1})\psi_{s'} \Leftrightarrow \psi_s = (P_-\delta_{s',s} + P_+\delta_{s',s+1})\eta_{s'}$$

$$\bar{\eta}_s = \bar{\psi}_s\gamma_5 Q_-^s \Leftrightarrow \bar{\psi}_s = \bar{\eta}_s (Q_-^s)^{-1}\gamma_5$$

$$Q_\pm^s \equiv \rho_s H_w P_\pm + \sigma_s H_w P_\mp \pm 1$$

$$T_s = -(Q_+^s)^{-1} Q_-^s = \frac{1 - H_s}{1 + H_s}$$

$$H_s = (\rho_s + \sigma_s) H_w [2 + (\rho_s - \sigma_s)\gamma_5 H_w]^{-1}$$

$$\begin{aligned} \mathcal{A}_f &= \bar{\eta}_0 (P_- - r m_q P_+)\eta_0 - \bar{\eta}_0\eta_0 + \sum_{s=1}^{N_s+2} [\bar{\eta}_s\eta_s - \bar{\eta}_s T_s^{-1}\eta_{s+1}] \\ &\quad + \bar{\eta}_{N_s+3}\eta_{N_s+3} - \bar{\eta}_{N_s+3}(P_+ - r m_q P_-)\eta_0, \end{aligned}$$

Generating Functional (cont.)

Including external sources

$$\bar{\eta}_n J_n + \bar{J}_{n+1}\eta_{n+1} + \bar{\eta}_{n+1} J_{n+1},$$

$$\bar{J}_q q + \bar{q} J_q = \bar{J}\eta_0 - \bar{\eta}_0 P_+ J + \bar{\eta}_{N_s+3} P_- J,$$

$$J \equiv \sqrt{r} J_q$$

$$\bar{J} \equiv \sqrt{r} \bar{J}_q$$

$$Z[J_q, \bar{J}_q, J_n, J_{n+1}, \bar{J}_{n+1}] = \mathcal{J} \int [d\bar{\eta}][d\eta] e^{-S_J}$$

$$S_J = A_f - \bar{J}\eta_0 + \bar{\eta}_0 P_+ J - \bar{\eta}_n J_n - \bar{J}_{n+1}\eta_{n+1} - \bar{\eta}_{n+1} J_{n+1} - \bar{\eta}_{N_s+3} P_- J$$

$\mathcal{J}$ is the Jacobian of the transformation

$$\mathcal{J} = \prod_{s=0}^{N_s+3} \det[\gamma_5(\rho_s H_w P_- + \sigma_s H_w P_+ - 1)]$$

Generating Functional (cont.)

Integrating $(\eta_s, \bar{\eta}_s)$ successively from $s = N_s + 3$ to $s = 0$:

$$Z[J_q, \bar{J}_q, J_n, J_{n+1}, \bar{J}_{n+1}]$$

$$= K \det[r(D_c + m_q)] \exp\left\{ \bar{J}_{n+1} T_U^{-1} P_- J + \bar{J}_{n+1} J_{n+1} + \right.$$
$$\left. + \left[\bar{J} + \bar{J}_{n+1} T_U^{-1}(P_+ - r m_q P_-)\right] (r D_c + r m_q)^{-1} \left[J + \widehat{T}^{-1} J_n + \widehat{T}^{-1} J_{n+1} \right] \right\}$$

$$T_L^{-1} \equiv \prod_{s=1}^{n} T_s^{-1}$$

$$T_U^{-1} \equiv \prod_{s=n+1}^{N_s+2} T_s^{-1}$$

$$T^{-1} \equiv \prod_{s=1}^{N_s+2} T_s^{-1} = T_L^{-1} T_U^{-1}$$

$$\widehat{T}^{-1} \equiv \left(-P_+ + T^{-1} P_-\right)^{-1} T_L^{-1}$$

$$K \equiv \mathcal{J} \det\left[-P_+ + T^{-1} P_-\right]$$

$$D_c = \frac{1}{r} \frac{1 + \gamma_5 S}{1 - \gamma_5 S}$$

$$S = \frac{1 - \prod_{s=0}^{N_s+3} T_s}{1 + \prod_{s=0}^{N_s+3} T_s}$$

$$T_s = \frac{1 - H_s}{1 + H_s}$$

$$H_s = (\rho_s + \sigma_s) H_w [2 + (\rho_s - \sigma_s)\gamma_5 H_w]^{-1}$$

Generating Functional (cont.)

(I) The valence quark propagator

$$\langle q(x)\bar{q}(y)\rangle = -\frac{1}{Z}\frac{\delta^2 Z}{\delta \bar{J}_q(x)\delta J_q(y)}\bigg|_0 = (D_c + m_q)^{-1}(x,y)$$

(II) The mixed correlator of the first kind

$$\begin{aligned}\langle q(x)\bar{\eta}_n(y)\rangle &= -\frac{1}{Z}\frac{\delta^2 Z}{\delta \bar{J}_q(x)\delta J_n(y)}\bigg|_0 \\ &= \sqrt{r}(rD_c + rm_q)^{-1}\left(-P_+ + T^{-1}P_-\right)^{-1} T_L^{-1} \\ &= -\frac{1}{\sqrt{r}} D^{-1}(m_q)\gamma_5 \frac{T_L^{-1}}{T^{-1}+1}\end{aligned}$$

$$D^{-1}(m_q) = (1 + rD_c)(D_c + m_q)^{-1} = r + (1 - rm_q)(D_c + m_q)^{-1}$$

the sea quark propagator

Generating Functional (cont.)

(III) The mixed correlator of the second kind

$$
\begin{aligned}
\langle q(x)\bar{\eta}_{n+1}(y)\rangle &= -\frac{1}{Z}\frac{\delta^2 Z}{\delta \bar{J}_q(x)\delta J_{n+1}(y)}\bigg|_0 \\
&= \sqrt{r}(rD_c + rm_q)^{-1}\left(-P_+ + T^{-1}P_-\right)^{-1} T_L^{-1} \\
&= -\frac{1}{\sqrt{r}} D^{-1}(m_q)\gamma_5 \frac{T_L^{-1}}{T^{-1}+1} = \langle q(x)\bar{\eta}_n(y)\rangle .
\end{aligned}
$$

(IV) The mixed correlator of the third kind

$$
\begin{aligned}
\langle \eta_{n+1}(x)\bar{q}(y)\rangle &= -\frac{1}{Z}\frac{\delta^2 Z}{\delta \bar{J}_{n+1}(x)\delta J_q(y)}\bigg|_0 \\
&= T_U^{-1}(-rm_q P_- + P_+)(rD_c + rm_q)^{-1}\sqrt{r} + T_U^{-1} P_- \sqrt{r} \\
&= T_U^{-1}\frac{1}{2\sqrt{r}}\left(1 + \frac{1+rm_q}{1-rm_q}\gamma_5\right) D^{-1}(m_q) - \frac{\sqrt{r}}{1-rm_q} T_U^{-1}\gamma_5
\end{aligned}
$$

A New Formula for the Residual Mass

$$m_{res}(y) = \frac{\sum_x \langle J_5^a(x,n)\bar{q}(y)\lambda^b\gamma_5 q(y)\rangle}{\sum_x \langle \bar{q}(x)\lambda^a\gamma_5 q(x)\bar{q}(y)\lambda^b\gamma_5 q(y)\rangle}$$

$$\sum_x \langle \bar{q}(x)\lambda^a\gamma_5 q(x)\bar{q}(y)\lambda^b\gamma_5 q(y)\rangle$$
$$= -\mathrm{tr}_F(\lambda^a\lambda^b)\mathrm{tr}_{DC}\{[(D_c+m_q)^{-1}]^\dagger (D_c+m_q)^{-1}\}(y,y)$$

$$\sum_x \langle J_5^a(x,n)\bar{q}(y)\lambda^b\gamma_5 q(y)\rangle \qquad \boxed{J_5^a(x,n) = -\bar{\psi}_n(x)\lambda^a P_- \psi_{n+1}(x) + \bar{\psi}_{n+1}(x)\lambda^a P_+ \psi_n(x)}$$

$$= \mathrm{tr}(\lambda^a\lambda^b)\left\{\sum_x \mathrm{tr}[\langle q(y)\bar{\psi}_n(x)\rangle P_- \langle \psi_{n+1}(x)\bar{q}(y)\rangle\gamma_5] - \sum_x \mathrm{tr}[\langle q(y)\bar{\psi}_{n+1}(x)\rangle P_+ \langle \psi_n(x)\bar{q}(y)\rangle\gamma_5]\right\}$$

$$= \mathrm{tr}(\lambda^a\lambda^b)\sum_x \mathrm{tr}[\langle q(y)\bar{\eta}_n(x)\rangle\langle \eta_{n+1}(x)\bar{q}(y)\gamma_5\rangle]$$

$$= -\mathrm{tr}(\lambda^a\lambda^b)\frac{1}{4r}\mathrm{tr}\{[D^{-1}(m_q)]^\dagger(1-S^2)D^{-1}(m_q)](y,y)$$

A New Formula for the Residual Mass

$$m_{res}(y) = \frac{\sum_x \langle J_5^a(x,n)\bar{q}(y)\lambda^b\gamma_5 q(y)\rangle}{\sum_x \langle \bar{q}(x)\lambda^a\gamma_5 q(x)\bar{q}(y)\lambda^b\gamma_5 q(y)\rangle}$$

$$= \frac{1}{4r}\frac{\mathrm{tr}\{[D^{-1}(m_q)]^\dagger(1-S^2)D^{-1}(m_q)\}(y,y)}{\mathrm{tr}\{[(D_c+m_q)^{-1}]^\dagger(D_c+m_q)^{-1}\}(y,y)}$$

$D^{-1}(m_q) = r + (1 - rm_q)(D_c + m_q)^{-1}$: sea quark propagator

$(D_c + m_q)^{-1}$: valence quark propagator

$$M_{res} = \frac{1}{4r}\frac{\mathrm{Tr}\{[D^{-1}(m_q)]^\dagger(1-S^2)D^{-1}(m_q)\}}{\mathrm{Tr}\{[(D_c+m_q)^{-1}]^\dagger(D_c+m_q)^{-1}\}}$$

However, it is tedious to use these formulas to compute the residual mass since they involve the multiplication of

$$S = (1 - \prod_s T_s)(1 + \prod_s T_s)^{-1} = H\sum_{i=1}^{n} b_i(H^2 + d_i)^{-1}$$

to the columns of the sea-quark propagator, requiring multi-shift CG.

A New Formula for the Residual Mass (cont.)

$$\mathrm{tr}\{[D^{-1}(m_q)]^\dagger(1-S^2)D^{-1}(m_q)\}(y,y)$$

$$= \mathrm{tr}\left\{[D^{-1}(m_q)]^\dagger D^{-1}(m_q)\right\}(y,y) - \mathrm{tr}\left\{[SD^{-1}(m_q)]^\dagger (SD^{-1}(m_q))\right\}(y,y)$$

Using

$$S = \gamma_5\left[2r\frac{D(m_q)-m_q}{1-rm_q}-1\right]$$

$$\begin{aligned} SD(m_q)^{-1} &= \gamma_5\left[\frac{2r}{1-rm_q}-\frac{1+rm_q}{1-rm_q}D(m_q)^{-1}\right] \\ &= \gamma_5\left[r-(1+rm_q)\left(D_c+m_q\right)^{-1}\right]. \end{aligned}$$

$$\begin{aligned} &\mathrm{tr}\left\{[SD^{-1}(m_q))]^\dagger (SD^{-1}(m_q)\right\}(y,y) \\ &= r^2\mathrm{tr}\,\mathbb{I} - 2r(1+rm_q)\mathrm{Re}\ \mathrm{tr}(D_c+m_q)^{-1}(y,y) \\ &\qquad +(1+rm_q)^2\mathrm{tr}\{[(D_c+m_q)^{-1}]^\dagger(D_c+m_q)^{-1}\}(y,y). \end{aligned}$$

A New Formula for the Residual Mass (cont.)

Using

$$D^{-1}(m_q) = (1 + rD_c)(D_c + m_q)^{-1} = r + (1 - rm_q)(D_c + m_q)^{-1}$$

$$\begin{aligned}
&\mathrm{tr}\left\{[D^{-1}(m_q)]^\dagger D^{-1}(m_q)\right\}(y,y) \\
&= r^2 \mathrm{tr}\,\mathbb{I} + 2r(1 - rm_q)\mathrm{Re}\ \mathrm{tr}(D_c + m_q)^{-1}(y,y) \\
&\qquad + (1 - rm_q)^2 \mathrm{tr}\left\{[(D_c + m_q)^{-1}]^\dagger (D_c + m_q)^{-1}\right\}(y,y)
\end{aligned}$$

Thus

$$\mathrm{tr}\{[D^{-1}(m_q)]^\dagger (1 - S^2) D^{-1}(m_q)\}(y,y)$$

$$= 4r\ \mathrm{Re}\ \mathrm{tr}\{(D_c + m_q)^{-1}(y,y)\} - 4rm_q \mathrm{tr}\{[(D_c + m_q)^{-1}]^\dagger (D_c + m_q)^{-1}\}(y,y)$$

$$\boxed{m_{res}(y) = \frac{\mathrm{Re}\ \mathrm{tr}\{(D_c + m_q)^{-1}(y,y)\}}{\mathrm{tr}\{[(D_c + m_q)^\dagger (D_c + m_q)]^{-1}(y,y)\}} - m_q}$$

which immediately gives the residual mass once the 12 columns of $(D_c + m_q)^{-1}(x,y)$ have been computed.

An Upper Bound for the Global Residual Mass

$$M_{res} = \frac{1}{4r}\frac{\mathrm{Tr}\{[D^{-1}(m_q)]^\dagger(1-S^2)D^{-1}(m_q)\}}{\mathrm{Tr}\{[(D_c+m_q)^{-1}]^\dagger(D_c+m_q)^{-1}\}}$$

$$= \frac{\mathrm{Re}\ \mathrm{Tr}\{(D_c+m_q)^{-1}\}}{\mathrm{Tr}\{[(D_c+m_q)^\dagger(D_c+m_q)]^{-1}\}} - m_q$$

$$\mathrm{Tr}\{[D(m_q)^{-1}]^\dagger(1-S^2)D^{-1}(m_q)\} = \mathrm{Tr}\{(1-S^2)(D^\dagger D)^{-1}(m_q)\} \le \sum_j \alpha_j\beta_j$$

von Neumann's trace inequality

α_j and β_j are the eigenvalues of $(1-S^2)$ and $(D^\dagger D)^{-1}(m_q)$ respectively

For ODWF, $S = S_{opt}$, $|\alpha_j| \le 2d_Z$. Thus

$$\mathrm{Tr}\{[D(m_q)^{-1}]^\dagger(1-S_{opt}^2)D^{-1}(m_q)\} \le 2d_Z\mathrm{Tr}\{(D^\dagger D)^{-1}(m_q)\}.$$

An Upper Bound for the Residual Mass (cont.)

$$M_{res} \le \frac{d_Z}{2r} \frac{\mathrm{Tr}\{[D(m_q)^{-1}]^\dagger D^{-1}(m_q)\}}{\mathrm{Tr}\{[(D_c+m_q)^{-1}]^\dagger (D_c+m_q)^{-1}\}}$$

$\because$ $$D^{-1}(m_q) = (1+rD_c)(D_c+m_q)^{-1} = r + (1-rm_q)(D_c+m_q)^{-1}$$

$\therefore$ $$\lambda_j = r + (1-rm_q)\xi_j$$

ξ_j is a singular value of $(D_c+m_q)^{-1}$

λ_j is the corresponding singular value of $D^{-1}(m_q)$

$\therefore$ $$\frac{\sum_j |\lambda_j|^2}{\sum_j |\xi_j|^2} = (1-rm_q)^2 + 2r(1-rm_q)\frac{\langle \mathrm{Re}(\xi)\rangle}{\langle |\xi|^2\rangle} + \frac{r^2}{\langle |\xi|^2\rangle}$$

$$\langle |\xi|^2 \rangle = \frac{1}{N}\sum_{j=1}^{N} |\xi_j|^2, \quad \langle \mathrm{Re}(\xi)\rangle = \frac{1}{N}\sum_{j=1}^{N} \mathrm{Re}(\xi_j)$$

N is the total number of singular values of $(D_c+m_q)^{-1}$

An Upper Bound for the Residual Mass (cont.)

$$\therefore \quad \frac{\mathrm{Tr}\{[D(m_q)^{-1}]^\dagger D^{-1}(m_q)\}}{\mathrm{Tr}\{[(D_c+m_q)^{-1}]^\dagger (D_c+m_q)^{-1}\}} = (1-rm_q)^2 + 2r(1-rm_q)\frac{\langle \mathrm{Re}(\xi)\rangle}{\langle|\xi|^2\rangle} + \frac{r^2}{\langle|\xi|^2\rangle}$$

$$\Rightarrow \quad M_{res} \le \frac{d_Z}{2r}\left[(1-rm_q)^2 + 2r(1-rm_q)\frac{\langle \mathrm{Re}(\xi)\rangle}{\langle|\xi|^2\rangle} + \frac{r^2}{\langle|\xi|^2\rangle}\right]$$

Thus, to obtain the upper bound of M_{res} amounts to working out

(i) an upper bound for $\langle \mathrm{Re}(\xi)\rangle / \langle|\xi|^2\rangle$

(ii) a lower bound for $\langle|\xi|^2\rangle$

It can be shown that

$$\frac{\langle \mathrm{Re}(\xi)\rangle}{\langle|\xi|^2\rangle} \le m + \frac{(1+m)d_Z}{2-(3-m)d_Z}$$

$$\langle|\xi|^2\rangle \ge \frac{r^2}{1+m}\left[\frac{2-(3-m)d_Z}{2m+(1-m)^2 d_Z}\right]$$

An Upper Bound for the Residual Mass (cont.)

$$M_{res} \le \frac{d_Z}{2r}\left\{(1-rm_q)^2 + 2r(1-rm_q)\left[rm_q + \frac{(1+rm_q)d_Z}{2-(3-rm_q)d_Z}\right] + (1+rm_q)\left[\frac{2rm_q + (1-rm_q)^2 d_Z}{2-(3-rm_q)d_Z}\right]\right\}$$

For light quarks, $rm_q \ll 1$

$$M_{res} \le \frac{d_Z}{2r}$$

For ODWF, $d_Z \ll 1$ in most cases

$$M_{res} \le \frac{d_Z}{2r}\left[(1+2r^2 m_q)^2(1-rm_q) + 2r^2 m_q^2\right] \equiv \frac{d_Z}{2r} F(r, m_q)$$

$$M_{res}[d_Z/(2r)]^{-1} = F(r, m_q)$$

An Upper Bound for the Residual Mass (cont.)

It is clear that the derivation also goes through for the conventional DWF with nonzero weights $\rho_s = c_1(\text{constant})$ and $\sigma_s = c_2(\text{constant})$

by replacing $||1 - S_{opt}|| \le d_Z$ with $||1 - S_{polar}|| < \Delta_{max}$

Δ_{max} can be determined for given λ_{min} and λ_{max}

$$M_{res} \le \frac{\Delta_{max}}{2r} \left\{ (1 - rm_q)^2 + 2r(1 - rm_q) \left[rm_q + \frac{(1 + rm_q)\Delta_{max}}{2 - (3 - rm_q)\Delta_{max}} \right] \right.$$
$$\left. +(1 + rm_q) \left[\frac{2rm_q + (1 - rm_q)^2 \Delta_{max}}{2 - (3 - rm_q)\Delta_{max}} \right] \right\}$$

if Δ_{max} is sufficiently small

$M_{res}[\Delta_{max}/(2r)]^{-1} \approx F(r, m_q)$ universal for any DWF

An Upper Bound for the Residual Mass (cont.)

How does the residual mass depend on the quark mass ?

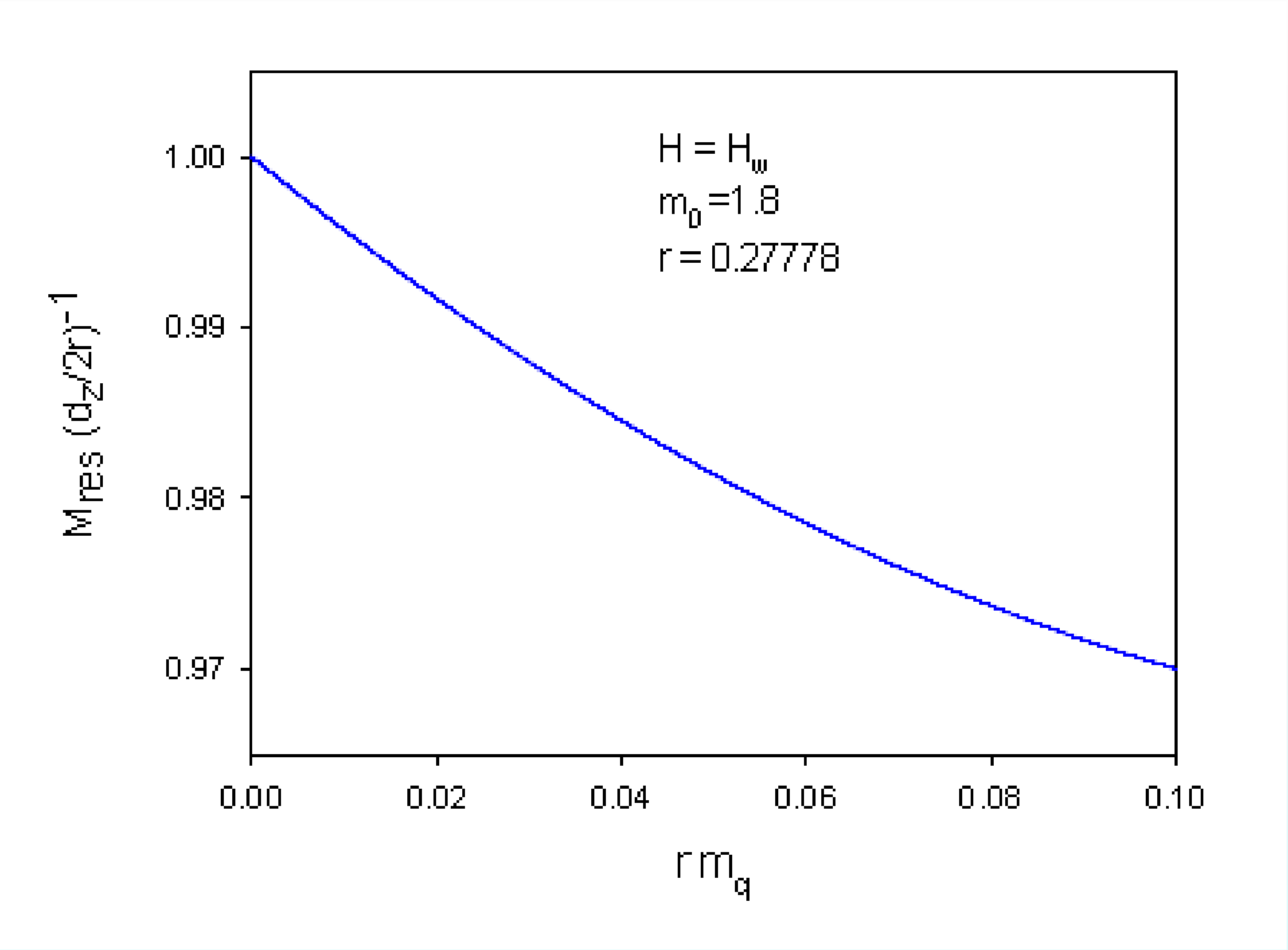
Consider $\rho_s = c\omega_s + d,\ \sigma_s = c\omega_s - d,$ with

$$H = cH_w(1 + d\gamma_5 H_w)^{-1},\ r = [2m_0(1 - dm_0)]^{-1}$$

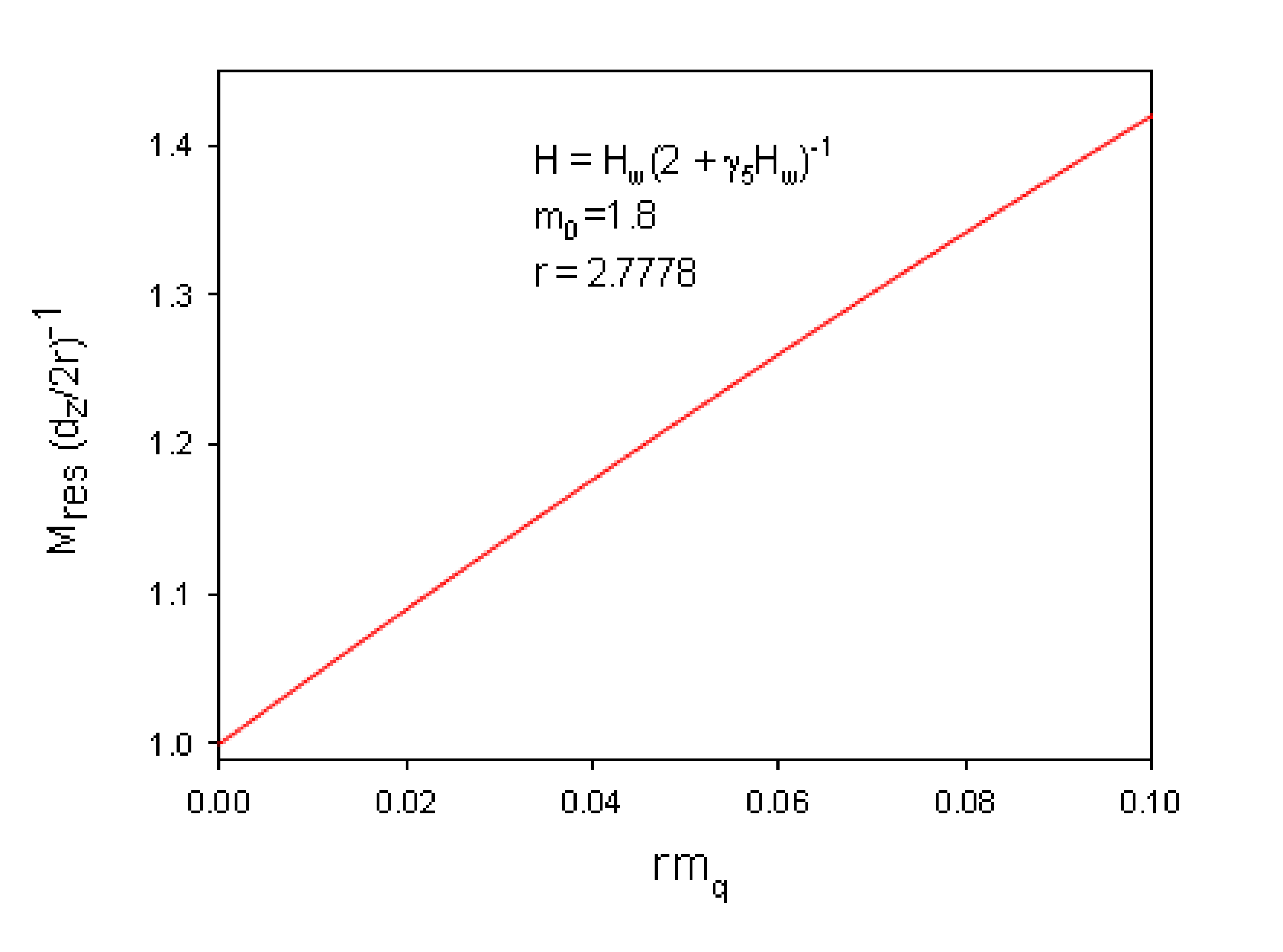
(i) $c = 1,\ d = 0,\ H = H_w,\ r = 1/(2m_0)$

(ii) $c = 1/2,\ d = 1/2,\ H = H_w(2 + \gamma_5 H_w)^{-1},\ r = [m_0(2 - m_0)]^{-1}$

An Upper Bound for the Residual Mass (cont.)



An Upper Bound for the Residual Mass (cont.)



Concluding Remarks

- Axial Ward identity is derived for LQCD with ODWF
- Z[J] for n-point Green's function is obtained
- A practical formula for the residual mass is obtained
- An upper bound for the residual mass is obtained
  - It provides a guideline for designing simulations with DWF
  - The normalized residual mass is expressed as

$$F(r, m_q) = (1 + 2r^2 m_q)(1 - r m_q) + 2r^2 m_q^2$$

  which is universal for any DWF with sufficiently small $\Delta_{\max}$
- The residual mass of quark for any observable O should be measured respectively.