Charge symmetry violation in hadrons: Electromagnetism & quark masses

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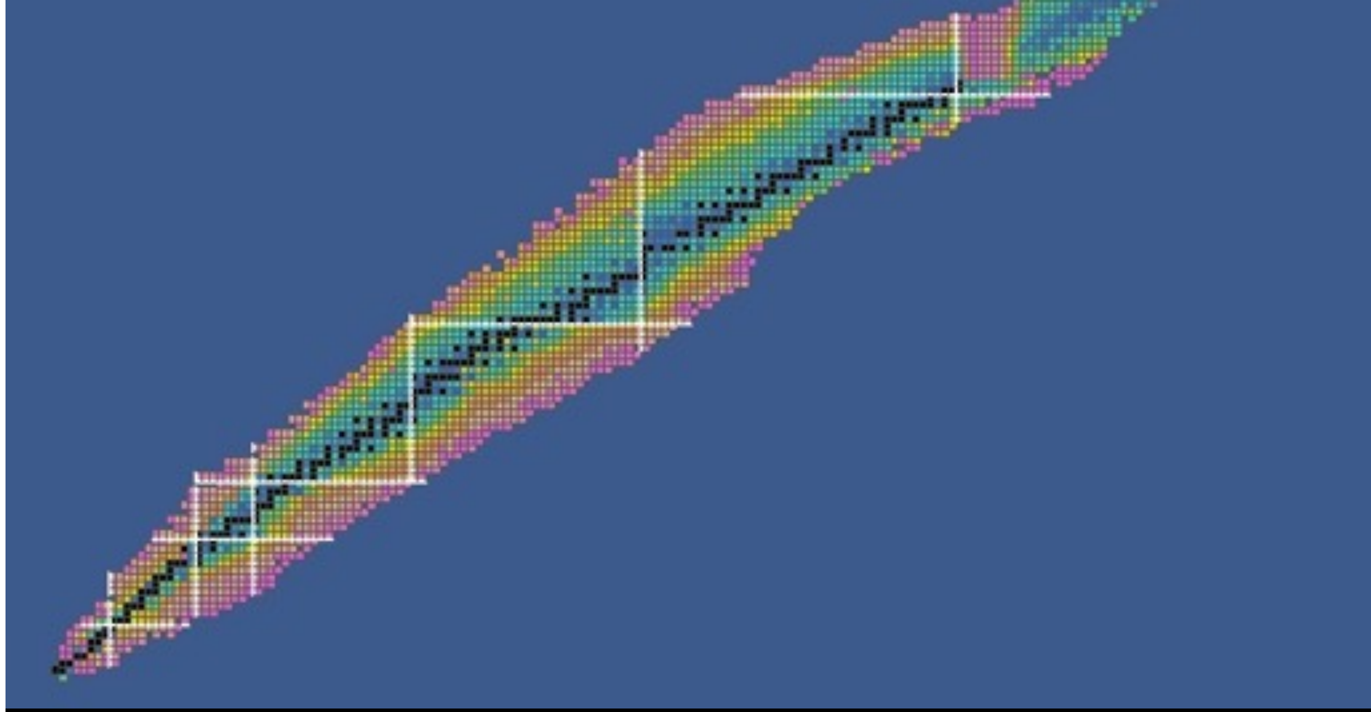
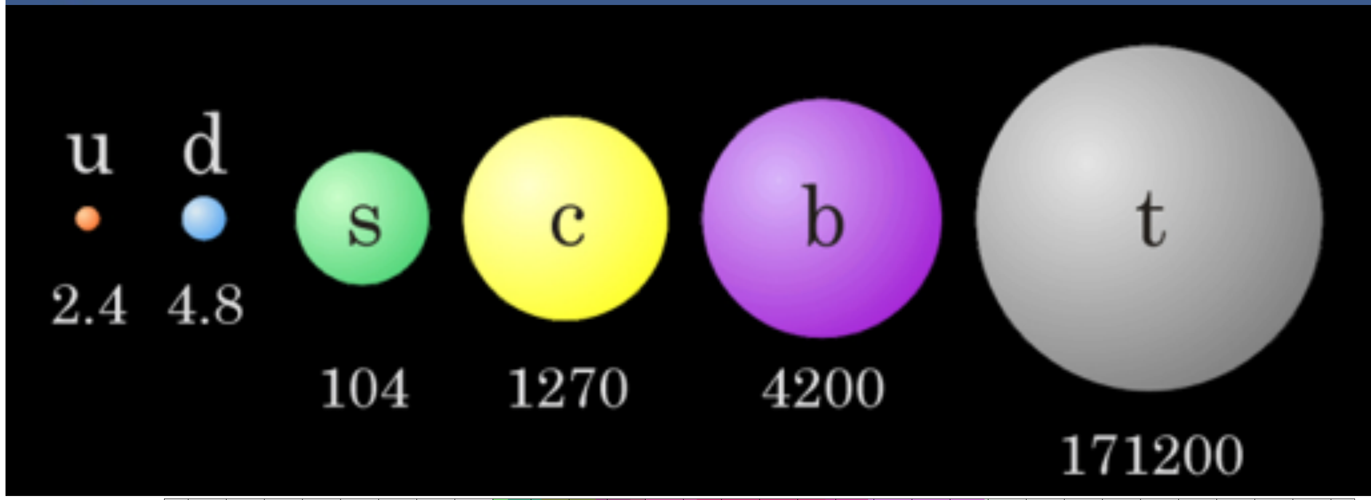
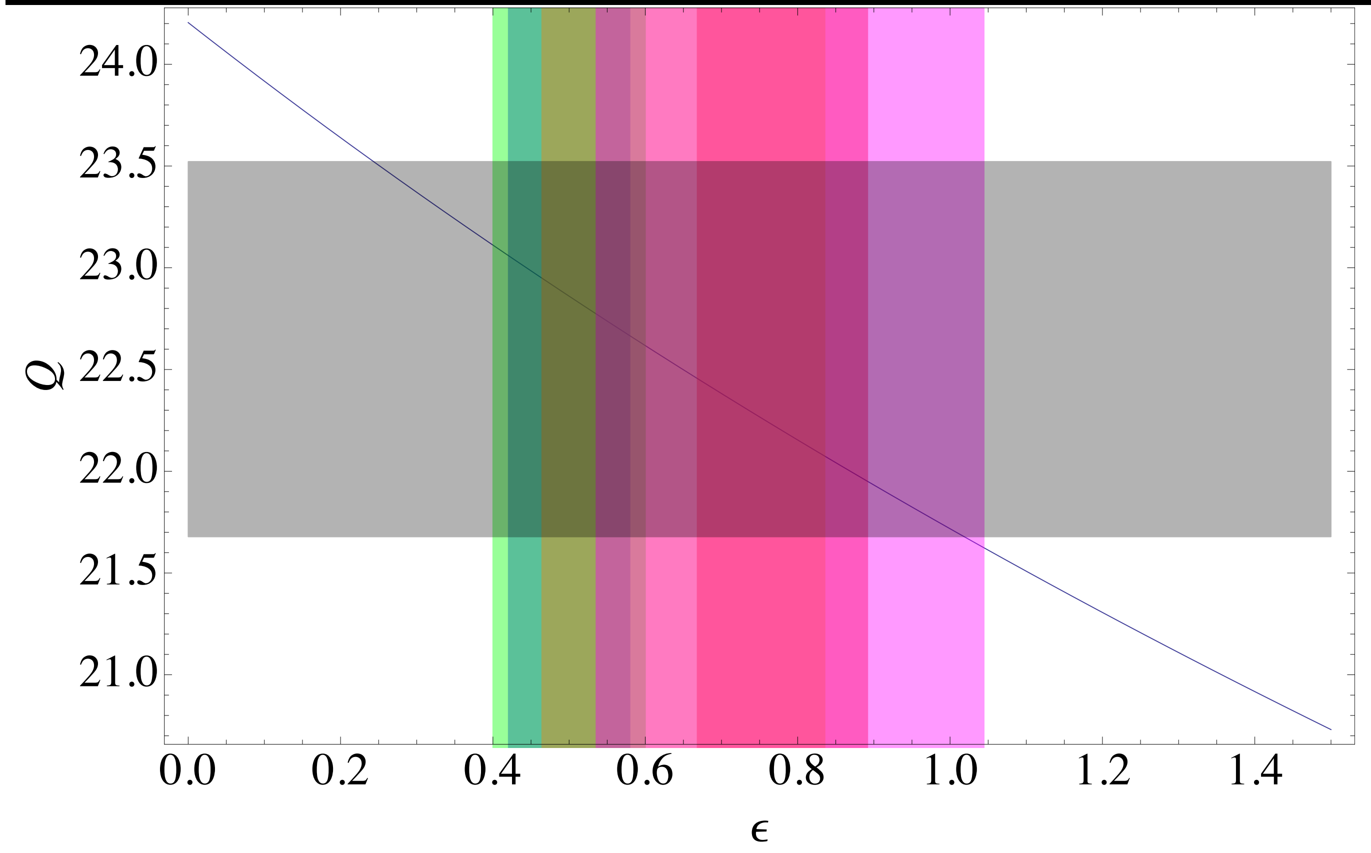
- QCDSF-UKQCD-CSSM
  - R. Horsley, Y. Nakamura, H. Perlt, D. Pleiter
  - P. Rakow, G. Schierholz, A. Schiller, R. Stokes
  - H. Stüben, J. Zanotti
- And:
  - F. Erben, P. Shanahan, A. Thomas

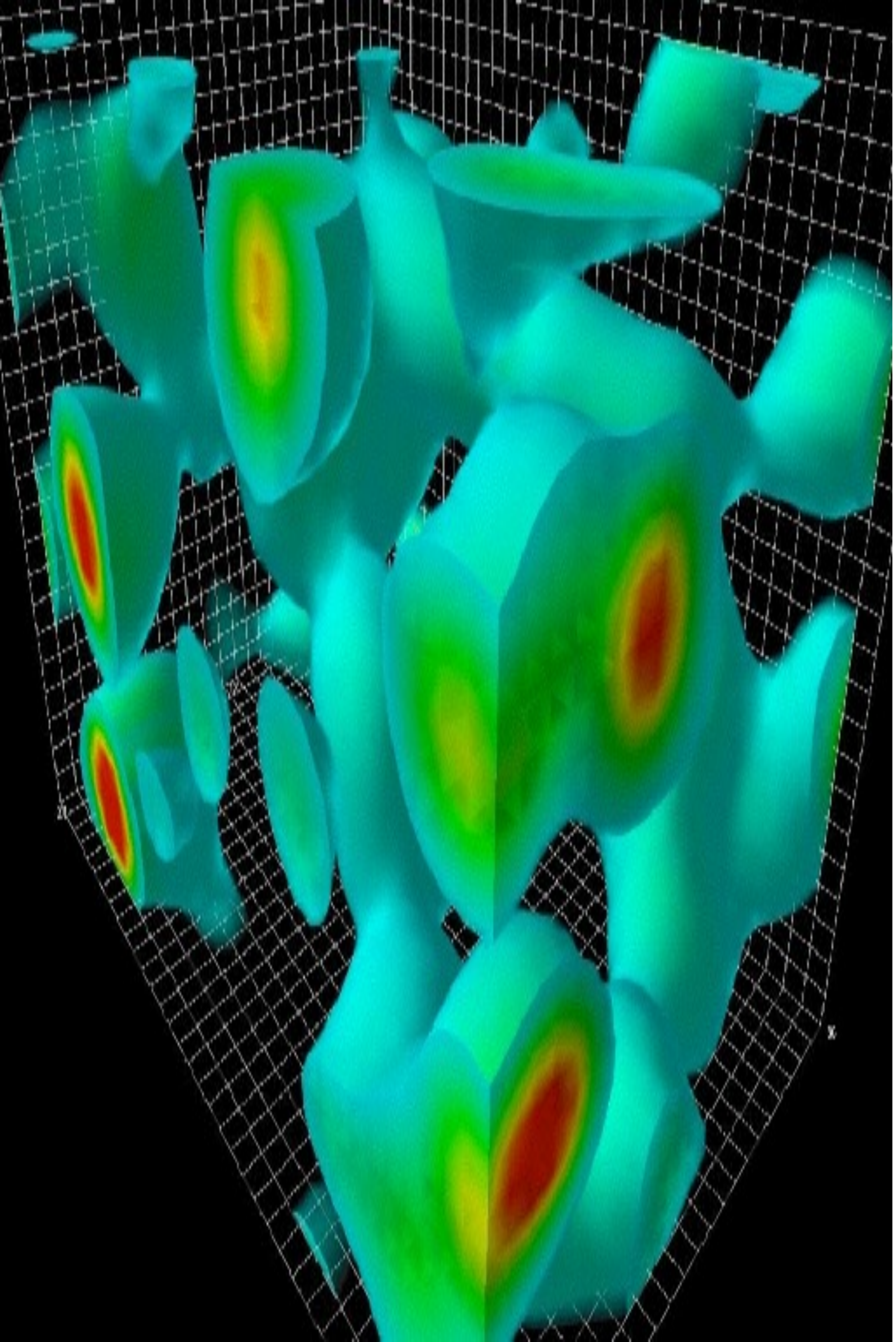
Outline: I

- Historical origins of isospin symmetry breaking in the strong nuclear force
- Determination of quark mass parameters from meson spectrum
    - Important to resolve electromagnetic effects
- Latest results on the Cottingham formula
    - Electromagnetic and strong contributions to the *p–n* mass difference



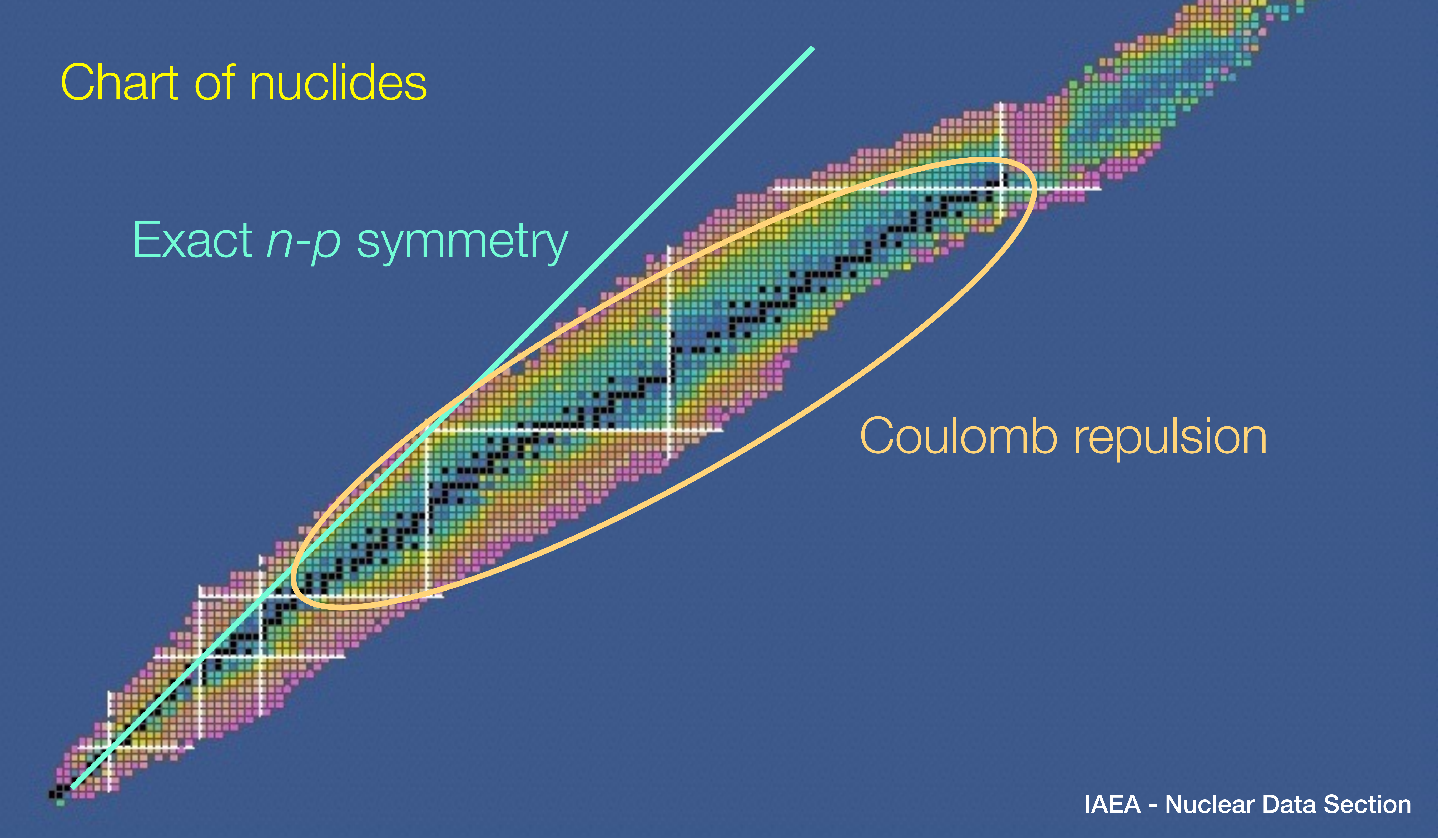






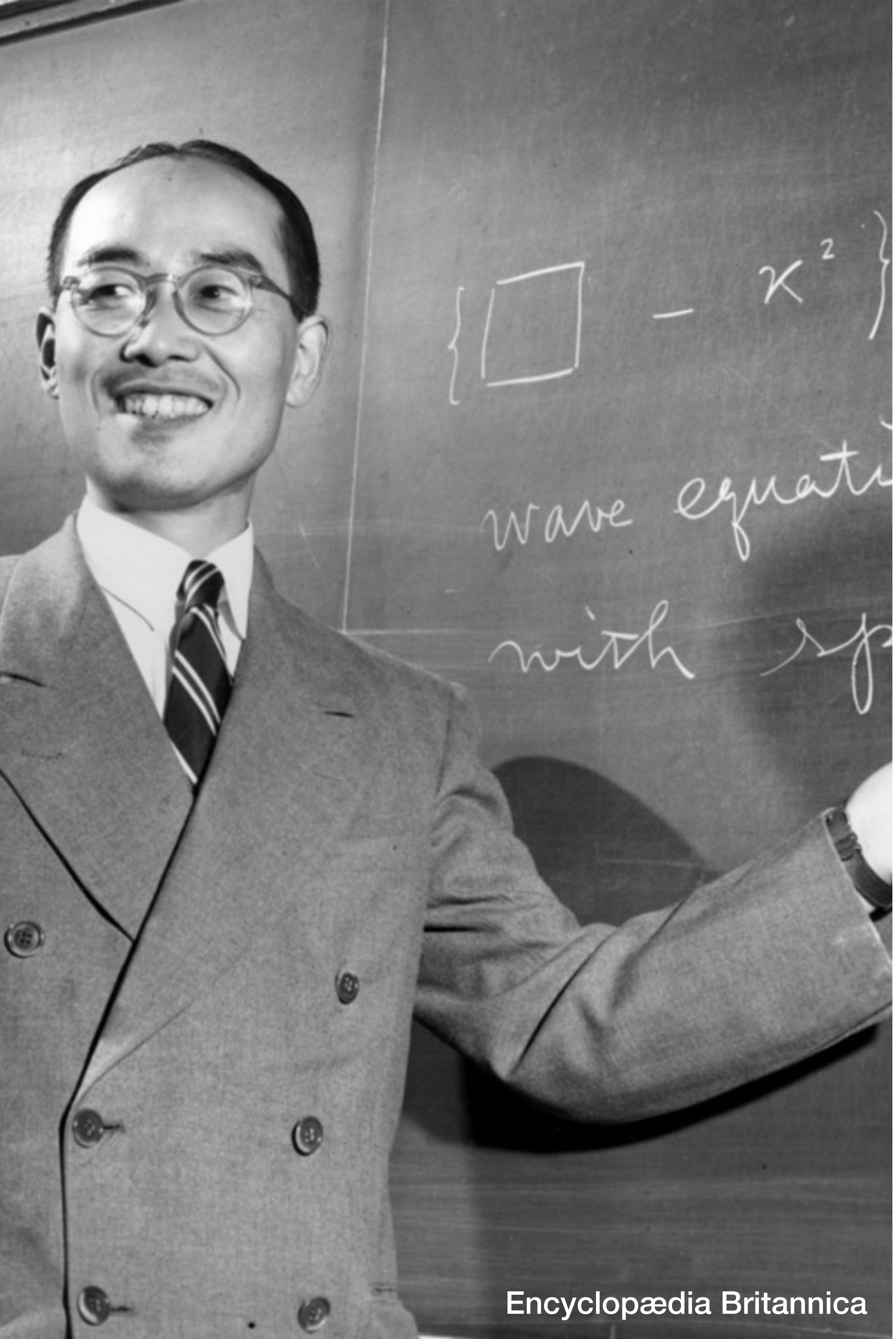
Outline: II

- Lattice Introduction
- SU(3) symmetry breaking in the hadron spectrum
  - "QCDSF trajectory"
- Including QED
  - Scheme dependence and matching
  - Finite-volume considerations
- EM in meson spectrum
- Proton–neutron separation



Symmetry of the strong force

Proton-neutron symmetry



Strong interaction

- Matter: Nucleons
- Force carrier: Pions
- approximate SU(2) symmetry

Early proposals:
SU(2) symmetry only broken **ONLY** by electromagnetic interaction?

Charged pion self-energy

IL NUOVO CIMENTO Vol. XXV, N. 3 1° Agosto 1962

Effect of Pion Resonances on the $(\pi^+ - \pi^0)$ and $(K^+ - K^0)$ Mass Differences.

S. K. Bose and R. E. Marshak

Department of Physics and Astronomy, University of Rochester - Rochester, N. Y.

(ricevuto il 12 Marzo 1962)

- One-loop electromagnetic self energy;
    - Form factor saturated by rho resonance:

$$\delta^{\pi^+}_{\rm EM} \simeq 4.1\,{\rm MeV}$$

$$\delta^{\pi^+}_{\rm EM}({\rm exp.}) \simeq 4.6\,{\rm MeV}$$

K^+–K^0 mass difference difficult to reconcile?

Cottingham formula

ANNALS OF PHYSICS: **25**, 424–432 (1963)

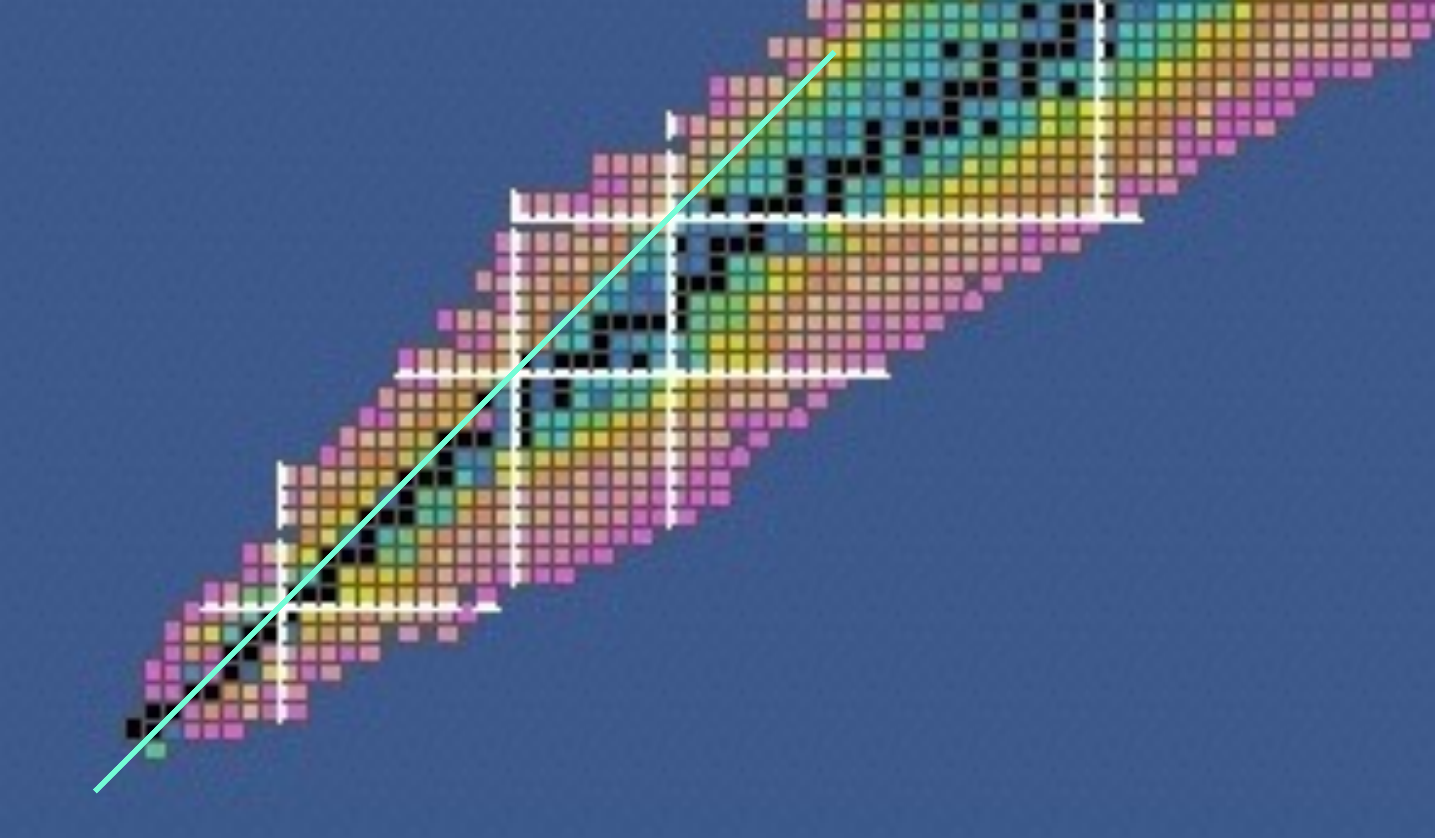
The Neutron Proton Mass Difference and Electron Scattering Experiments

W. N. Cottingham

Department of Mathematical Physics, The University of Birmingham, England

The calculations show that, using the elastic scattering data up to energies presently available, the "elastic" contribution is of the wrong sign to explain the nucleon mass difference. The correct sign can be obtained only if particular extrapolations of $f_i(q^2)$ are made to values of q^2 very far from those presently explored.

- IF isospin invariance is ONLY broken by electromagnetism, then the proton should be heavier than the neutron.



Charge symmetry violation in the absence of electromagnetism?

Strip down to single nucleons in the absence of EM.

1975

IMPLICATIONS OF SCALING FOR THE PROTON-NEUTRON MASS DIFFERENCE

J. GASSER * and H. LEUTWYLER
Institut für theoretische Physik der Universität Bern, Bern, Switzerland

Received 17 February 1975

- In renormalisation of Cottingham formula, Gasser & Leutwyler introduce an isospin-violating "mass" operator

We assume, following Wilson [2], that the Lagrangian contains generalized mass terms, in particular a term proportional to $\sigma(x)$ ("u_3-term", "tadpole", ...). The full Lagrangian is written as

$$\mathcal{L}(x) = \mathcal{L}_0(x) - e\, j_\mu(x) A^\mu(x) - g_0\, \sigma(x)\,. \tag{2.6}$$

"Isospin-invariant strong Lagrangian"

EM interaction

Isospin-violating operator

Quark-model language:

$$\sigma(x) = \overline{q}(x) Q^2 \mathcal{M} q(x)$$

1975: Gasser & Luetwyler

- Describe a prescription for regularising the divergent dispersion integral
  - Expressed in terms of (in principle) measurable structure functions
- With available data at the time, they determine:

$$\Delta M^{\mathrm{p-n}}_{\mathrm{n.t.}} = 0.7 \pm 0.3\ \mathrm{MeV}\,.$$

~electromagnetic

- And quark model with octet hyperon masses:

$$\frac{(g+\gamma_{\mathrm{fit}})}{2M}\{\langle p|\sigma|p\rangle - \langle n|\sigma|n\rangle\} = -2.0 \pm 0.3\ \mathrm{MeV}\,.$$

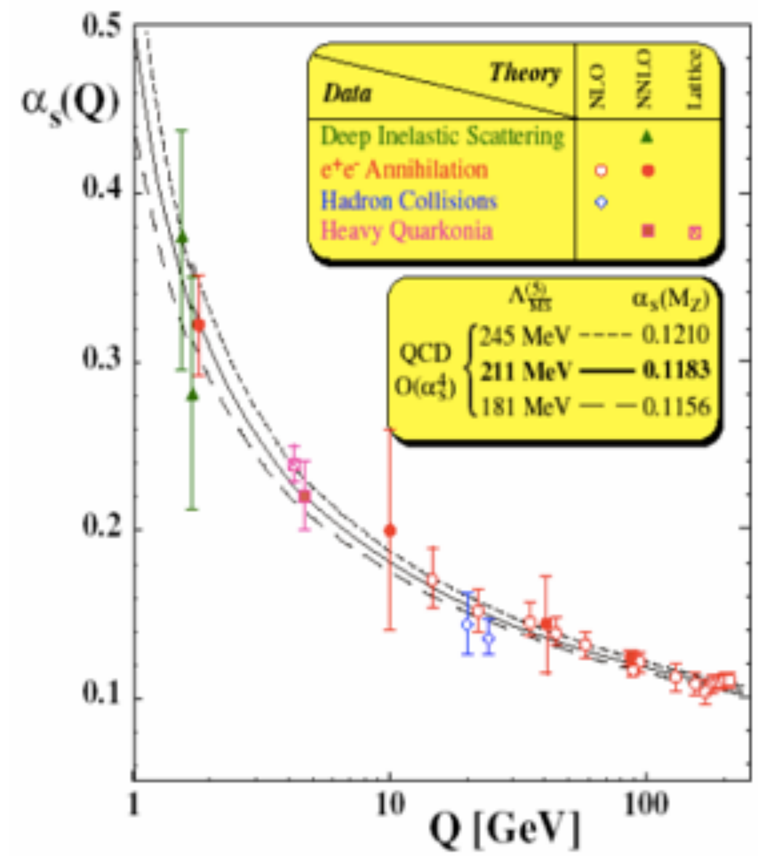
~quark mass

- Agreement with experiment:

$$\Delta M^{p-n} \sim -1.3\,\mathrm{MeV}$$

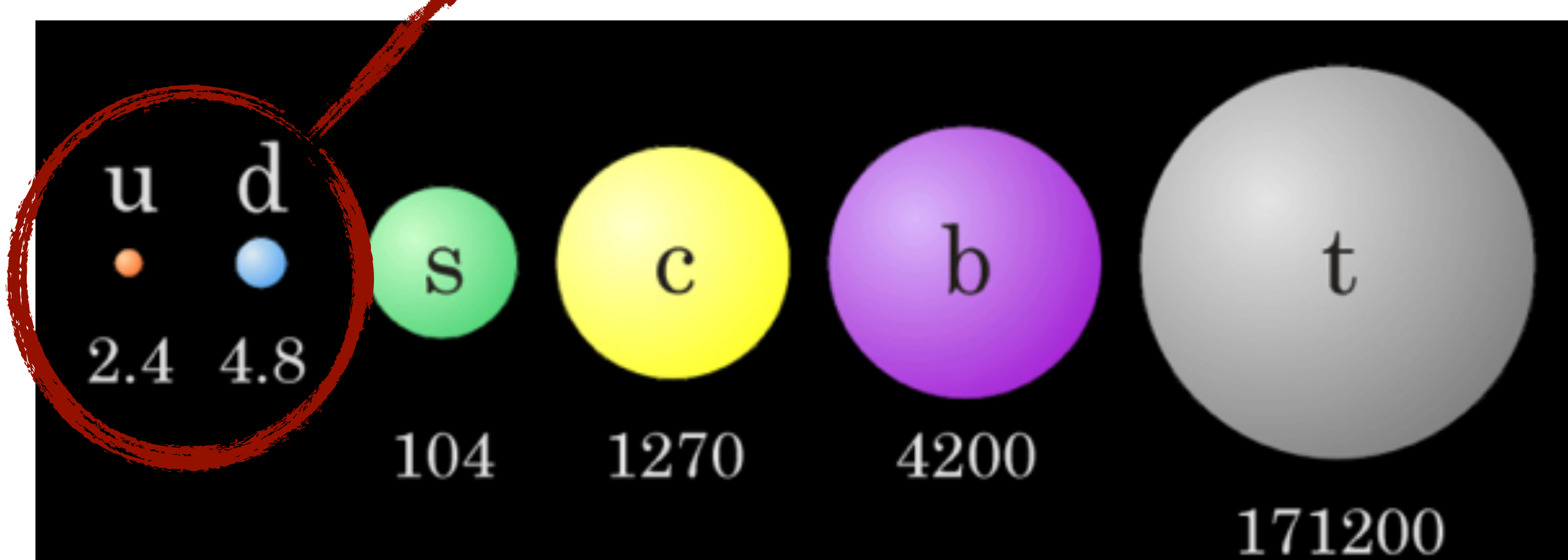
Quark Masses

- SU(3) Yang-Mills (coupled to Nf massless quarks) is a beautiful parameter-free theory [ignoring Nc, Nf]



- The reality of the strong nuclear force, and nature as we know it, relies on the quark mass parameters

Especially these guys!!



Determining m_u–m_d

- *Leading-order* pseudo scalar masses:

$$\begin{aligned} m_\pi^2 &= B_0(m_u + m_d) \\ m_{K^+}^2 &= B_0(m_u + m_s) \\ m_{K^0}^2 &= B_0(m_d + m_s) \end{aligned}$$

- ⇒ Quark mass ratios:

$$\frac{m_u}{m_d} = \frac{m_\pi^2 + m_{K^+}^2 - m_{K^0}^2}{m_\pi^2 + m_{K^0}^2 - m_{K^+}^2} \simeq 0.67$$

$$\frac{m_s}{m_d} = \frac{m_{K^+}^2 + m_{K^0}^2 - m_\pi^2}{m_\pi^2 + m_{K^0}^2 - m_{K^+}^2} \simeq 20$$

Determining *m_u*–*m_d*: Electromagnetic effects

- *Leading-order* pseudo scalar masses, with EM correction:

$$
\begin{aligned}
m_{\pi^0}^2 &= B_0(m_u + m_d) + \Delta_{\mathrm{EM}}^{\pi^0} \\
m_{\pi^+}^2 &= B_0(m_u + m_d) + \Delta_{\mathrm{EM}}^{\pi^+} \\
m_{K^+}^2 &= B_0(m_u + m_s) + \Delta_{\mathrm{EM}}^{K^+} \\
m_{K^0}^2 &= B_0(m_d + m_s) + \Delta_{\mathrm{EM}}^{K^0}
\end{aligned}
$$

"Dashen"

$$
\Delta_{\mathrm{EM}}^{\pi^0} \simeq \Delta_{\mathrm{EM}}^{K^0} \simeq 0
$$

$$
\Delta_{\mathrm{EM}}^{\pi^+} \simeq \Delta_{\mathrm{EM}}^{K^+}
$$

- ⇒ Quark mass ratios with Dashen correction:

$$
\frac{m_u}{m_d} = \frac{2m_{\pi^0}^2 - m_{K^0}^2 - m_{\pi^+}^2 + m_{K^+}^2}{m_{\pi^+}^2 + m_{K^0}^2 - m_{K^+}^2} = 0.56
$$

$$
\frac{m_s}{m_d} = \frac{m_{K^+}^2 + m_{K^0}^2 - m_{\pi}^2}{m_{\pi}^2 + m_{K^0}^2 - m_{K^+}^2} = 20.1
$$

Determining m_u–m_d: Beyond leading order

- Second order in quark mass expansion (pure QCD): [Gasser & Leutwyler 1985]

$$\frac{m_K^2}{m_\pi^2} = \frac{m_s + \hat{m}}{2\hat{m}} \left[1 + \Delta_M\right]$$

$$\frac{m_{K^0}^2 - m_{K^+}^2}{m_K^2 - m_\pi^2} = \frac{m_d - m_u}{m_s - \hat{m}} \left[1 + \Delta_M\right]$$

Chiral logs + LECs

- Double ratio:

$$Q^2 \equiv \frac{m_s^2 - \hat{m}^2}{m_d^2 - m_u^2} = \frac{m_K^2}{m_\pi^2} \frac{m_K^2 - m_\pi^2}{m_{K^0}^2 - m_{K^+}^2} \left[1 + \mathcal{O}(m_q^2)\right]$$

- And with electromagnetic corrections (assuming Dashen):

$$Q_D^2 \equiv \frac{(m_{K^0}^2 + m_{K^+}^2 - m_{\pi^+}^2 + m_{\pi^0}^2)(m_{K^0}^2 + m_{K^+}^2 - m_{\pi^+}^2 - m_{\pi^0}^2)}{4m_{\pi^0}^2(m_{K^0}^2 - m_{K^+}^2 + m_{\pi^+}^2 - m_{\pi^0}^2)} = (24.2)^2$$

Violation of Dashen's theorem

- Define pseudoscalar electromagnetic contribution to mass(-square):

$$\Delta_P^\gamma \equiv m_P^2(g^2, e^2) - m_P^2(g^2, 0)$$

  - Dimensionless epsilon parameters:

$$\epsilon_P \equiv \frac{\Delta_P^\gamma}{\Delta_\pi}; \qquad \Delta_\pi \equiv \left[m_{\pi^+}^2 - m_{\pi^0}^2\right]^{\text{phys.}}$$

- Dashen theorem:

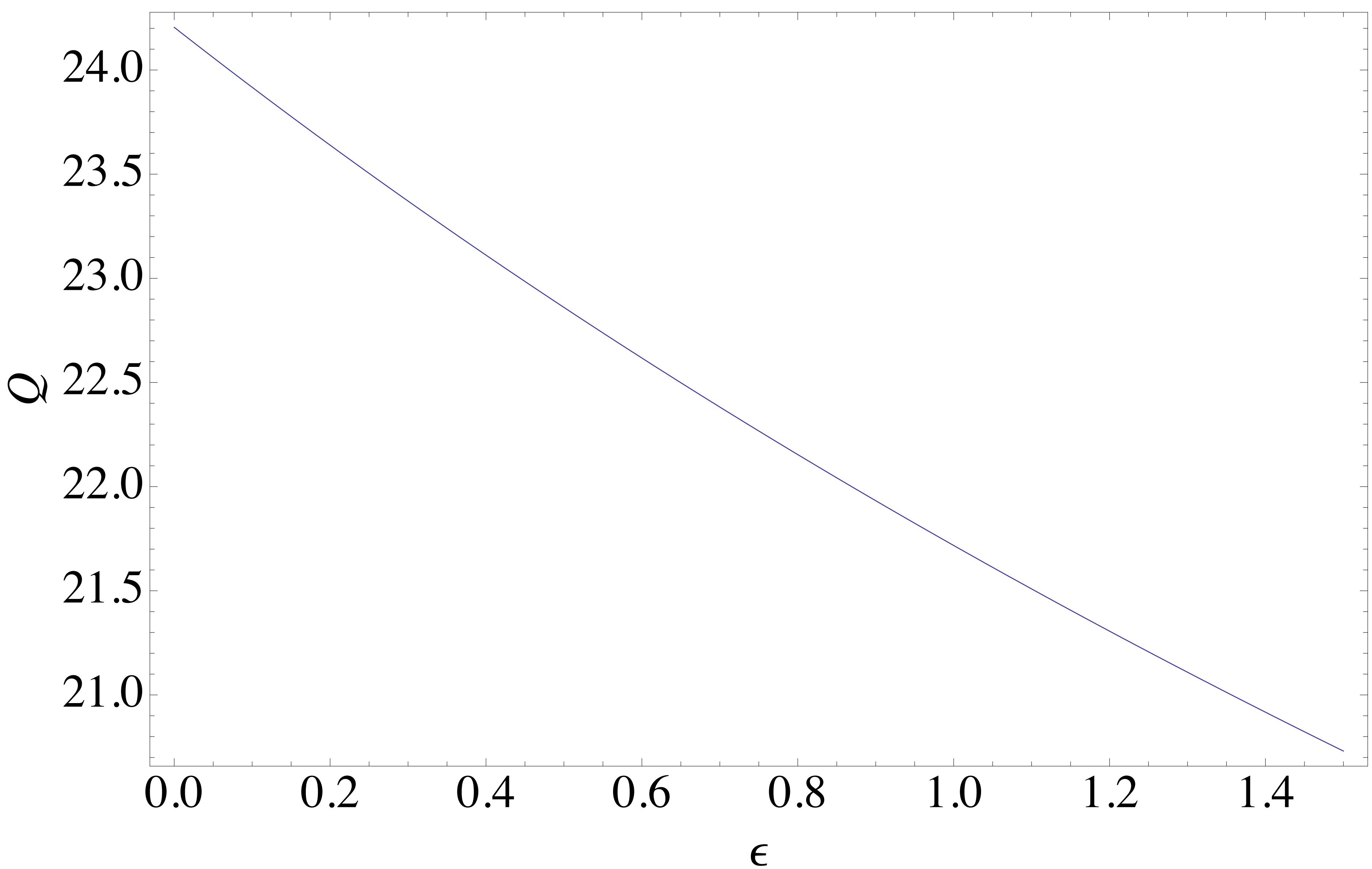
$$\Delta_{K^+}^\gamma = \Delta_{\pi^+}^\gamma$$

  - Violation encoded by:

$$\Delta_{K^+}^\gamma - \Delta_{K^0}^\gamma - \Delta_{\pi^+}^\gamma + \Delta_{\pi^0}^\gamma = \epsilon\Delta_\pi$$

Violation of Dashen’s theorem: Lattice estimates

- Illustrative* sensitivity to Dashen violation epsilon parameter
  [*Dashen correction in denominator only]



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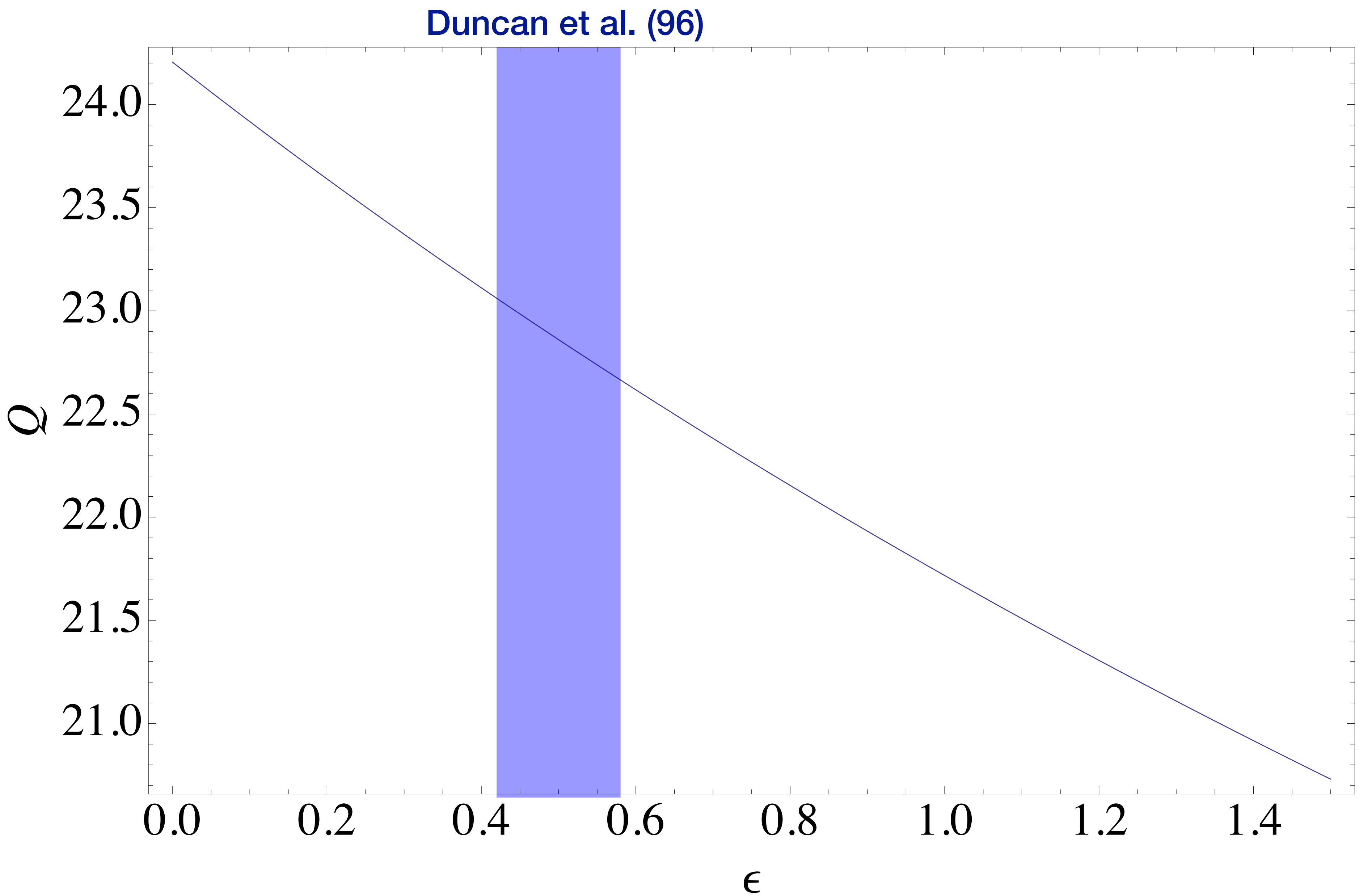

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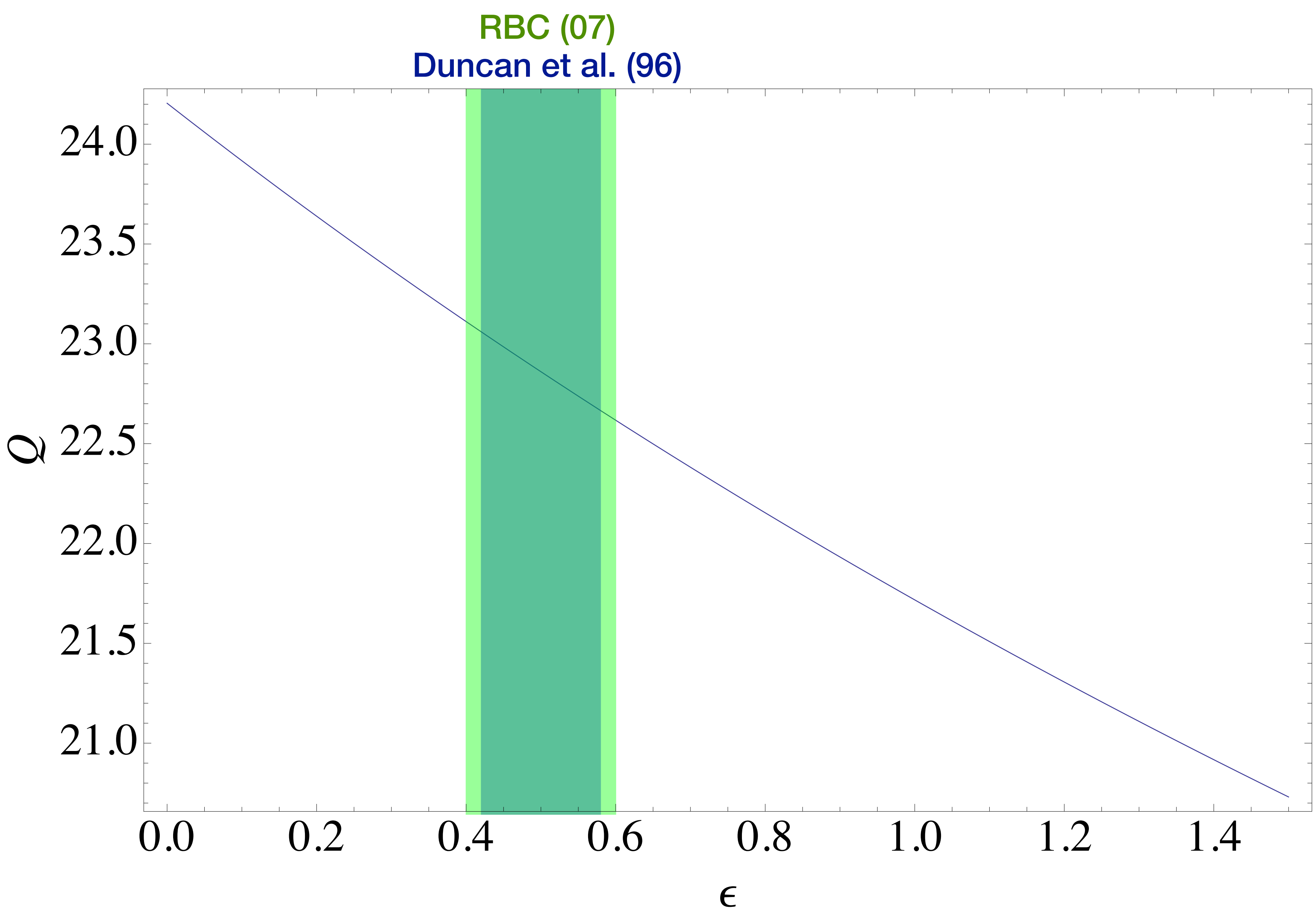

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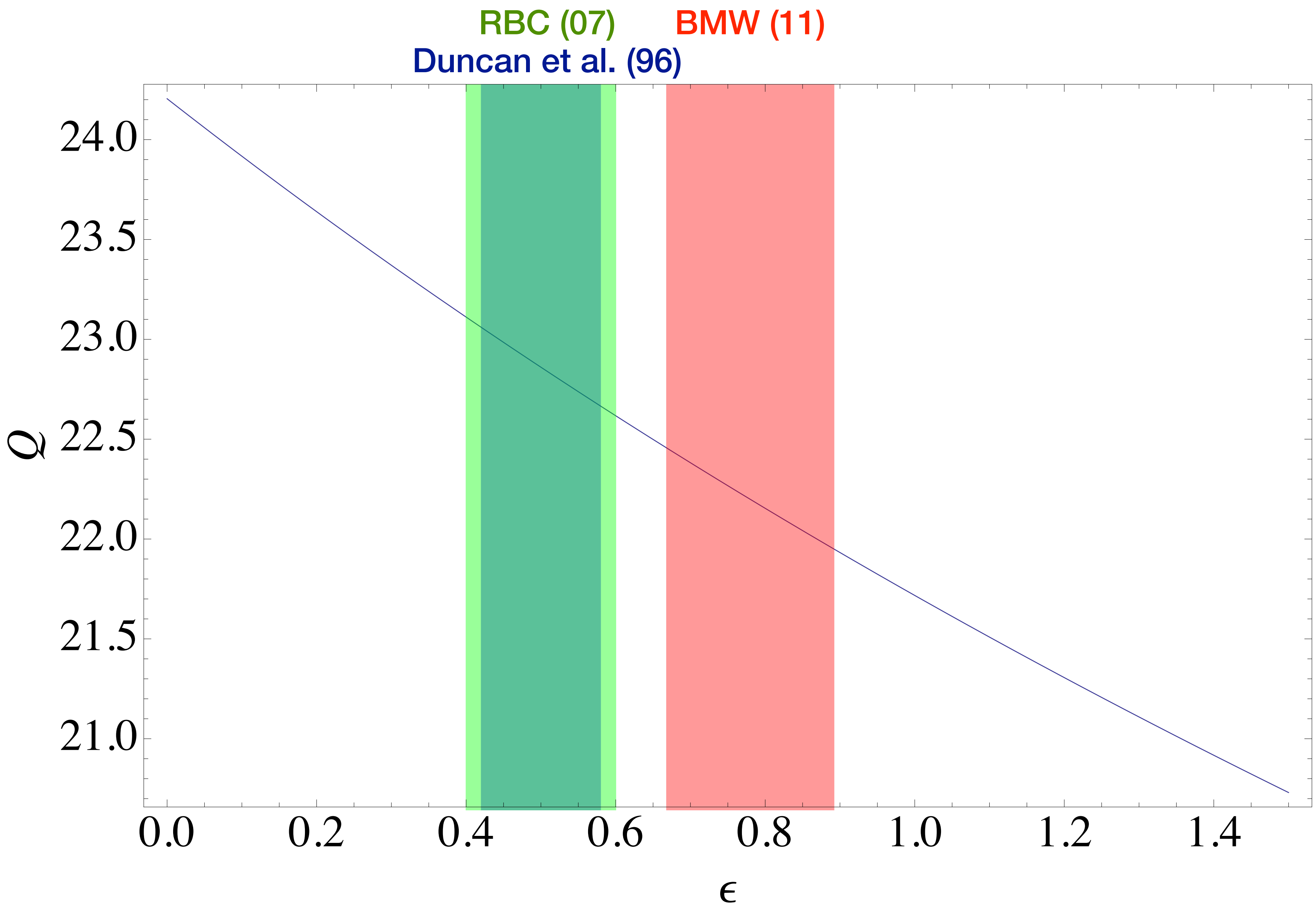

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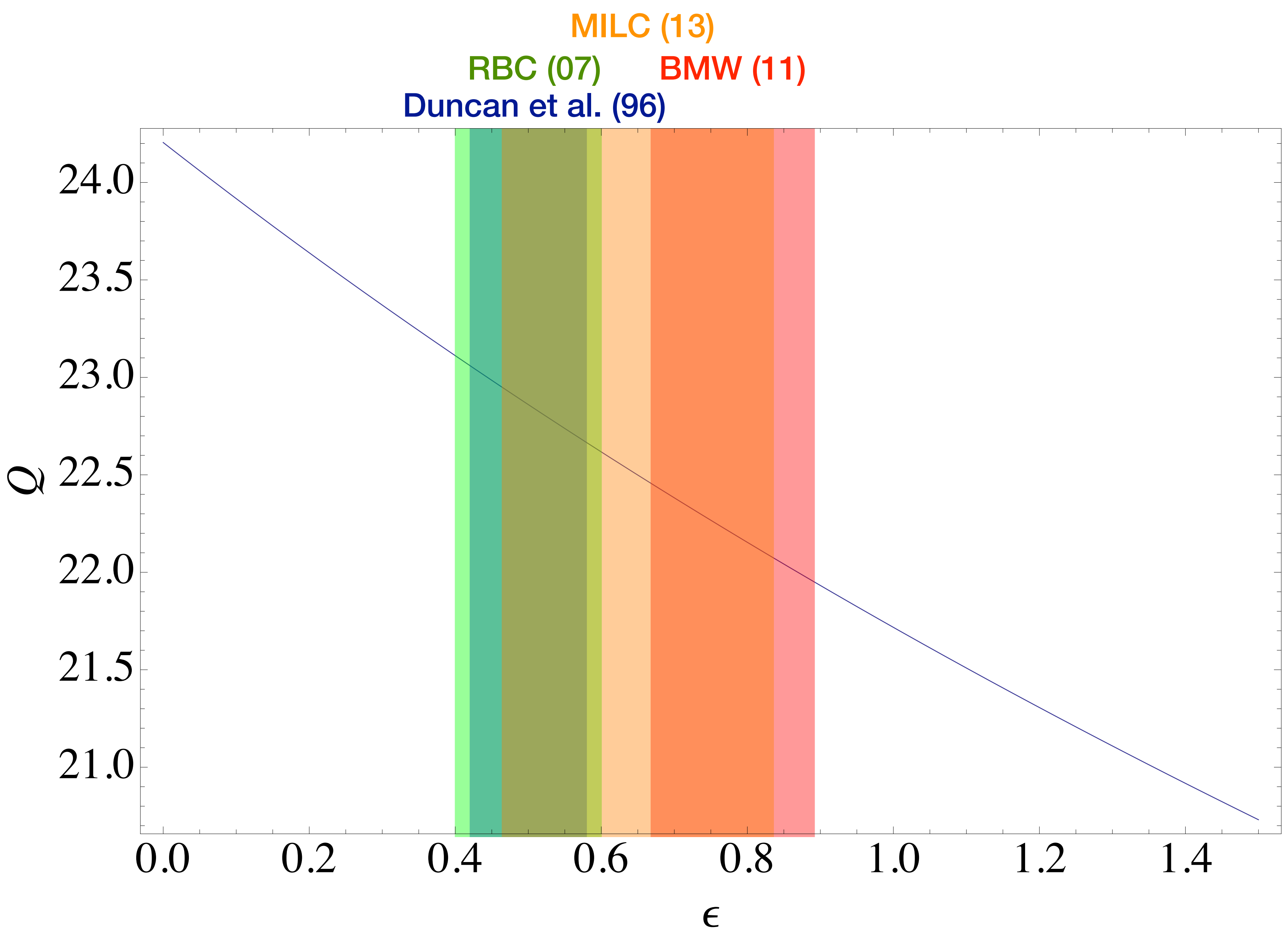

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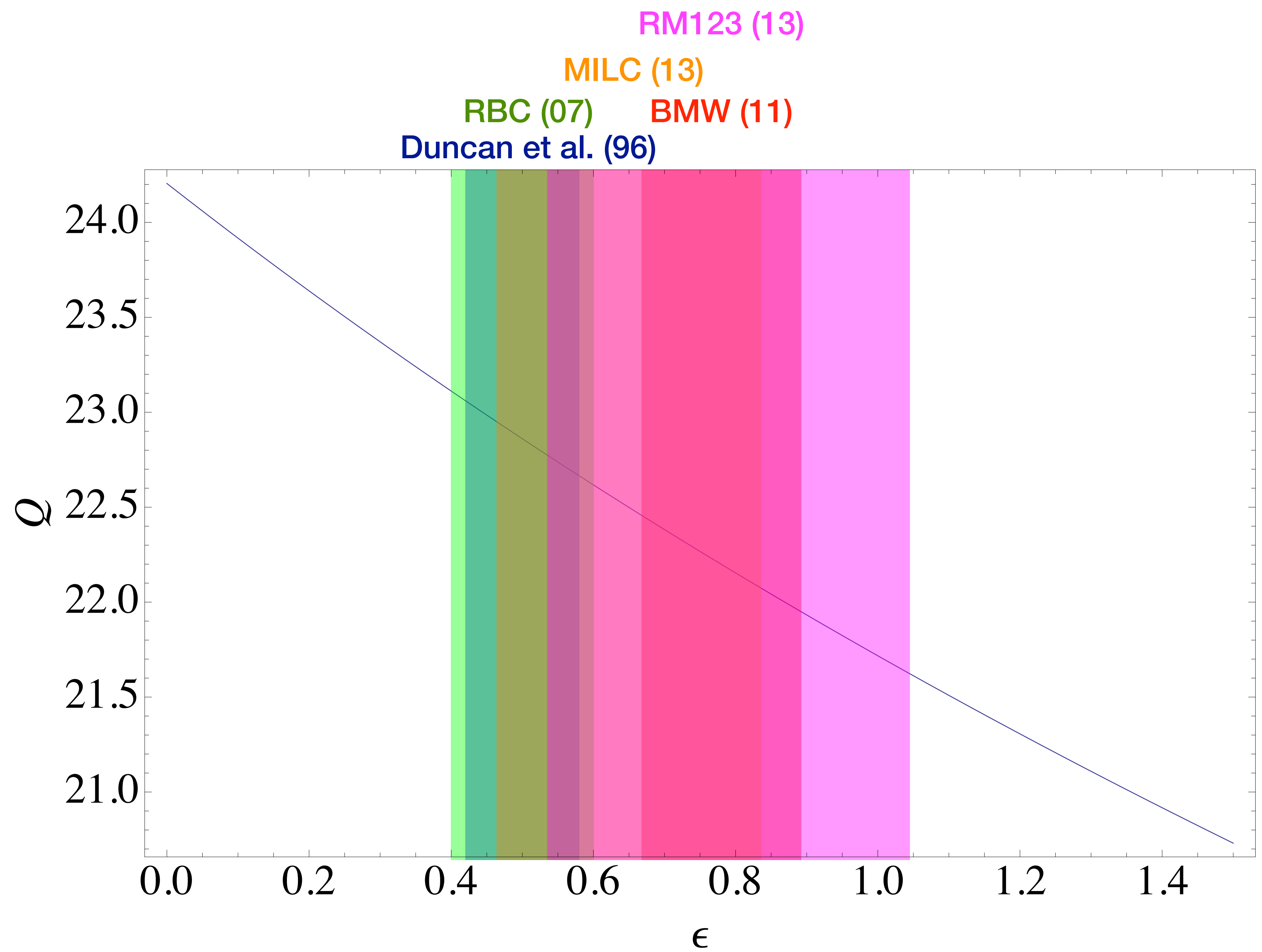

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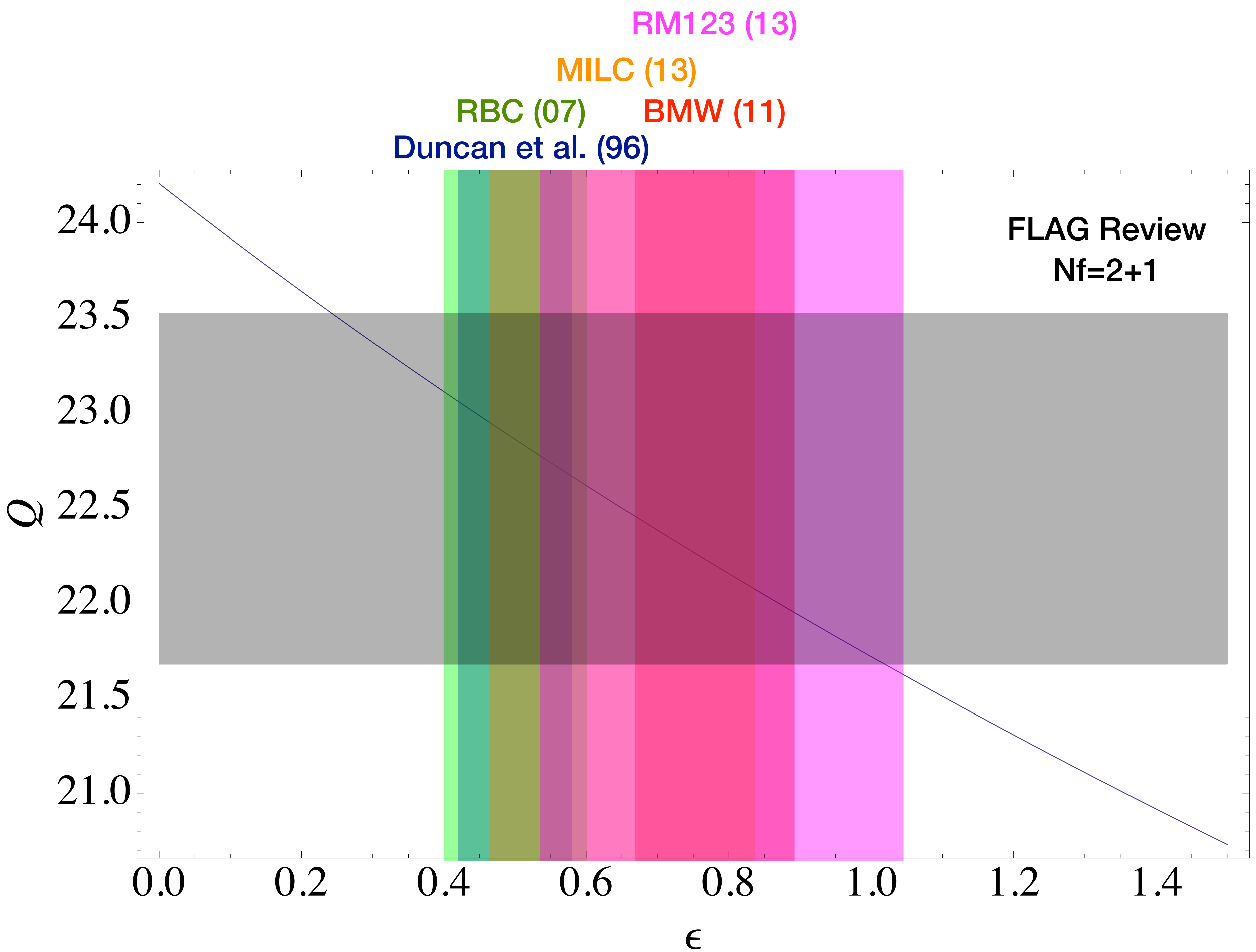

Lattice studies, *including electromagnetism*, essential for precision resolution of quark mass parameters

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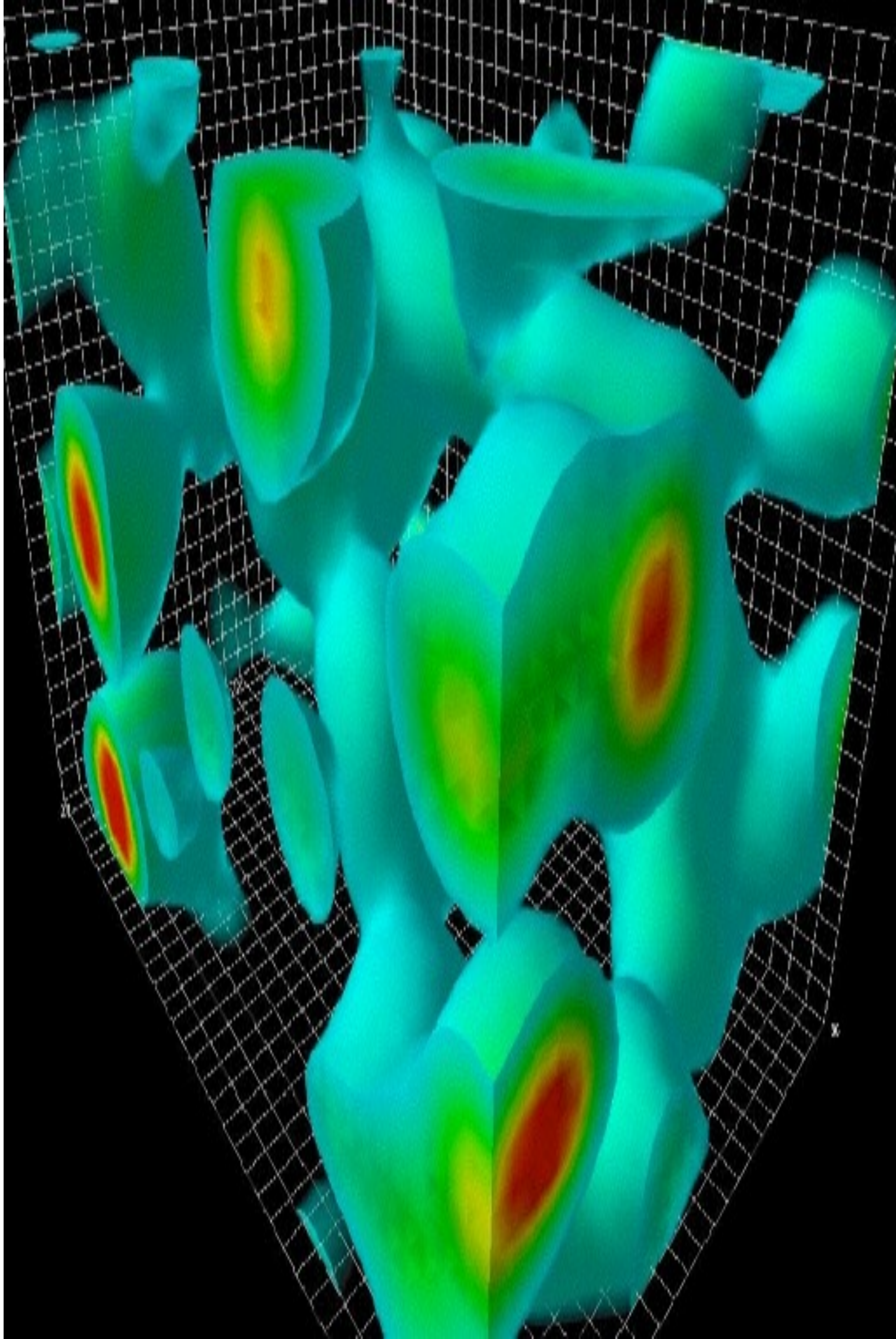
Story to be continued in next session

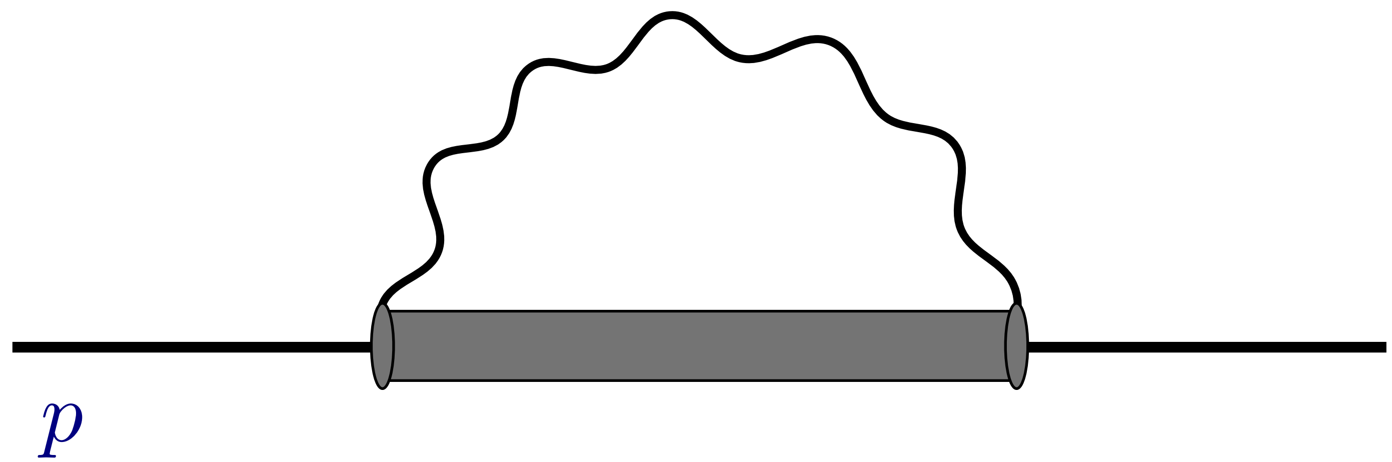


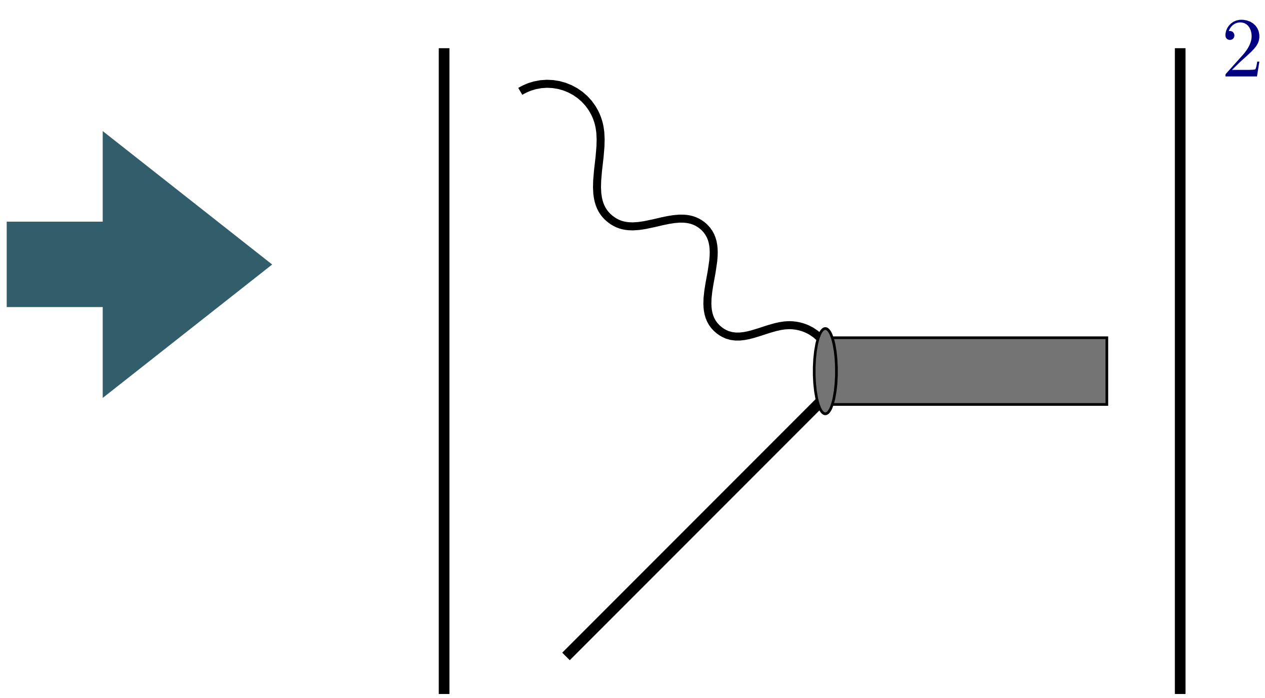
Cottingham formula and the proton–neutron mass splitting

Cottingham formula

[Cottingham 1963]

- Electromagnetic self-energy of the nucleon





Self energy computable in terms of measurable structure functions

Cottingham formula: Modern update

- **2012: Walker-Loud, Carlson & Miller**
  - *Alternative* description of subtraction term in dispersion relation
  - Modern data set

$$\delta M^{\gamma} = 1.30 \pm 0.47\,\mathrm{MeV}$$

Uncertainty dominated by inelastic subtraction

- **2014: Thomas, Wang & RY**
  - Use RBC lattice simulations (2010) to improve determination of subtraction term

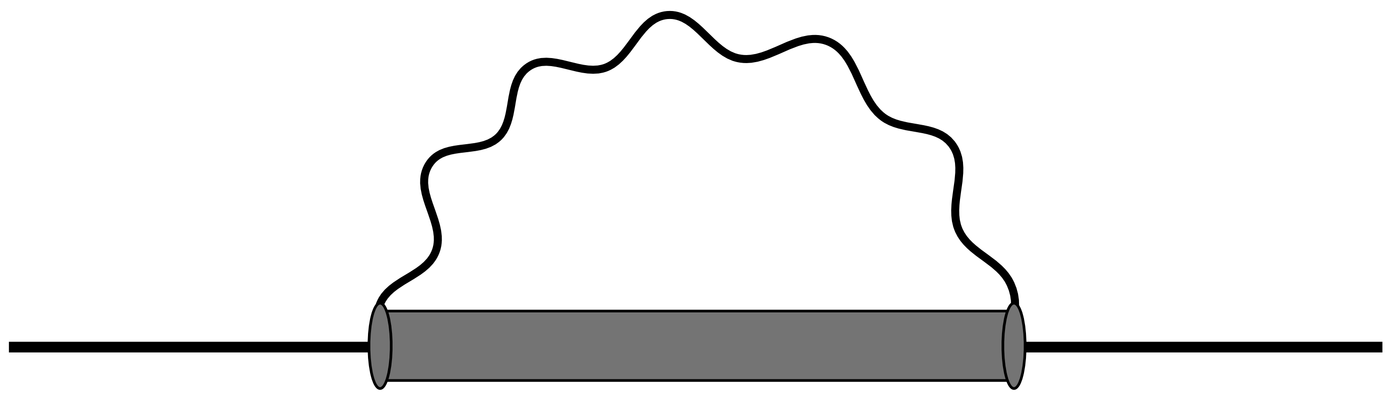
$$\delta M^{\gamma} = 1.04 \pm 0.11\,\mathrm{MeV}$$

- **2014: Erben, Shanahan, Thomas & RY**
  - Revised phenomenological extraction: OPE constraint on subtraction term

$$\delta M^{\gamma} = 0.95 \pm 0.26\,\mathrm{MeV}$$

Includes improved polarisability measurement

Cottingham Formula



- Photon self energy

$$\Sigma(p) = -ie^2 \int \frac{d^4q}{(2\pi)^4} \frac{T^{\mu}_{\mu}(p,q)}{q^2 + i\varepsilon} \qquad \delta M^{\gamma} \simeq \frac{\Sigma(p)}{2m}$$

- Forward Compton scattering tensor

$$T^{\mu\nu}(p,q) = \frac{i}{2} \sum_s \int d^4x \, e^{iq.x} \langle p, s | \mathrm{T}\left\{ j^{\mu}(x) j^{\nu}(0) \right\} | p, s \rangle$$

Compton tensor

- Tensor decomposition

$$T^{\mu\nu}(p,q) = \left(g^{\mu\nu}q^2 - q^\mu q^\nu\right) t_1(-q^2, p.q)$$
$$+ \frac{1}{M^2}\left[(p^\mu q^\nu + p^\nu q^\mu)p.q - g^{\mu\nu}(p.q)^2 - p^\mu p^\nu q^2\right] t_2(-q^2, p.q)$$

- Nucleon rest frame $\quad p = (M, \vec{0})$

$$q = (\omega, \vec{q})$$

$$T^\mu_\mu(p,q) = 3q^2 t_1(-q^2, M\omega) - (2\omega^2 + q^2)t_2(-q^2, M\omega)$$

$$\boxed{F(-q^2,\omega) \equiv 3q^2 t_1(-q^2, M\omega) - (2\omega^2 + q^2)t_2(-q^2, M\omega)}$$

Cottingham self energy

- Evaluate self energy in nucleon rest frame

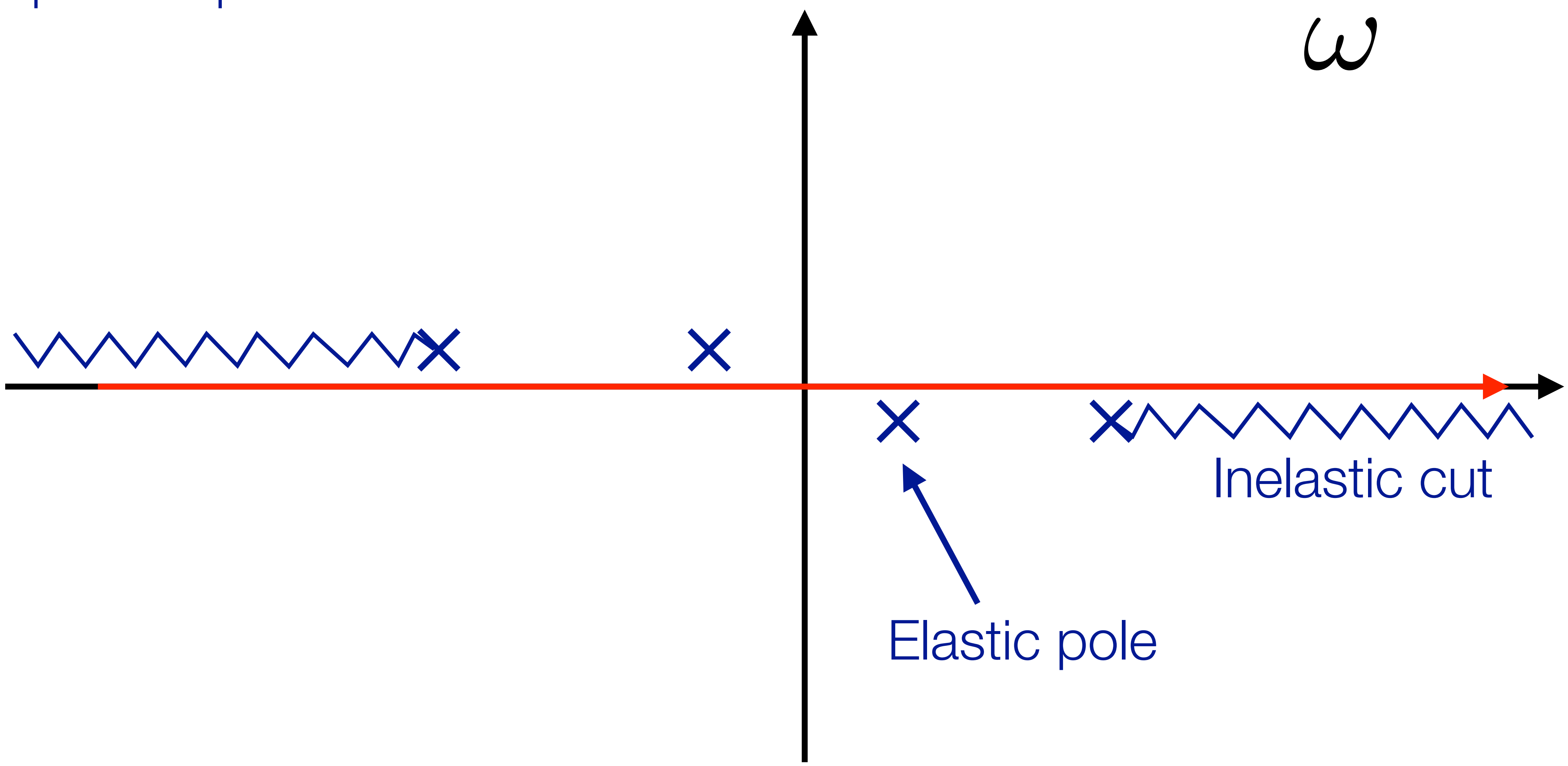
$$\Sigma(p) = -ie^2 \int \frac{d^4q}{(2\pi)^4} \frac{T^\mu_\mu(p,q)}{q^2 + i\varepsilon}$$

$$\Rightarrow \quad \Sigma(m) = i\frac{\alpha}{(2\pi)^3} \int d\vec{q} \int_{-\infty}^{\infty} d\omega \frac{F(-q^2,\omega)}{q^2 + i\varepsilon}$$

Want a Wick rotation to move away from pole

Complex energy plane

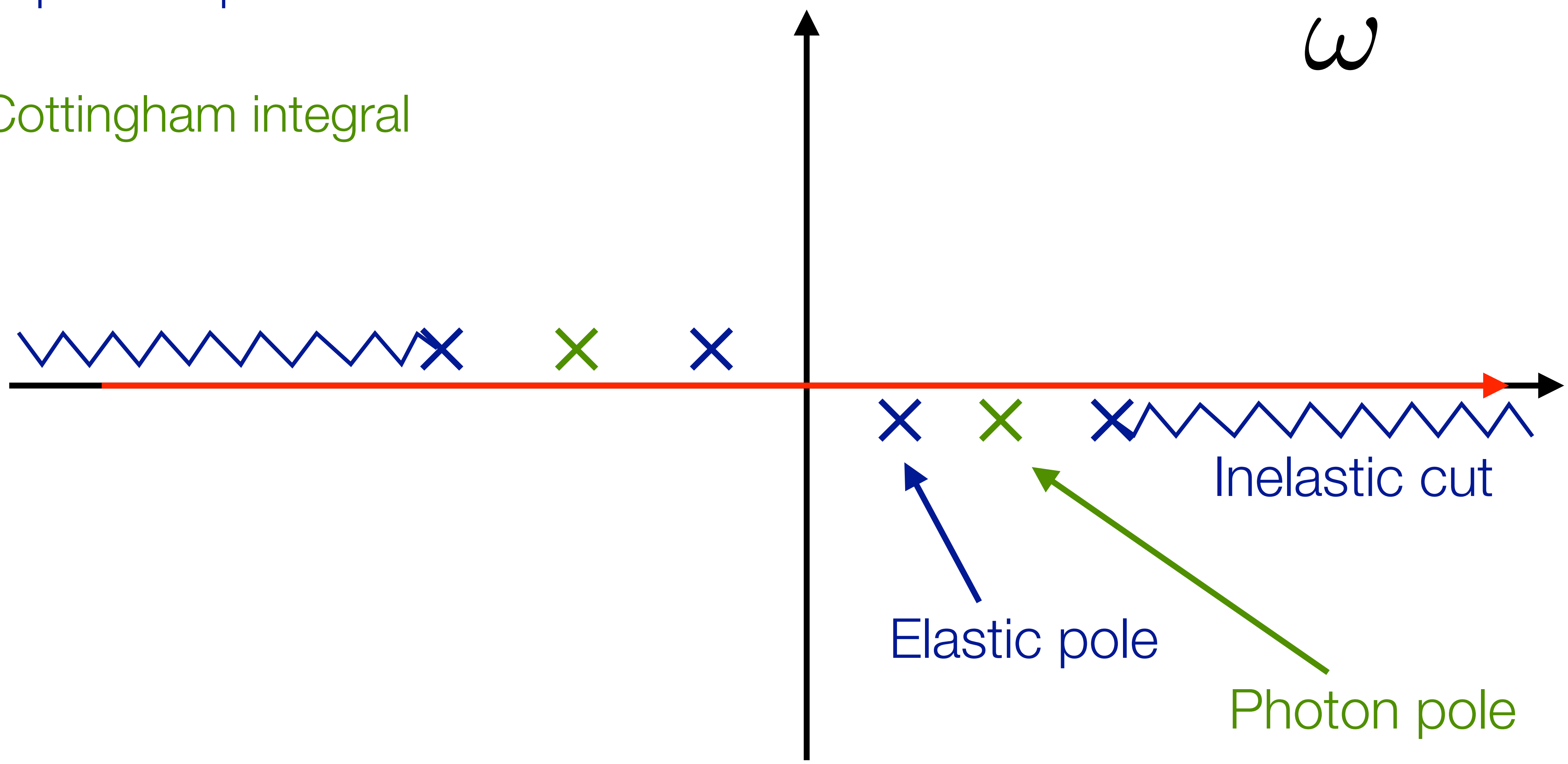
Singularity structure of
Compton amplitude



Complex energy plane

Singularity structure of Compton amplitude

and Cottingham integral



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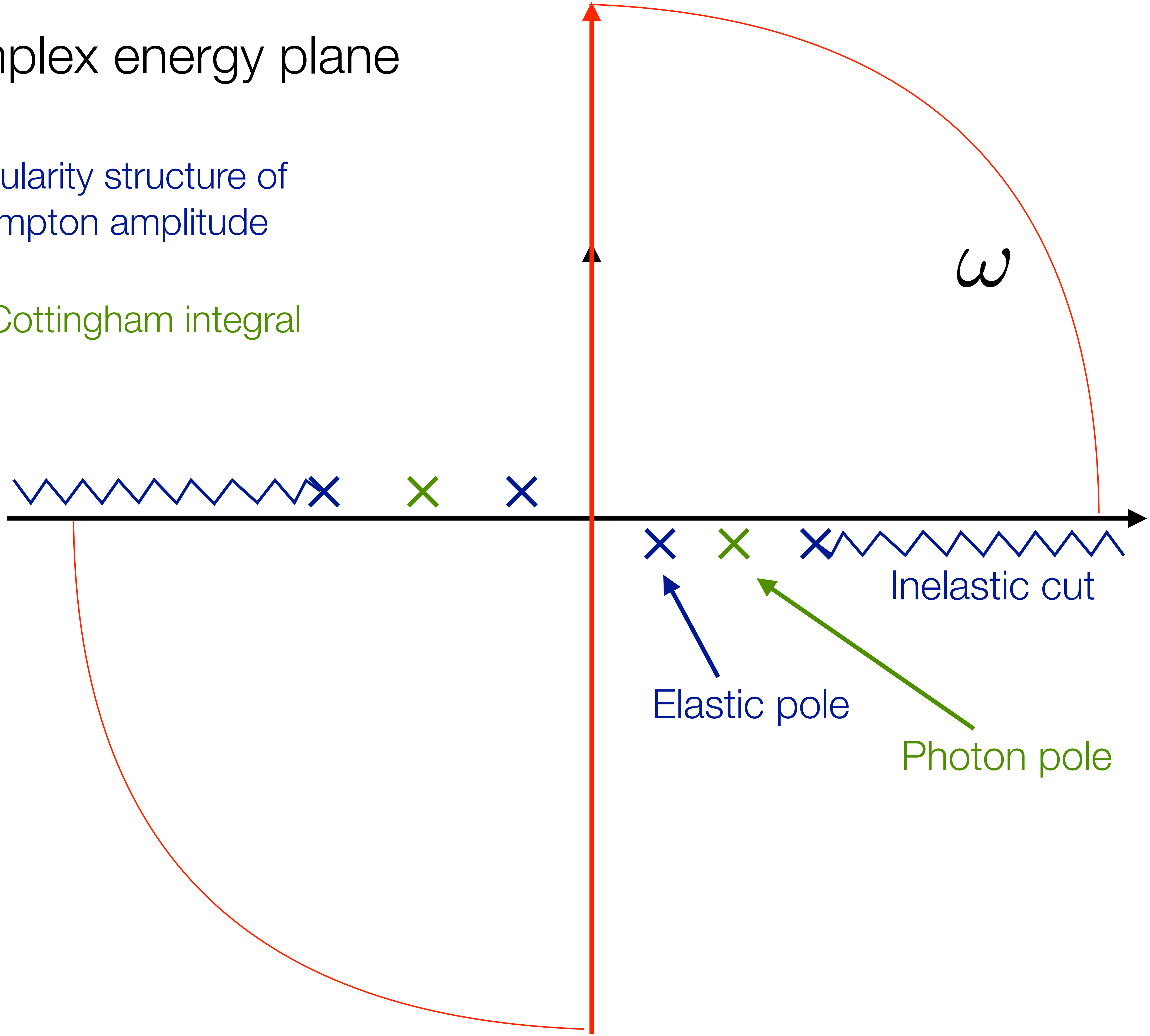

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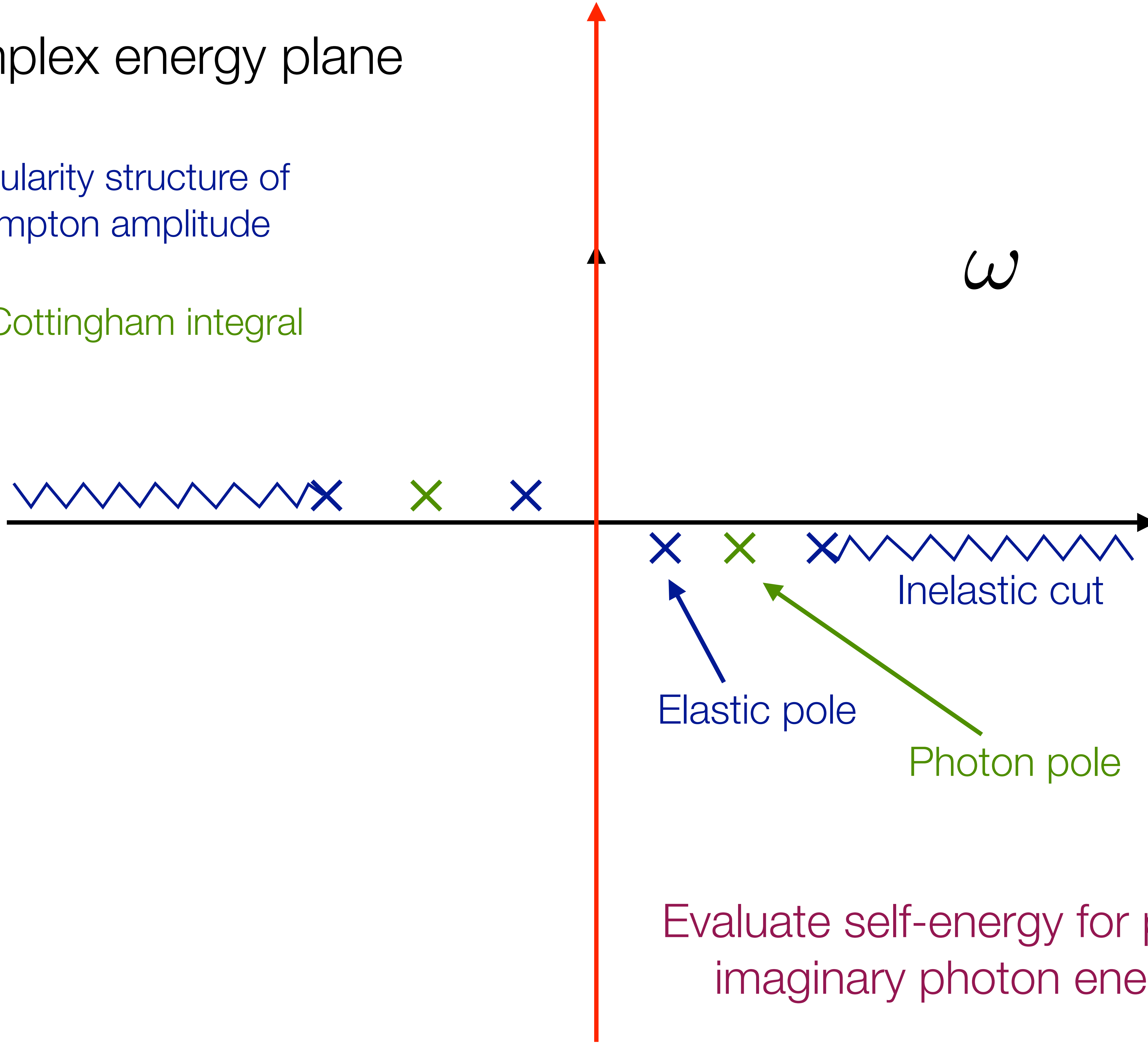


Evaluate self-energy for purely imaginary photon energy

Wick-rotated self energy

- Integrate along imaginary axis:

$$\omega \to i\omega$$

$$Q^2 = -q^2 = |\vec{q}|^2 - (i\omega)^2 = |\vec{q}|^2 + \omega^2$$

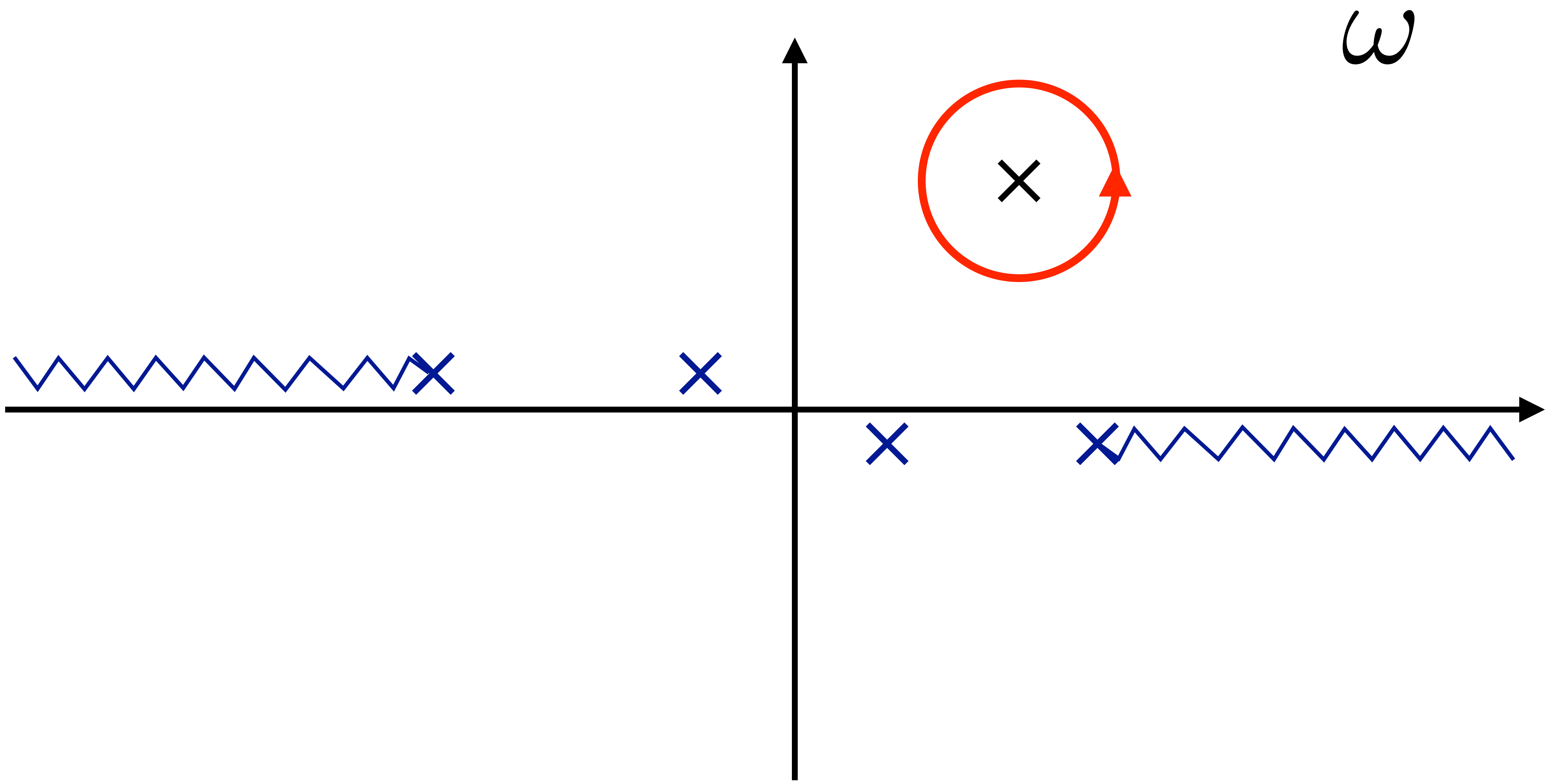
$$d\vec{q} \to 2\pi|\vec{q}|d|\vec{q}|^2 = 2\pi\sqrt{Q^2 - \omega^2}dQ^2$$

Use dispersion to evaluate Compton amplitude for imaginary energy

$$\Sigma(m) = i\frac{\alpha}{(2\pi)^3}\int d\vec{q}\int_{-\infty}^{\infty} d\omega \frac{F(-q^2,\omega)}{q^2 + i\varepsilon}$$

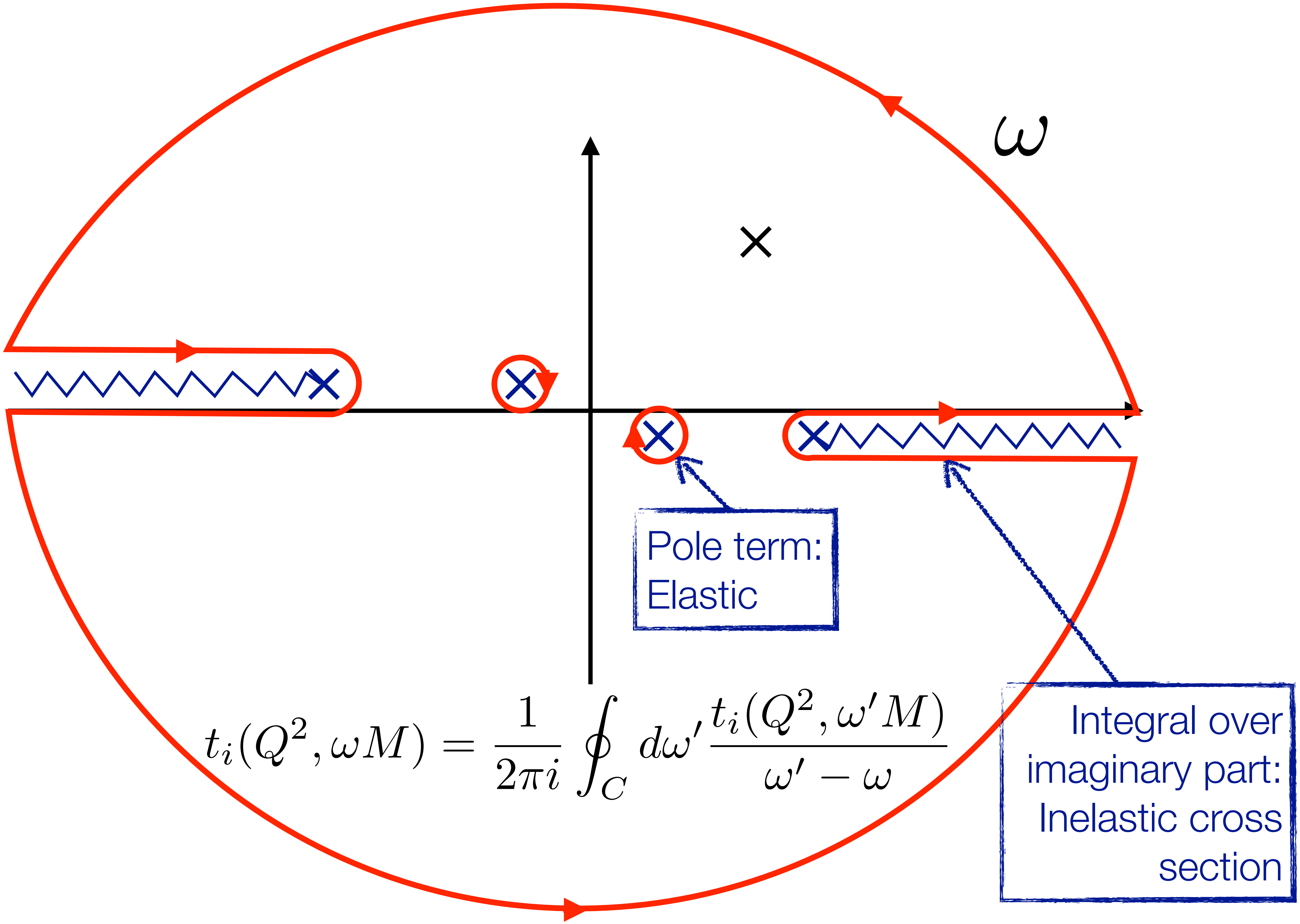
$$= -i\frac{\alpha}{(2\pi)^2}\int_0^{\Lambda^2}\frac{dQ^2}{Q^2}\int_{-Q}^{Q} d\omega\sqrt{Q^2-\omega^2}F(Q^2, i\omega)$$

Want to evaluate $t_i(Q^2, i\omega M)$



$$t_i(Q^2, \omega M) = \frac{1}{2\pi i} \oint_C d\omega' \frac{t_i(Q^2, \omega' M)}{\omega' - \omega}$$

Want to evaluate $t_i(Q^2, i\omega M)$



Subtractions?

- IF t_i vanishes fast enough for $\omega \to \infty$, we can neglect arc contributions

$$\omega \to \infty : \quad t_1 \sim \omega^{\alpha}$$

$$t_2 \sim \omega^{\alpha-2}$$

α : Regge parameter

$$\Sigma(m) = -i\frac{\alpha}{(2\pi)^2}\int_0^{\Lambda}\frac{dQ^2}{Q^2}\int_{-Q}^{Q} d\omega\sqrt{Q^2-\omega^2}F(Q^2,i\omega)$$

$$F(Q^2,i\omega) = -3Q^2 t_1(Q^2,i\omega M) + (2\omega^2+Q^2)t_2(Q^2,i\omega M)$$

Require subtraction term to define t_1 contribution

Implementing subtraction

a la Walker-Loud *et al*.

- Subtract structure function at zero energy

$$t_1(Q^2, i\omega M) - t_1(Q^2, 0) = \frac{1}{2\pi i}\oint_C d\omega' \frac{t_i(Q^2, \omega' M)}{\omega' - i\omega} - \frac{1}{2\pi i}\oint_C d\omega' \frac{t_i(Q^2, \omega' M)}{\omega'}$$

$$t_1(Q^2, i\omega M) = t_1(Q^2, 0) + \frac{1}{2\pi i}\oint_C d\omega' \frac{\omega}{\omega'^2 - i\omega'\omega} t_i(Q^2, \omega' M)$$

- Evaluate dispersion integral at poles and along cut

$$\Rightarrow t_1(Q^2, i\omega M) = \underbrace{t_1(Q^2, 0)}_{\text{“Subtraction” term}} - \underbrace{\frac{2i\omega}{\omega^2 + \omega_{\rm el}^2} t_1(Q^2, \omega_{\rm el} M)}_{\text{Elastic part}} + \underbrace{\frac{2}{\pi}\int_{\omega_{\rm th}}^{\infty} d\omega' \frac{\omega' \,\mathrm{Im}\, t_1(Q^2, \omega')}{\omega'^2 - i\omega'\omega}}_{\text{Inelastic part}}$$

Putting it all together

- Elastic:

$$\delta M^{\mathrm{el}} = \frac{\alpha}{\pi}\int_0^{\Lambda_0^2} dQ\left\{\frac{3\sqrt{\tau_{\mathrm{el}}}G_M^2}{2(1+\tau_{\mathrm{el}})} + \frac{[G_E^2 - 2\tau_{\mathrm{el}}G_M^2]}{1+\tau_{\mathrm{el}}} \times\left[(1+\tau_{\mathrm{el}})^{3/2} - \tau_{\mathrm{el}}^{3/2} - \frac{3}{2}\sqrt{\tau_{\mathrm{el}}}\right]\right\}$$

- Inelastic:

$$\delta M^{\mathrm{inel}} = \frac{\alpha}{\pi}\int_0^{\Lambda_0^2}\frac{dQ^2}{2Q}\int_{\nu_{th}}^{\infty} d\nu \times\left\{\frac{3F_1(\nu,Q^2)}{M}\left[\frac{\tau^{3/2} - \tau\sqrt{1+\tau} + \sqrt{\tau}/2}{\tau}\right] + \frac{F_2(\nu,Q^2)}{\nu}\left[(1+\tau)^{3/2} - \tau^{3/2} - \frac{3}{2}\sqrt{\tau}\right]\right\},$$

- Subtraction:

$$\delta M^{\mathrm{sub}} = -\frac{3\alpha}{16\pi M}\int_0^{\Lambda_0^2} dQ^2 T_1(0,Q^2),$$

Numerical estimates

$\Lambda^2 = 2\,\mathrm{GeV}^2$

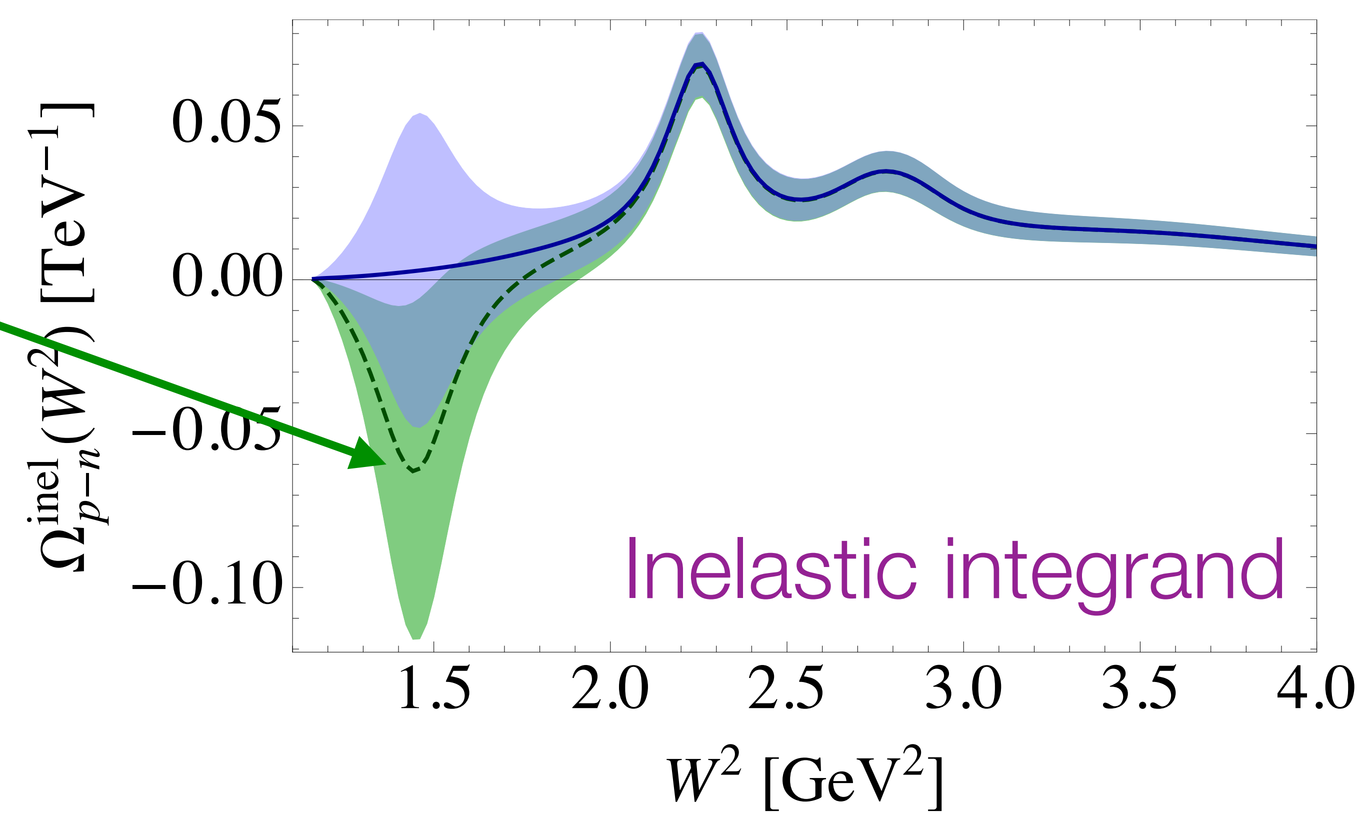
- Elastic:

$$\delta M^{\gamma}_{\mathrm{el}} = 1.39(02)\,\mathrm{MeV} \qquad \text{WCM(2012)}$$
$$\delta M^{\gamma}_{\mathrm{el}} = 1.40(01)\,\mathrm{MeV} \qquad \text{ESTY(2014)}$$

- Inelastic:

$$\delta M^{\gamma}_{\mathrm{inel}} = 0.057(16)\,\mathrm{MeV} \qquad \text{WCM(2012)}$$
$$\delta M^{\gamma}_{\mathrm{inel}} = 0.089(42)\,\mathrm{MeV} \qquad \text{ESTY(2014)}$$

Christy–Bosted parameterisation of structure functions



$\gamma^* p \to \Delta^+$
$\gamma^* n \to \Delta^0$

$\sim 18\%$ violation of charge symmetry

Numerical estimates

- Subtraction term:

$$\delta M^{\rm sub} = -\frac{3\alpha}{16\pi M}\int_0^{\Lambda_0^2} dQ^2 T_1(0, Q^2),$$

  - Two pieces (WCM), based on low-energy expansion:

$$T_1(0,Q^2) \simeq \underline{2G_M^2(Q^2) - 2F_1^2(Q^2)} + Q^2 2M \frac{\beta_M}{\alpha}\left(\frac{m_0^2}{m_0^2+Q^2}\right)^2,$$

"Elastic"

"Form factor" to give correct asymptotic scaling dimension

Polarisability

$\delta M^{\gamma}_{\rm sub\ el} = -0.62(2)\,\mathrm{MeV}$ WCM(2012)

$\delta M^{\gamma}_{\rm sub\ el} = -0.635(7)\,\mathrm{MeV}$ ESTY(2014)

Inelastic subtraction term

- Walker-Loud et al.:

$$T_1^{\mathrm{inel}}(Q^2,0) = Q^2 2M \frac{\beta_M}{\alpha}\left(\frac{m_0^2}{m_0^2+Q^2}\right)^2$$

- Renormalisation of Cottingham formula [Collins]

$$T_1(Q^2,0) \sim \frac{1}{Q^2}$$

  - Coefficient*:

$$-\frac{8}{9}M_N\left(\frac{4m_u-m_d}{m_u+m_d}\right)(\sigma_u-\sigma_d) \qquad \mathcal{O}(\alpha(m_u-m_d))$$

Coefficient* from polarisability factor ~400 too big!!

$$T_1^{\mathrm{inel}}(Q^2,0) \sim Q^2 2M \frac{\beta_M}{\alpha}\left(\frac{m_0^2}{m_0^2+Q^2}\right)^3$$

*Note: term involving isovector momentum fraction missing from ESTY paper; numerical effect ~0.02 MeV.

Inelastic subtraction term

- Numerical estimates:

$$\delta M^{\gamma}_{\text{sub inel}} = 0.47(47)\,\text{MeV} \qquad \text{WCM(2012)}$$

$$\delta M^{\gamma}_{\text{sub inel}} = 0.18(35)\,\text{MeV} \qquad \text{ESTY(2014)}$$

With improved constraint from OPE

Summary phenomenological determination

- Walker-Loud, Carlson & Miller (2012)

$$\delta M^{\gamma} = 1.30 \pm 0.47\,\mathrm{MeV}$$

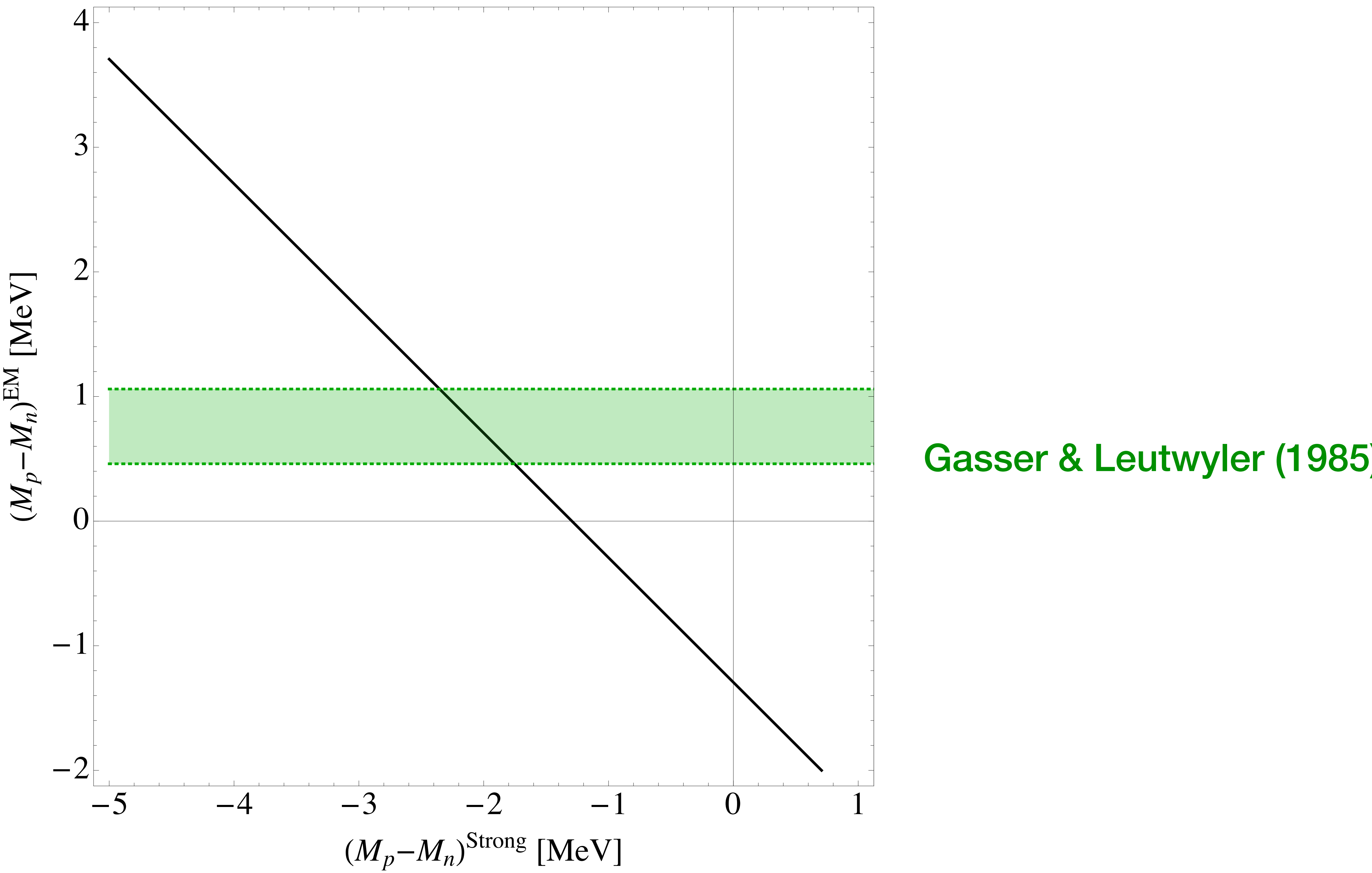
- Erben, Shanahan, Thomas & RY (2014)

$$\delta M^{\gamma} = 1.04 \pm 0.35\,\mathrm{MeV}$$

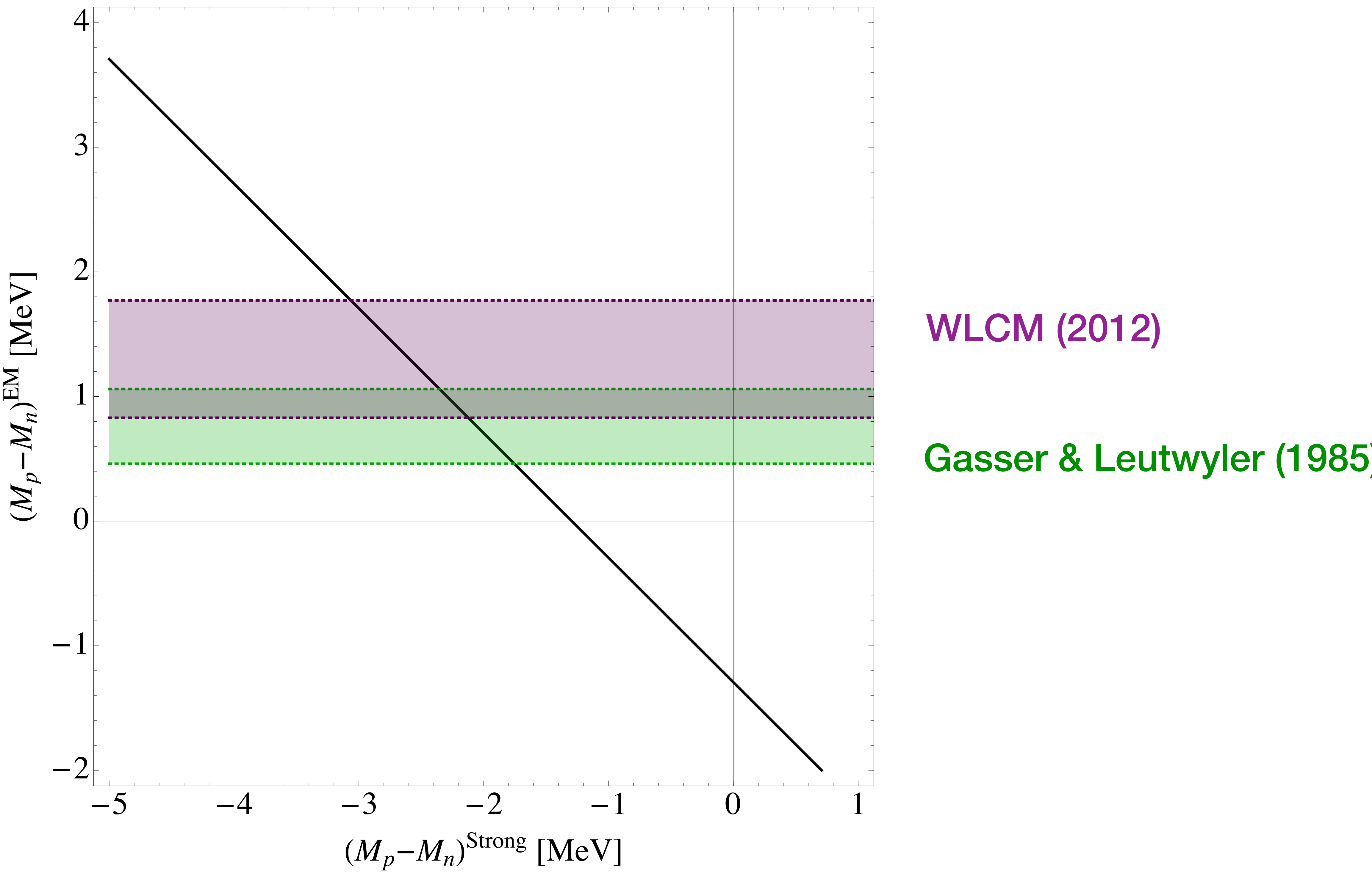
* Suppressed large CSV in Delta region
* Improved constraint from OPE

With COMPTON@MAX-lab result

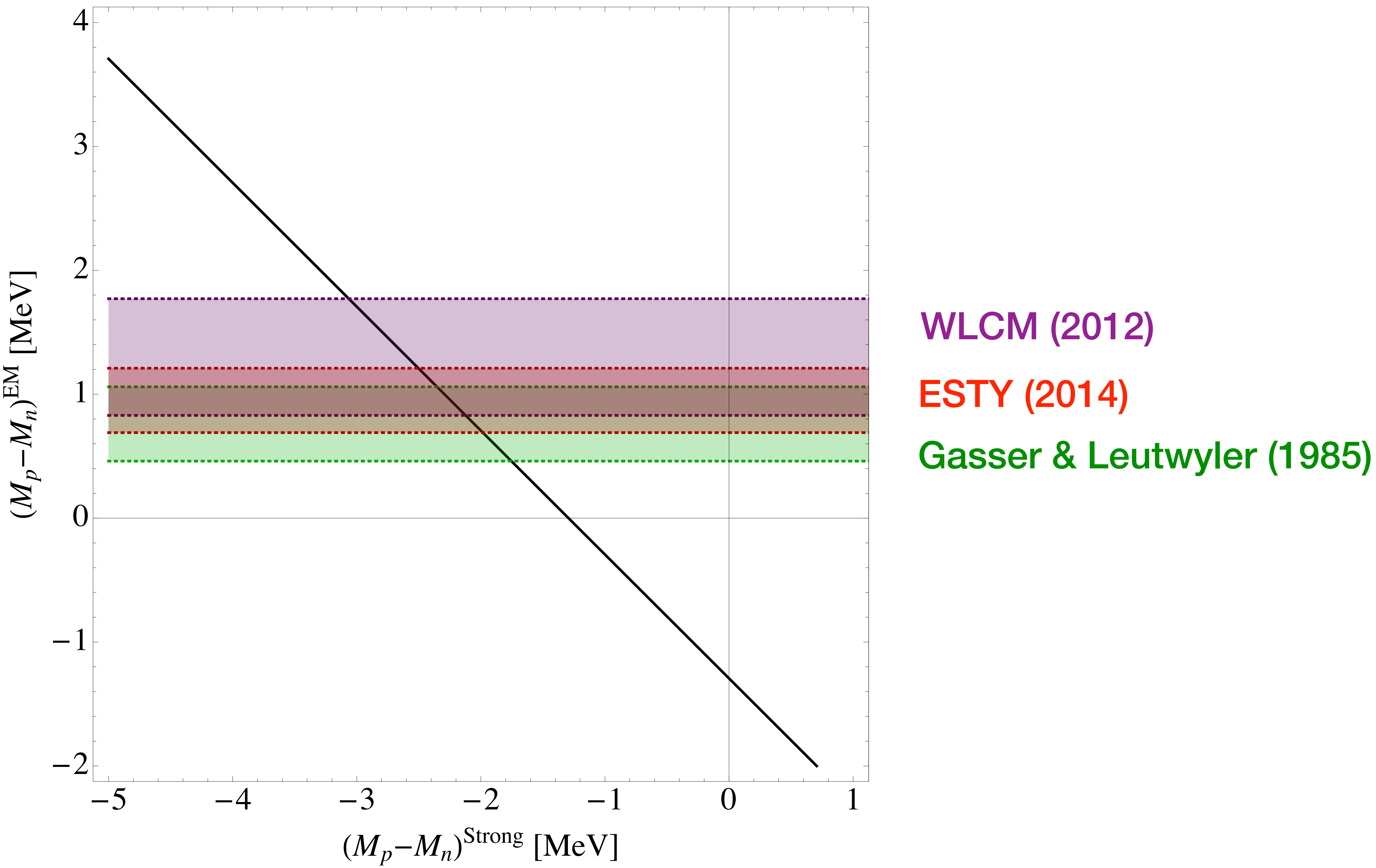
$$\boxed{\delta M^{\gamma} = 0.95 \pm 0.26\,\mathrm{MeV}}$$



p-*n* summary | Cottingham results



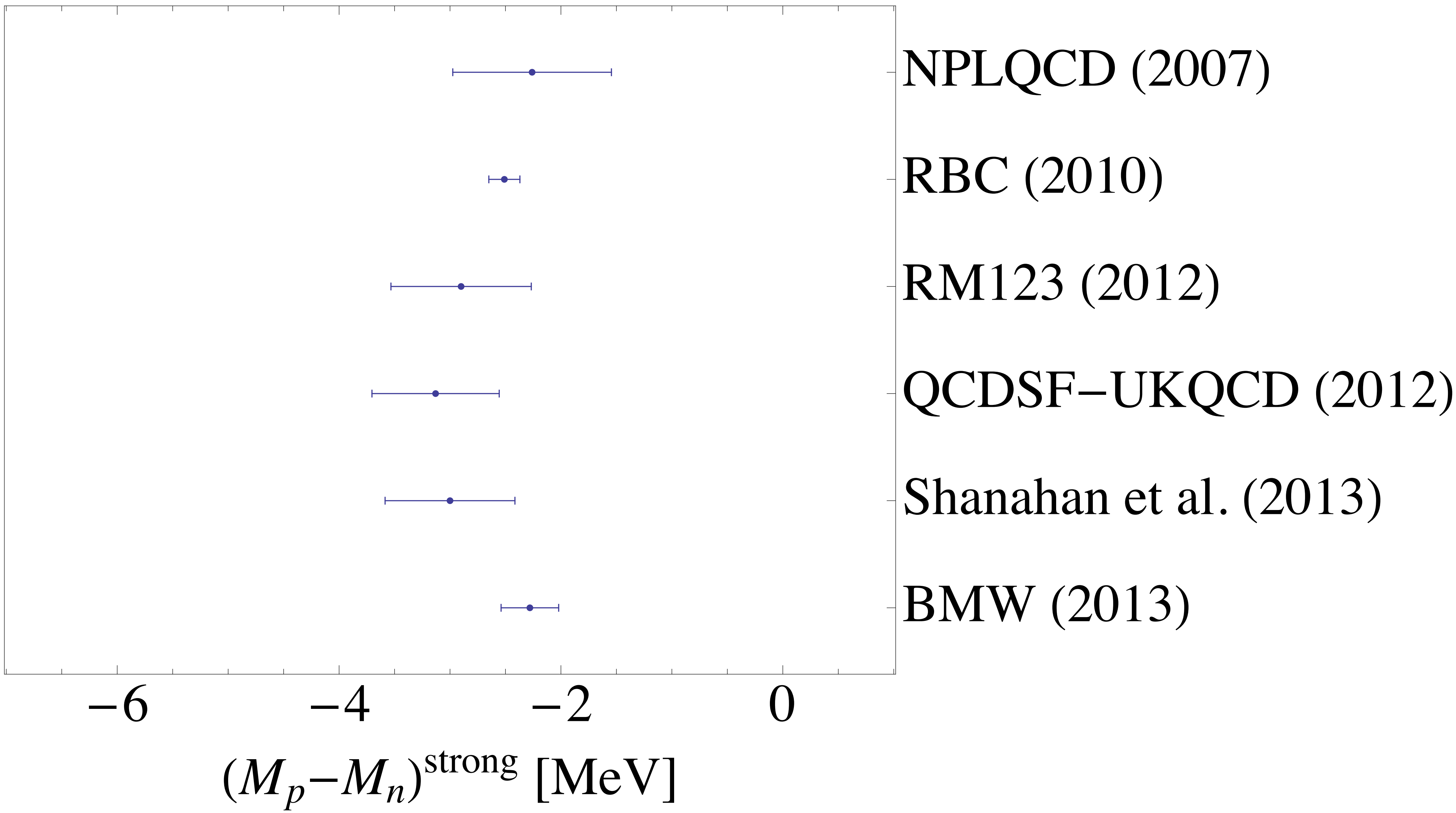
p-n summary | Cottingham results



p-n summary

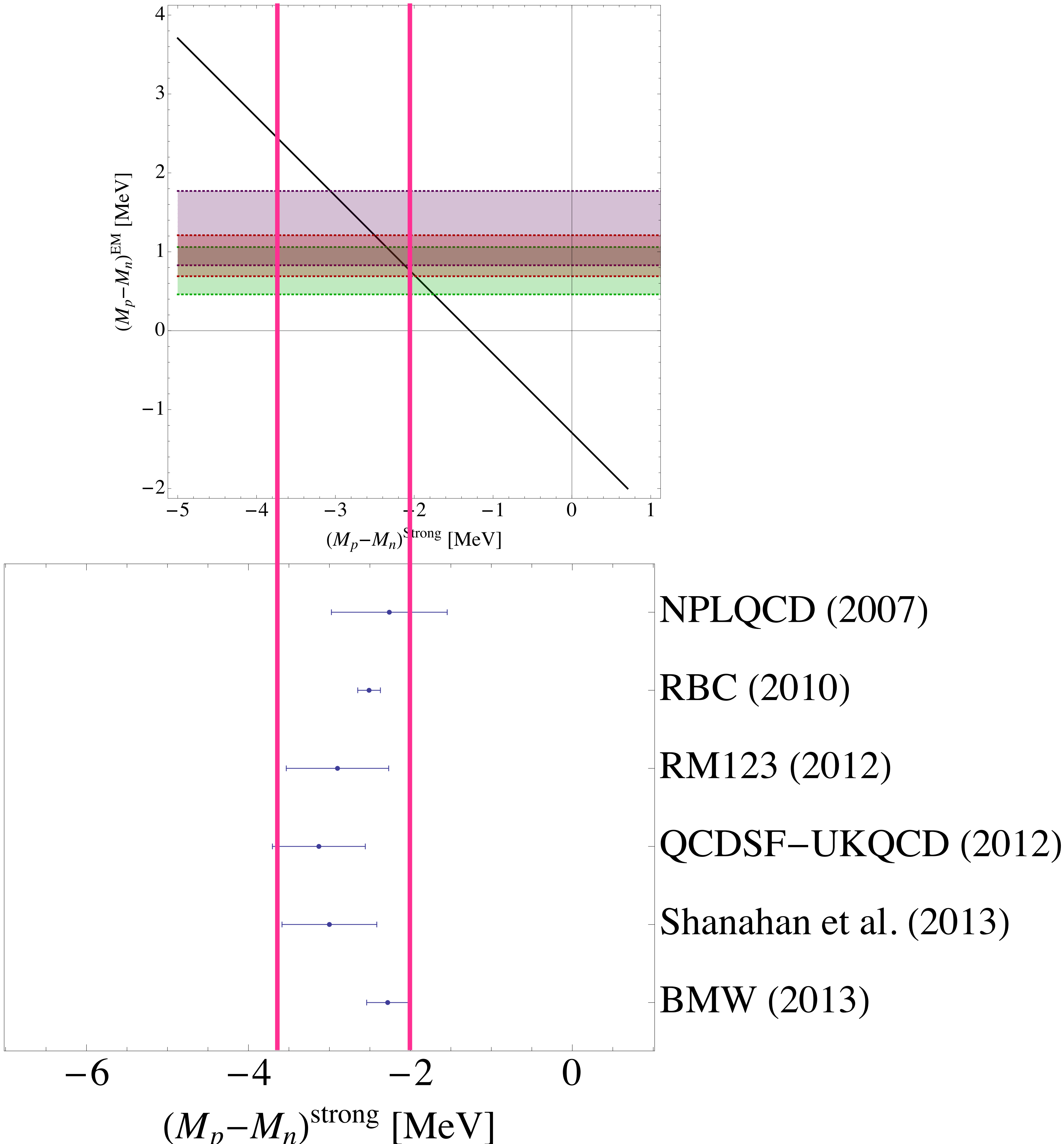
Cottingham results

Proton–neutron:
Strong mass difference



Lattice QCD: Strong *p*–*n*

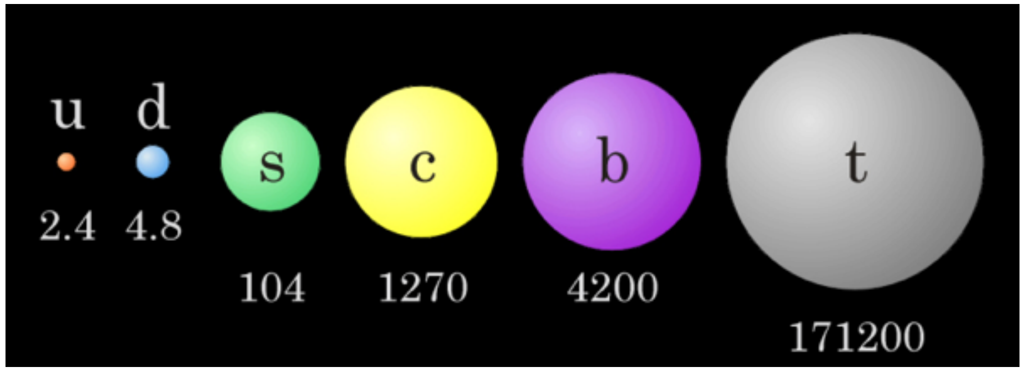
Status ~2013



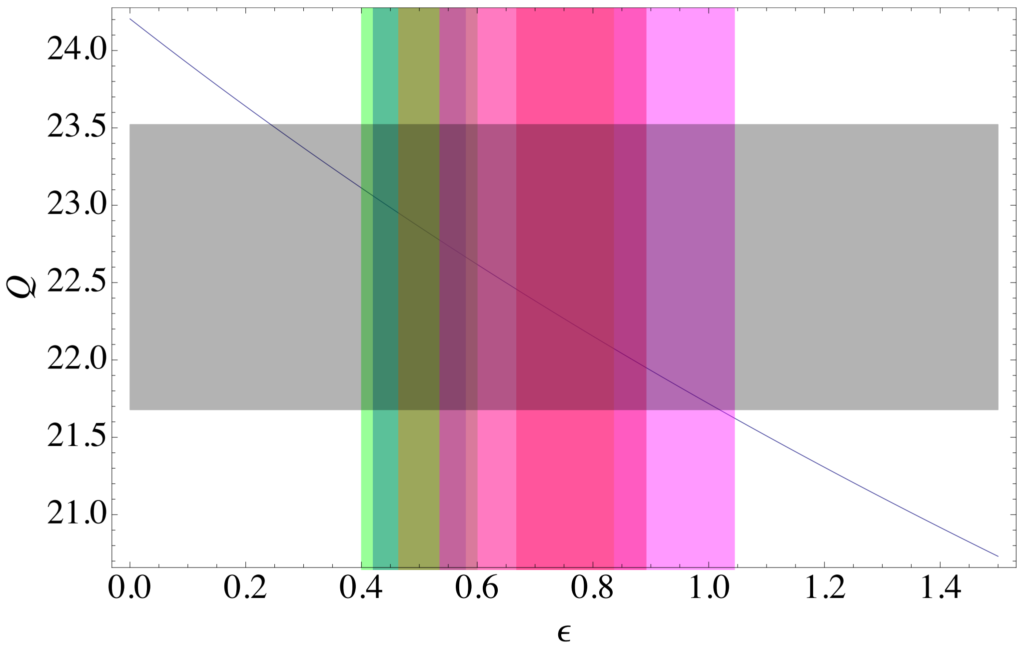
$(M_p - M_n)^{\mathrm{EM}}$ [MeV]
$(M_p - M_n)^{\mathrm{Strong}}$ [MeV]
NPLQCD (2007)
RBC (2010)
RM123 (2012)
QCDSF−UKQCD (2012)
Shanahan et al. (2013)
BMW (2013)
$(M_p - M_n)^{\mathrm{strong}}$ [MeV]

Summary: Part I

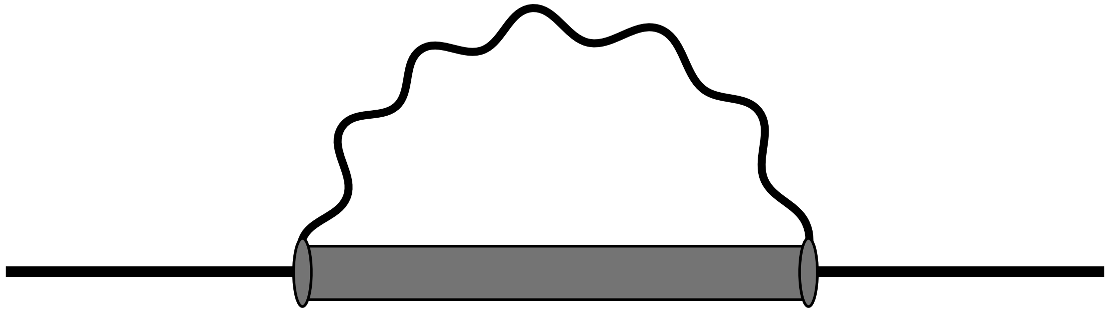
- Quark masses are the **exciting** parameters of QCD



- Violation of Dashen's theorem vital input to resolving quark mass parameters from spectrum

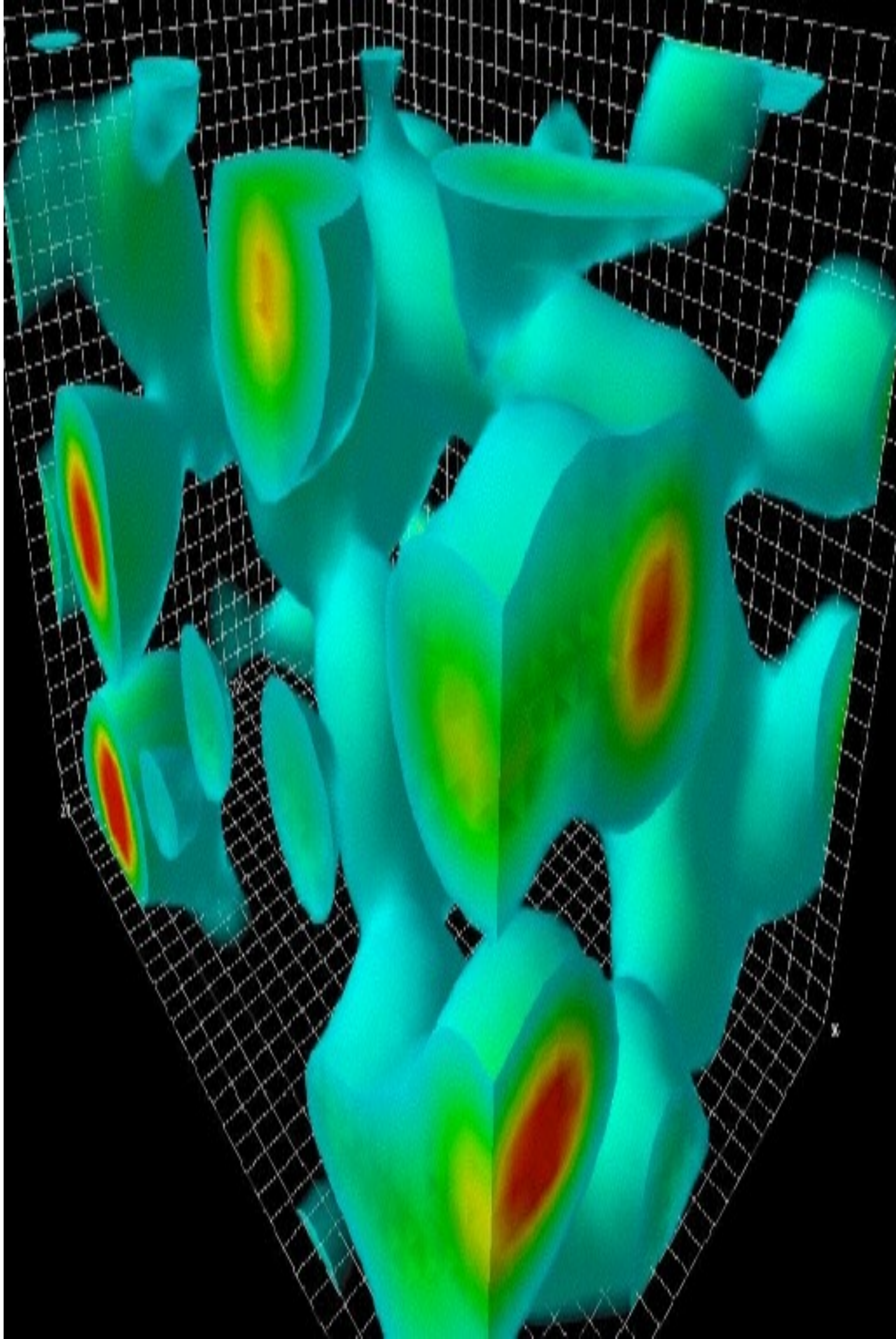


- Cottingham formula isolates electromagnetic component of *p*–*n* mass splitting
    - Compatible with strong determinations in lattice QCD



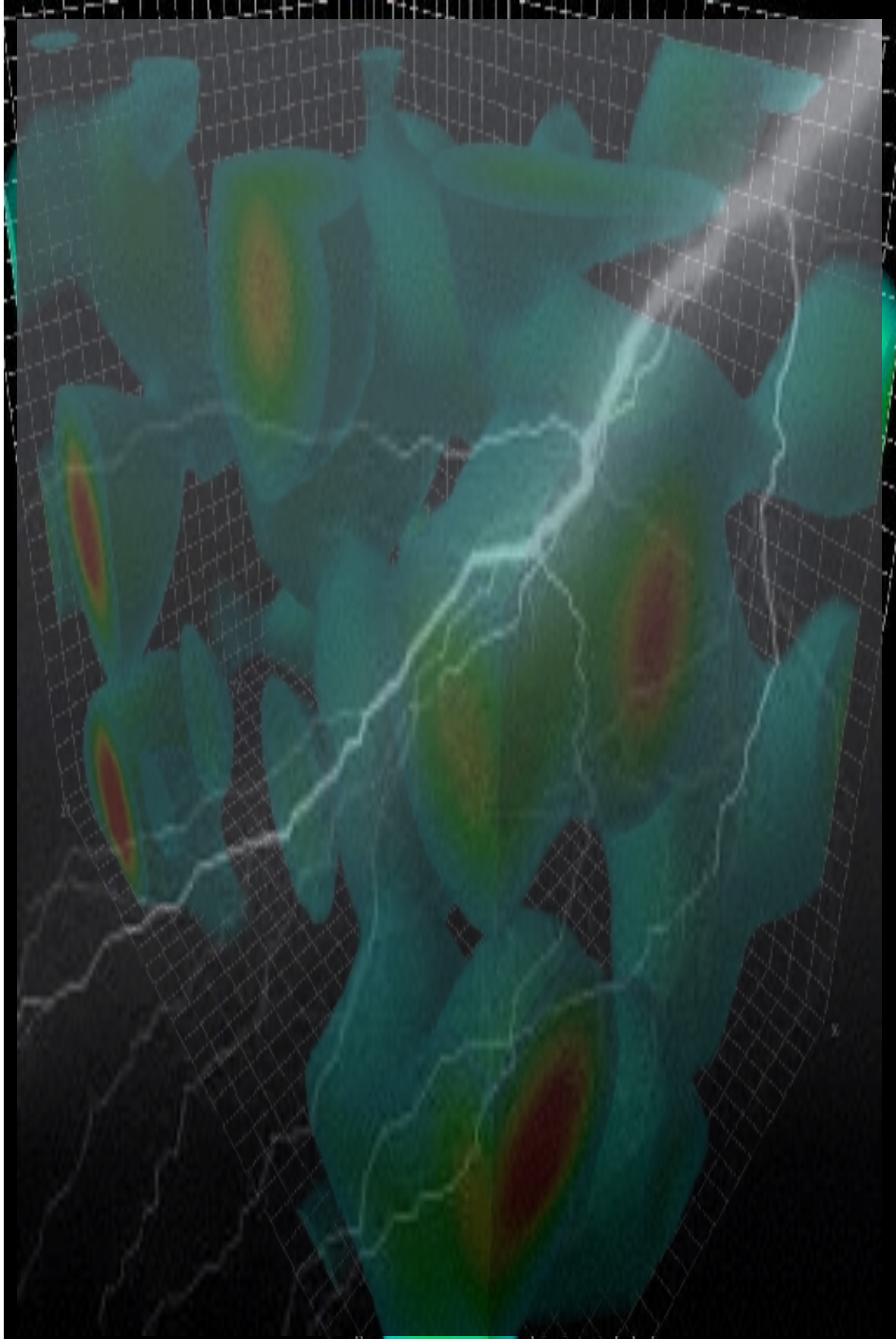
Part II

Electromagnetism in lattice simulations



Part II

Electromagnetism in lattice simulations



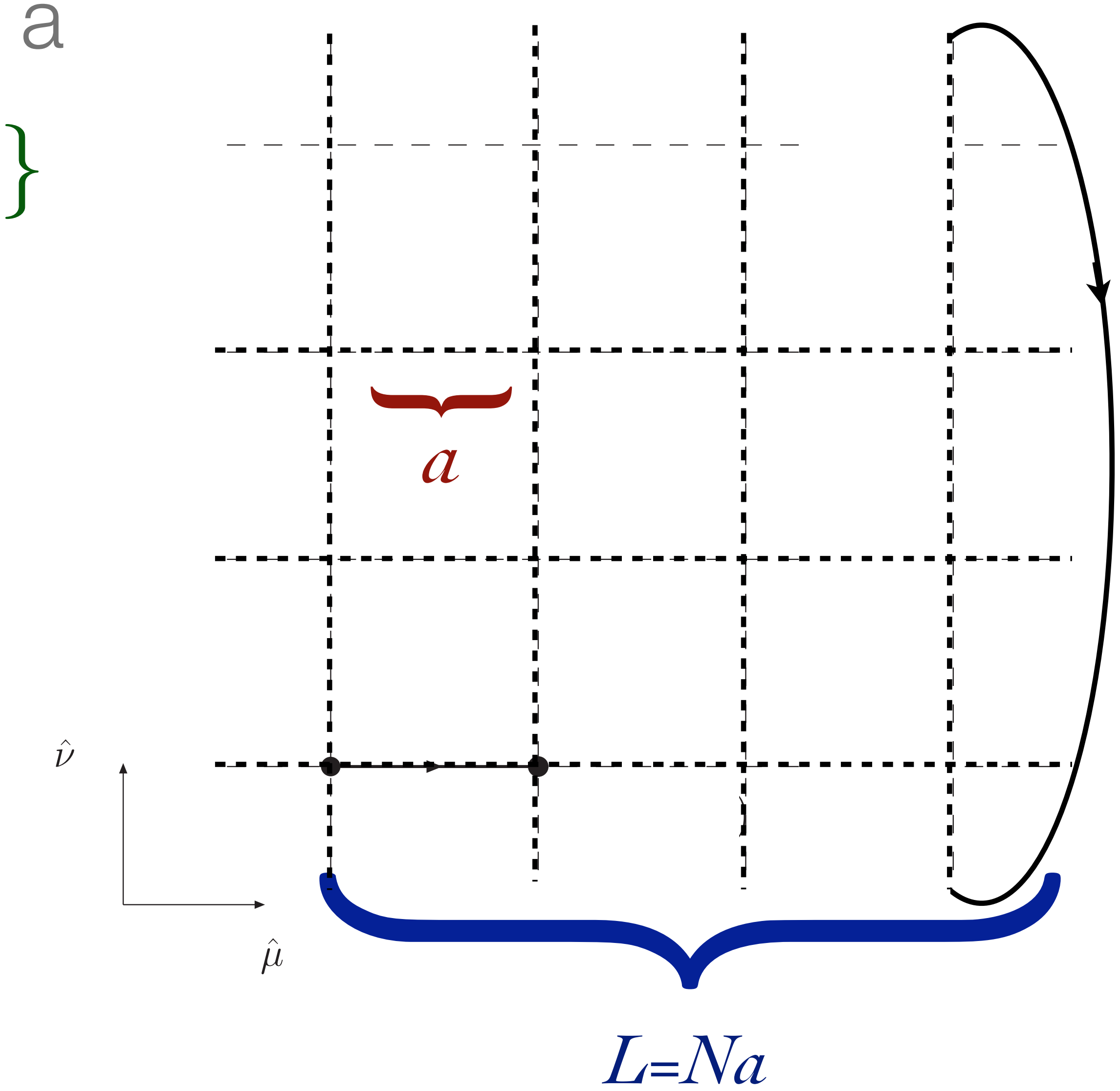
Ken Wilson (1974)

Lattice QCD

- Work in Euclidean space $t \to i\tau$
- Discretise spacetime, lattice spacing, a

$$\mathbb{L} \subset a\mathbb{Z}^4 = \{x | x^\mu = a n^\mu,\, n \in \mathbb{Z}^4\}$$

- Finite lattice:
  - Typically periodic boundary conditions
  - Theory formulated on "4-torus"



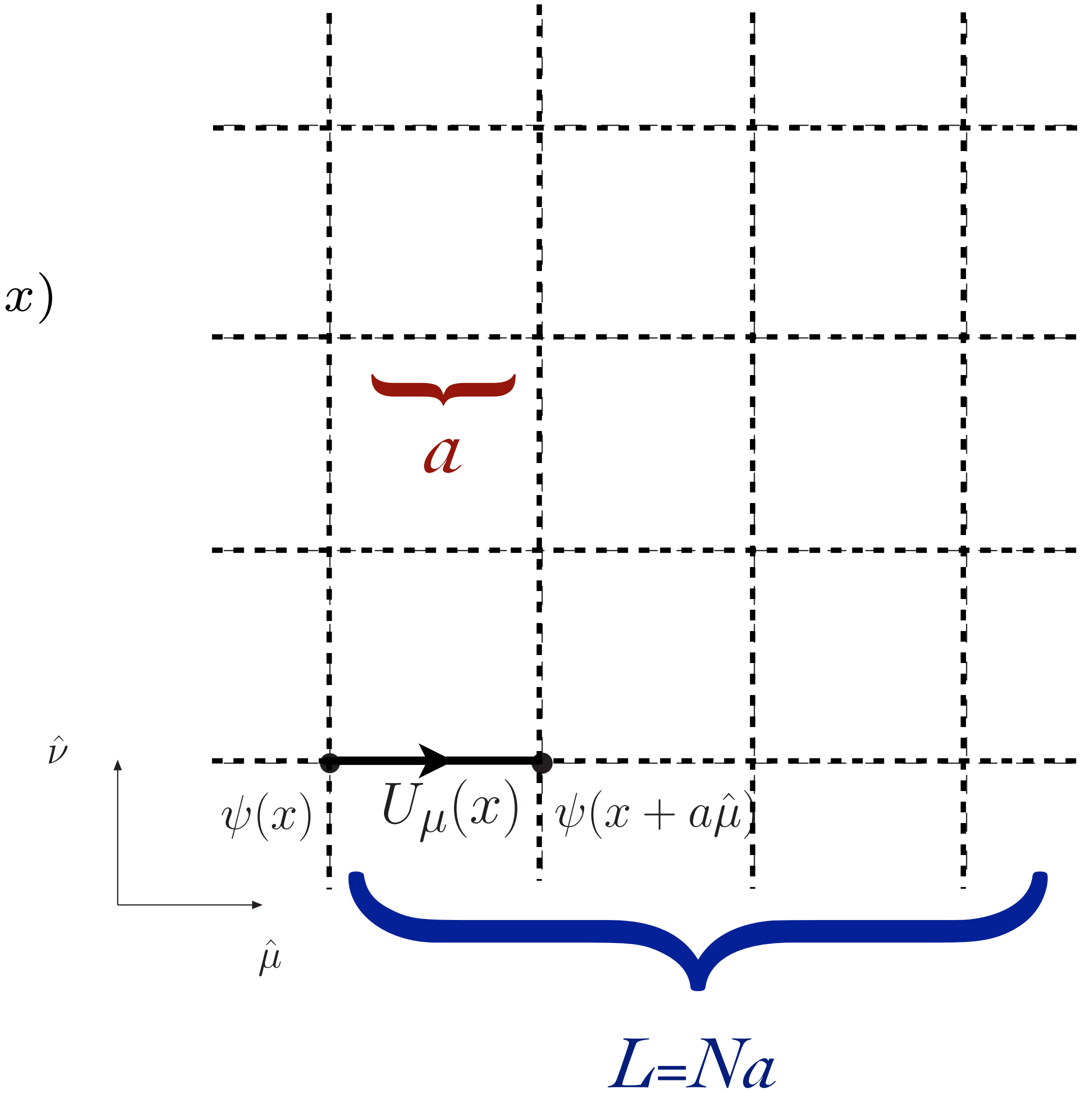
Ken Wilson (1974)

Lattice QCD

- Quark fields reside on sites: $\psi(x)$
- Gauge fields on links: $U_\mu(x) = e^{-iagA_\mu(x)}$
- Correlation functions evaluated as expectation values of path integral

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A\mathcal{D}\bar{\psi}\mathcal{D}\psi\, \mathcal{O}[A,\bar{\psi},\psi]\, e^{-S[A,\bar{\psi},\psi]}$$

- Compute approximately by Monte Carlo methods



$$\langle \mathcal{O} \rangle \simeq \frac{1}{N_{\rm conf}} \sum_i^{N_{\rm conf}} \mathcal{O}([U^{[i]}])$$

Field configurations statistically sampled according to weight: $\exp\left(-S[U]\right)$

Masses in Lattice QCD

- Correlation function
  - $$C_N(t,\vec{p}) = \sum_{\vec{x}} e^{i\vec{p}.\vec{x}} \langle \Omega | \chi_N(x) \overline{\chi}_N(0) | \Omega \rangle$$

Insert a complete set of states; integrate x; use translational inv.

$$= \sum_{\alpha} e^{-E_\alpha(\vec{p})t} \langle \Omega | \chi_N(0) | \alpha(\vec{p}) \rangle \langle \alpha(\vec{p}) | \overline{\chi}_N(0) | \Omega \rangle \ .$$

- Sum of exponentials; as $t \longrightarrow \infty$, project out lowest-lying eigenstates

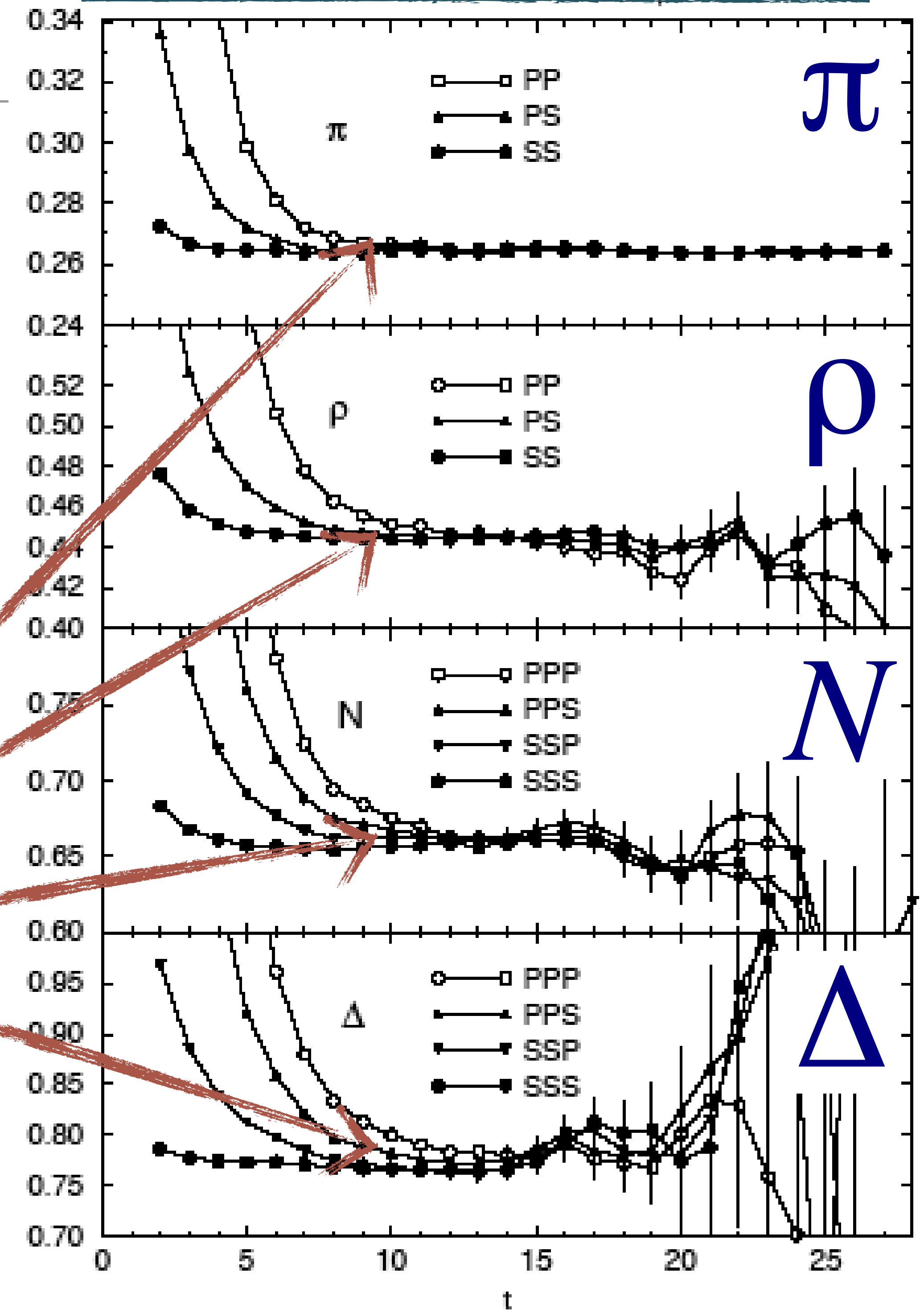
$$\lambda_0 e^{-m_0 t} + \lambda_1 e^{-m_1 t} + \ldots$$

Masses in Lattice QCD

Effective mass plots

$$M_{\text{eff}} = \log \frac{C(t)}{C(t+1)}$$

Ground-state masses from plateau

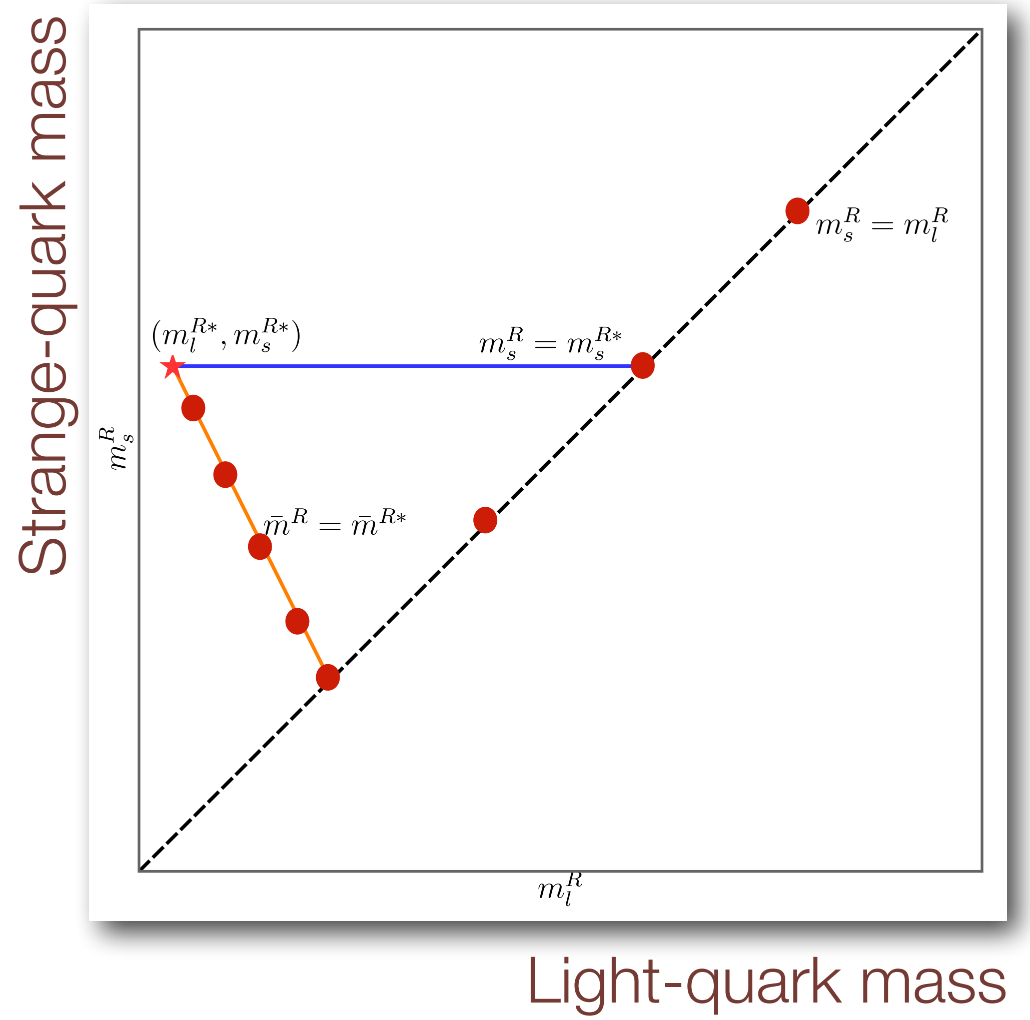


[Aoki et al. [CP-PACS] PRD67 (2003), 034503]

Tuning Nf = 2+1

- Choosing path to physical point
- Start on SU(3)-symmetric line
- Approach physical point by:
    - eg. keeping m_s fixed
- Keep the singlet quark mass fixed:

$$\overline{m}^R = \frac{1}{3}(2m_l^R + m_s^R)$$



Constant singlet-mass trajectory

- Flavour singlet quantities are "flat" at the symmetric point
    - Consider flavour-singlet observable X_S, then at SU(3)-symmetric point:

$$\frac{\partial X_S}{\partial m_u} = \frac{\partial X_S}{\partial m_d} = \frac{\partial X_S}{\partial m_s}$$

    - along our trajectory $(d\bar{m} = 0)$

$$dm_s = -dm_u - dm_d = -2dm_l$$

$$\boxed{dX_S = dm_u \frac{\partial X_S}{\partial m_u} + dm_d \frac{\partial X_S}{\partial m_d} + dm_s \frac{\partial X_S}{\partial m_s} = 0}$$

- Singlet quantities will therefore be close to their physical values at the SU(3) symmetric "starting point"
    - Good scale determination

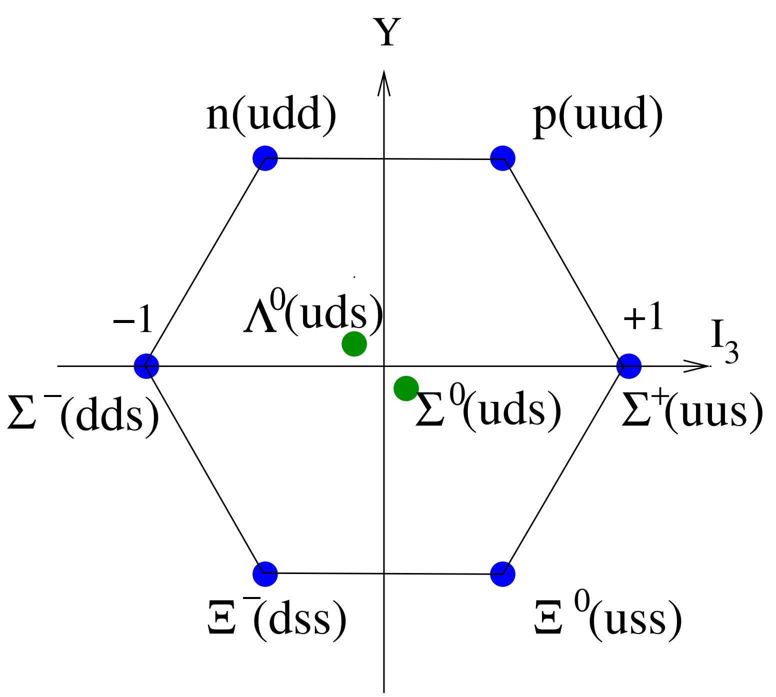
Flavour-singlet tuning

- Choose flavour-singlet observables, eg.
  - Octet baryons (centre of mass):

$$X_N = \frac{1}{3}\left(m_N + m_\Sigma + m_\Xi\right) = 1.15\,\mathrm{GeV}$$

  - Octet mesons (centre of mass):

$$X_\pi = \sqrt{\tfrac{1}{3}(2m_K^2 + m_\pi^2)} = 0.411\,\mathrm{GeV}$$



- Tune along SU(3) symmetric line to point

$$X_\pi / X_N = 0.357$$

- Can then determine lattice scale
  - Stable to a range of observables

Lattice scale:

$[aX_n]^{\mathrm{latt}}$ dimensionless

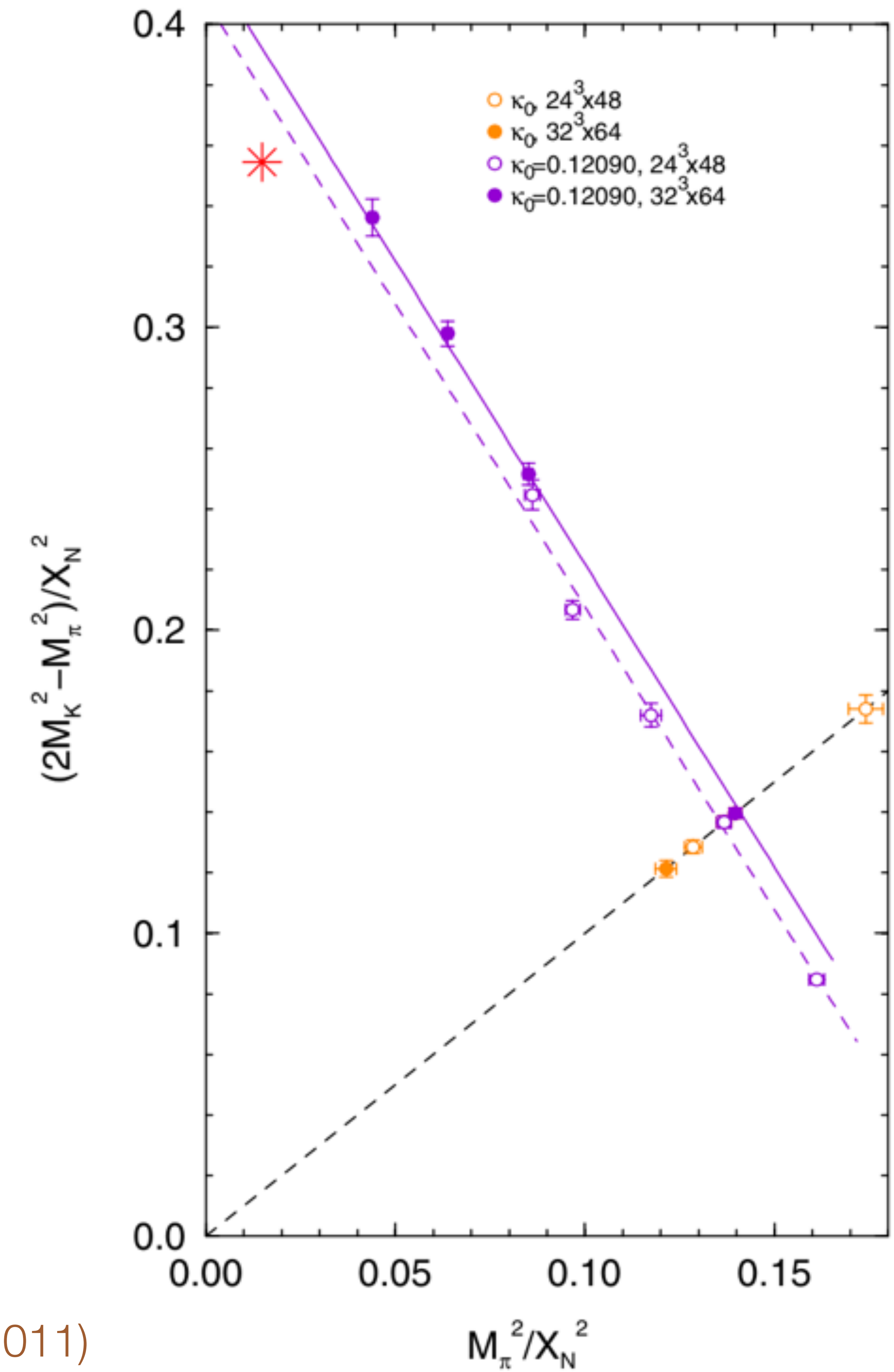
$$\Rightarrow a = [aX_N]^{\mathrm{latt}} / X_N^{\mathrm{phys}}$$

m_l–m_s trajectory

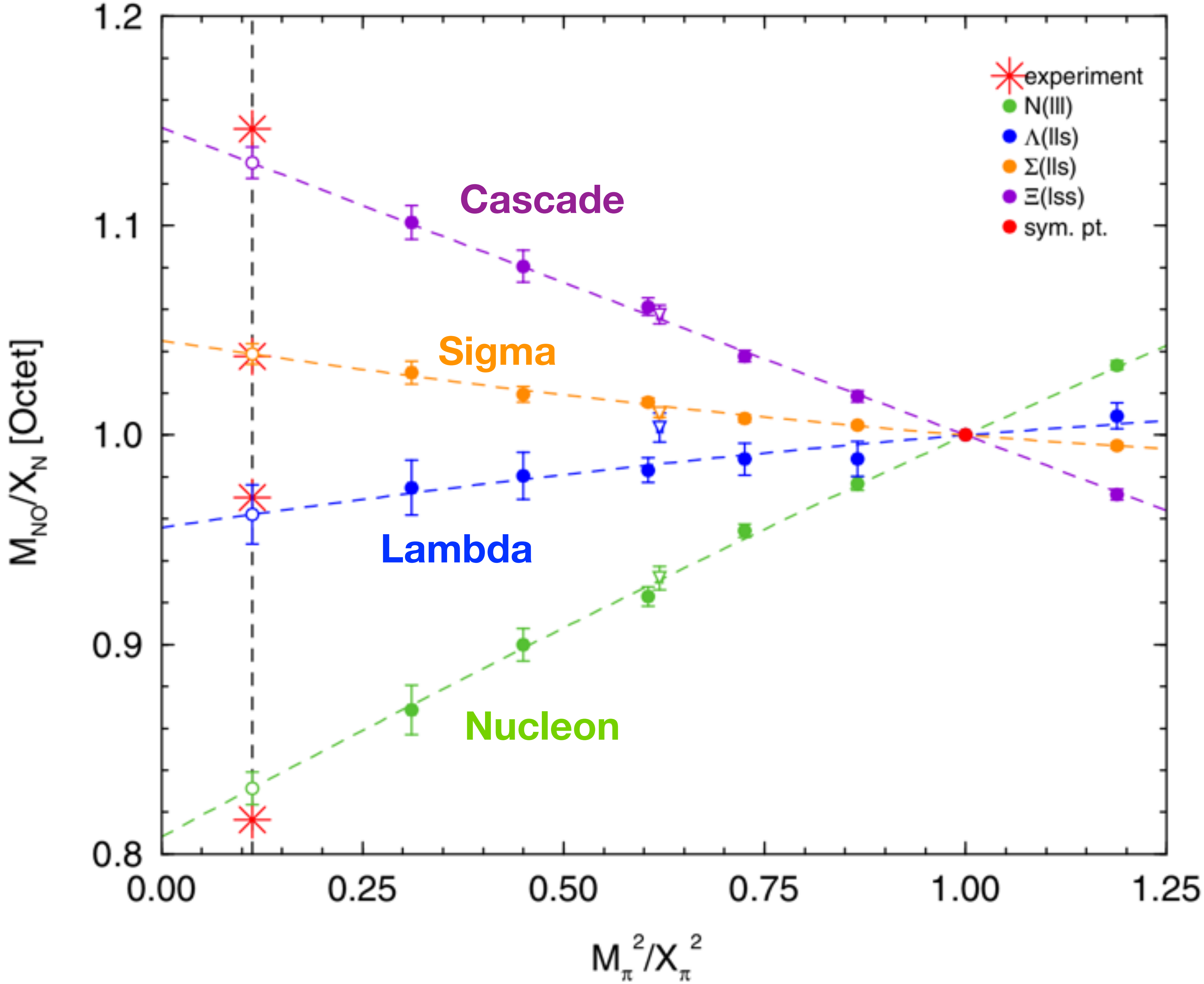
- QCDSF-UKQCD approach to the physical point
- Finite-volume effects: 24^3 & 32^3
- Singlet quark mass a little heavy:

$$[aX_\pi/aX_N]^{\mathrm{latt}} = 0.3751(13)$$

$$\text{cf. } [X_\pi/X_N]^{\mathrm{phys}} = 0.357$$



Bietenholz et al. [QCDSF-UKQCD], PRD (2011)



“Fan” plot

Octet-baryon masses

Extrapolation: Taylor expansion in SU(3)-breaking parameter

Bietenholz et al. [QCDSF-UKQCD], PRD (2011)

Bietenholz et al. [QCDSF-UKQCD], PRD (2011)

Flavour expansions

- S_3, SU(3) classification

$$\delta m_q = \bar{m} - m_l$$

Polynomial		S_3	$SU(3)$		
1	✓	A_1	1		
$(\overline{m} - m_0)$		A_1	1		
δm_s	✓	E^+		8	
$(\delta m_u - \delta m_d)$	✓	E^-		8	
$(\overline{m} - m_0)^2$		A_1	1		
$(\overline{m} - m_0)\delta m_s$		E^+		8	
$(\overline{m} - m_0)(\delta m_u - \delta m_d)$		E^-		8	
$\delta m_u^2 + \delta m_d^2 + \delta m_s^2$	✓	A_1	1		27
$3\delta m_s^2 - (\delta m_u - \delta m_d)^2$	✓	E^+		8	27
$\delta m_s(\delta m_d - \delta m_u)$	✓	E^-		8	27

- All quark-mass polynomials up to $O(\delta m^2)$
- A tick indicates relevant polynomial on constant mbar surface

Flavour expansions

- Mass combinations for different SU(3) irreps (2+1 case)

n	p	Σ^-	Σ^0	Λ	Σ^+	Ξ^-	Ξ^0	$SU(3)$
1	1	1	1	1	1	1	1	1
−1	−1	0	0	0	0	1	1	8_a
1	1	−2	−2	2	−2	1	1	8_b
3	3	−1	−1	−9	−1	3	3	27

O(δmq)	Phys [GeV]
0	9.21
1	0.76
1	-0.41
2	-0.077

Hierarchy of mass combinations

- Expansion in terms of mass eigenstates

$$\begin{aligned}
M_N &= M_0 + 3A_1\,\delta m_l + (B_0 + 3B_1)\delta m_l^2 \\
M_\Lambda &= M_0 + 3A_2\,\delta m_l + (B_0 + 6B_1 - 3B_2 + 9B_4)\delta m_l^2 \\
M_\Sigma &= M_0 - 3A_2\,\delta m_l + (B_0 + 6B_1 + 3B_2 + 9B_3)\delta m_l^2 \\
M_\Xi &= M_0 - 3(A_1 - A_2)\,\delta m_l + (B_0 + 9B_1 - 3B_2 + 9B_3)\delta m_l^2
\end{aligned}$$

$$\boxed{\delta m_l = -2\delta m_s}$$

Extrapolation to physical point

- Determine expansion parameters by constrained fit to baryon and meson masses

- Evaluate expressions at physical point: δm_l^*

$$\text{eg. } M_N^{\text{extrap}} = M_0 + 3A_1\,\delta m_l^* + (B_0 + 3B_1)(\delta m_l^*)^2$$

Further improvements in precision:

- Finite-volume effects
- Discretisation artefacts (finite *a*)
- Use of partially-quenched results
- Correction in singlet mass

Including QED

arXiv:1508.06401: “Isospin splittings of meson and baryon masses from three-flavor lattice QCD + QED”

arXiv:1509.00799: “QED effects in the pseudoscalar meson sector”

third paper on finite-volume effects: *soon!*

Lattice QCD+QED

"Continuum-like" language

- Remember, Monte Carlo sampling according to weight $\exp\left(-S[U]\right)$
- QCD action: $S_{\rm eff}^{\rm QCD}[U] = S^{\rm gluon} - \sum_q \operatorname{Tr}\log\mathcal{M}_q$
- QCD fermion matrix: $\mathcal{M}_q = \not{D}^{\rm SU(3)} + m_q$
- For QED, we modify the path integral sampling:

$$S_{\rm eff}^{\rm QCD+QED}[U,A] = S^{\rm gluon}[U] + S^{\rm photon}[A] - \sum_q \operatorname{Tr}\log\mathcal{M}'_q$$

$$\mathcal{M}'_q = \not{D}^{\rm SU(3)\times U(1)} + m_q$$

Lattice QCD+QED

$$S = S_G + S_{QED} + S_F^u + S_F^d + S_F^s \,.$$

$$S_{QED} = \frac{1}{2e^2} \sum_{x,\mu<\nu} \left(A_\mu(x) + A_\nu(x+\mu) - A_\mu(x+\nu) - A_\nu(x)\right)^2$$

noncompact

$$S_F^q = \sum_x \Big\{ \sum_\mu \Big[\overline{q}(x)\frac{\gamma_\mu - 1}{2} e^{-iQ_q A_\mu(x)} \tilde{U}_\mu(x) q(x+\hat{\mu})$$
$$-\overline{q}(x)\frac{\gamma_\mu + 1}{2} e^{iQ_q A_\mu(x)} \tilde{U}^\dagger_\mu(x-\hat{\mu}) q(x-\hat{\mu})\Big]$$
$$+\frac{1}{2\kappa_q}\overline{q}(x)q(x) - \frac{1}{4} c_{SW} \sum_{\mu\nu} \overline{q}(x)\sigma_{\mu\nu}F_{\mu\nu}(x)q(x) \Big\}$$

$$Q_u = \frac{2}{3}, \; Q_d = Q_s = -\frac{1}{3}$$

We work with a gauge coupling corresponding to $\alpha_{QED} = 0.1$

Lattice QCD+QED summary

- We are carrying out simulations in fully-dynamical QCD+QED
- QED stronger than the real world $\alpha_{\mathrm{QED}} \simeq 0.1$
  - Scale back results for physical comparison
- Partially quenched
  - Using *u*, *d*, *s* quarks; and a fictitious neutral-charge *n* quark
- Single set of sea parameters; tuned to SU(3) symmetric point
  - Three volumes: 24^3, 32^3 & 48^3
- No disconnected graphs — no mixing of neutral mesons
  - To a good approximation: $m^2_{\pi^0} = \left[m^2(\bar{u}u) + m^2(\bar{d}d)\right]/2$

Scheme dependence:
Separating QED and QCD

Scheme dependence

- Consider the $K^0 - K^+$ mass difference
- Can we separate the electromagnetic from strong?
- Simulate (or interpolate) to the point $m_u = m_d$
  - ⇒ Splitting is then pure QED contribution
- In pure QCD: scheme independent
- In QCD+QED, quark masses run differently:

$$\gamma_m = 6C_F g^2 + 6Q_f^2 e^2 + \ldots$$

  - $m_u = m_d$ in one scheme is not necessarily so in another.

Scheme dependence

- Also, how does one compare with the theory with QED “turned off”?

$$m_\gamma^2 = m^2(g^2, e^2, m_q^{\mathrm{phys}}) - m^2(g^2, 0, m_q^{?})$$

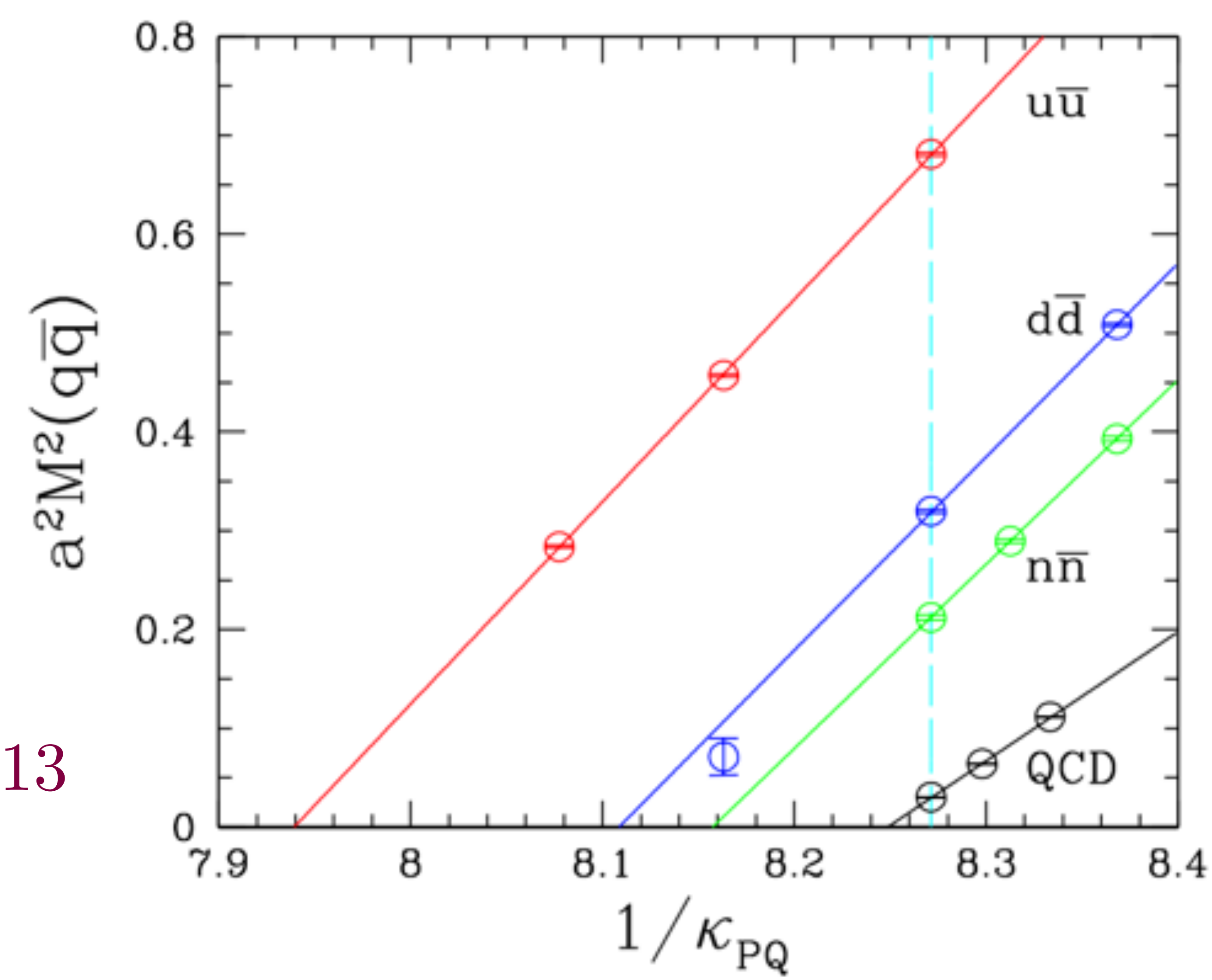
- Common choice: Same quark masses in MS-bar (at some prescribed scale)

- We propose alternative
    - Based on SU(3) symmetric point described above

Symmetric point: "Dashen scheme"

- In the spirit of Dashen's theorem, we define all neutral mesons to have no electromagnetic contribution

- We tune our lattice simulations to recover the SU(3) symmetric point
  - neutral mesons can therefore act as a proxy for "quark mass"
  - distance from symmetric point measures amount of SU(3) breaking



- Tuned parameters:

$$\beta_{QCD} = 5.50, \quad \beta_{QED} = 0.8,$$
$$\kappa_u = 0.124362, \quad \kappa_d = \kappa_s = 0.121713$$

Quark mass and charge expansion

Extension of SU(3)-breaking analysis

- Consider SU(3) breaking in both quark masses and charges
  - Expression includes partial-quenching (masses and charges)

$$\begin{aligned} M^2(a\bar{b}) \;=\;& M^2 + \alpha(\delta\mu_a + \delta\mu_b) \\ & + \beta_0 \tfrac{1}{6}(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) + \beta_1(\delta\mu_a^2 + \delta\mu_b^2) + \beta_2(\delta\mu_a - \delta\mu_b)^2 \\ & + \beta_0^{EM}(e_u^2 + e_d^2 + e_s^2) + \beta_1^{EM}(e_a^2 + e_b^2) + \beta_2^{EM}(e_a - e_b)^2 \\ & + \gamma_0^{EM}(e_u^2\delta m_u + e_d^2\delta m_d + e_s^2\delta m_s) + \gamma_1^{EM}(e_a^2\delta\mu_a + e_b^2\delta\mu_b) \\ & + \gamma_2^{EM}(e_a - e_b)^2(\delta\mu_a + \delta\mu_b) + \gamma_3^{EM}(e_a^2 - e_b^2)(\delta\mu_a - \delta\mu_b) \\ & + \gamma_4^{EM}(e_u^2 + e_d^2 + e_s^2)(\delta\mu_a + \delta\mu_b) \end{aligned}$$

  - Only one sea-quark ensemble; many PQ charge/kappa combinations
    - Can't determine all parameters: BUT not needed for charge-neutral splitting

$$\begin{aligned} M^2(a\bar{b}) - [M^2(a\bar{a}) + M^2(b\bar{b})]/2 = \beta_2(\delta\mu_a - \delta\mu_b)^2 + \beta_2^{EM}(e_a - e_b)^2 \\ + \gamma_2^{EM}(e_a - e_b)^2(\delta\mu_a + \delta\mu_b) + \gamma_3^{EM}(e_a^2 - e_b^2)(\delta\mu_a - \delta\mu_b) \end{aligned}$$

Extension of SU(3)-breaking analysis

- Consider SU(3) breaking in both quark masses and charges
  - Expression includes partial-quenching (masses and charges)

$$
\begin{aligned}
M^2(a\bar{b}) \;=\;& M^2 + \alpha(\delta\mu_a + \delta\mu_b) \\
& + \beta_0 \tfrac{1}{6}(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) + \beta_1(\delta\mu_a^2 + \delta\mu_b^2) + \beta_2(\delta\mu_a - \delta\mu_b)^2 \\
& + \beta_0^{EM}(e_u^2 + e_d^2 + e_s^2) + \beta_1^{EM}(e_a^2 + e_b^2) + \beta_2^{EM}(e_a - e_b)^2 \\
& + \gamma_0^{EM}(e_u^2\delta m_u + e_d^2\delta m_d + e_s^2\delta m_s) + \gamma_1^{EM}(e_a^2\delta\mu_a + e_b^2\delta\mu_b) \\
& + \gamma_2^{EM}(e_a - e_b)^2(\delta\mu_a + \delta\mu_b) + \gamma_3^{EM}(e_a^2 - e_b^2)(\delta\mu_a - \ldots \\
& + \gamma_4^{EM}(e_u^2 + e_d^2 + e_s^2)(\delta\mu_a + \delta\mu_b)
\end{aligned}
$$

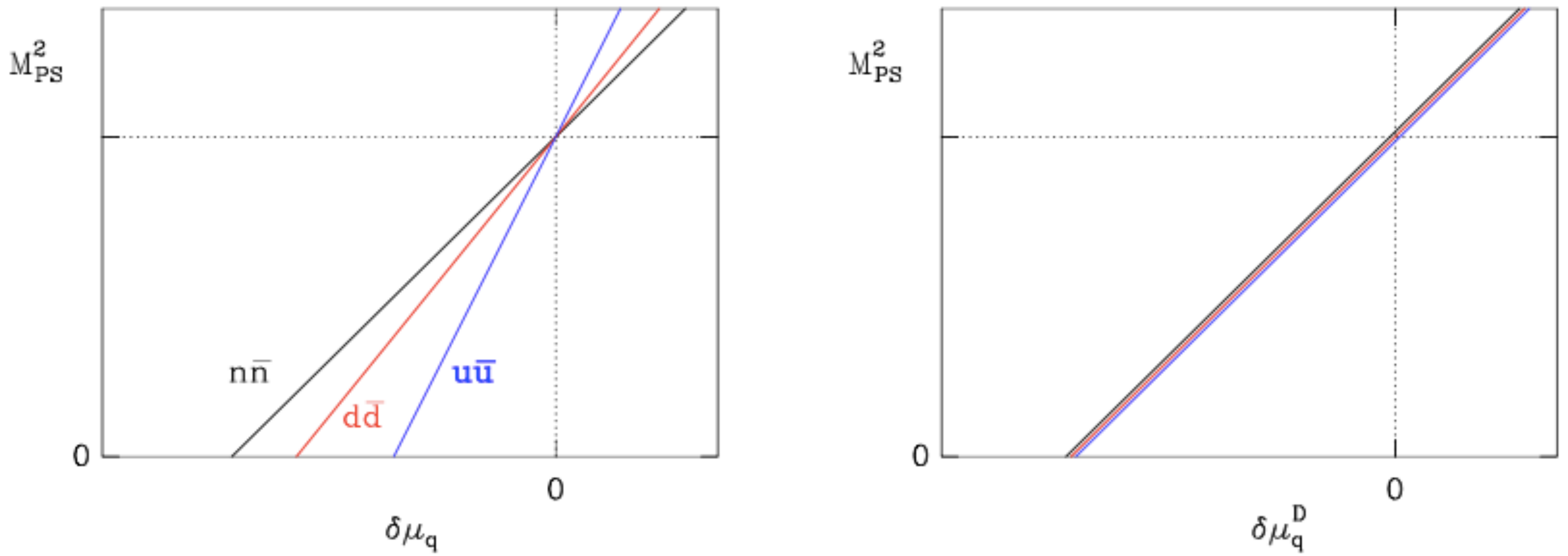
- Only one sea-quark ensemble; many PQ charge/… …ations
  - Can't determine all parameters: BUT n… charge-neutral splitting

$$
\begin{aligned}
M^2(a\bar{b}) - [M^2(a\bar{a}) + M^2(\ldots & \ldots \delta\mu_a - \delta\mu_b)^2 + \beta_2^{EM}(e_a - e_b)^2 \\
+ \gamma_2^{EM}(e_a - e_b)^2 \ldots & \ldots \gamma_3^{EM}(e_a^2 - e_b^2)(\delta\mu_a - \delta\mu_b)
\end{aligned}
$$

Note: symmetry pattern independent of scheme;
parameter values are not.

More on quark masses and scheme

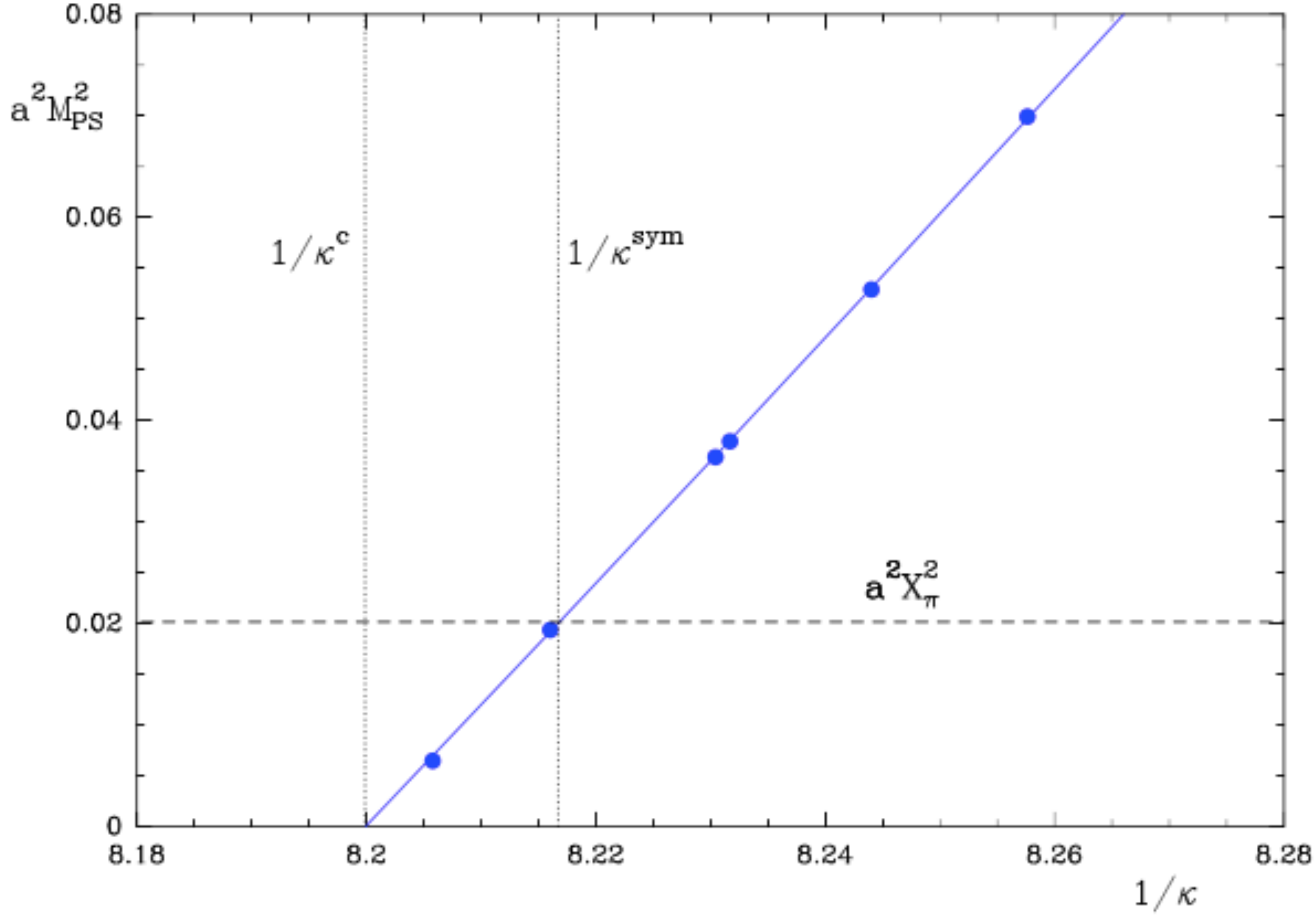
- Cartoon illustrating the different running of the bare quark masses



- Once tuned to the symmetric point, different charge quarks run differently to the chiral limit
  - Dashen scheme: rescale the horizontal axis so that all meson masses depend on the "Dashen mass" in the same way

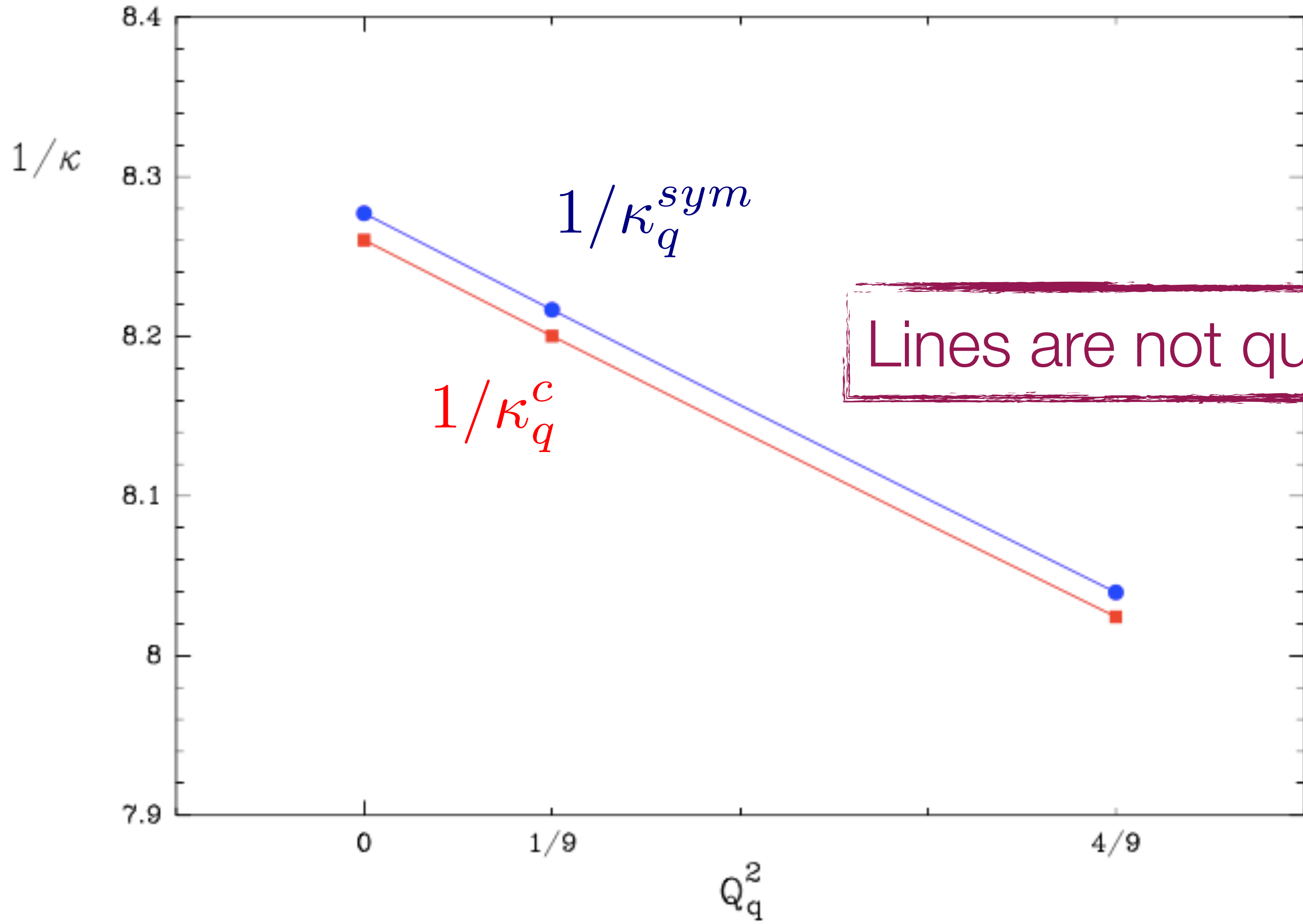
More on quark masses and scheme

- Tuning the down-quark mass



$$\kappa^{sym}: \quad m_{PS}^2 = X_\pi^2$$

More on quark masses and scheme



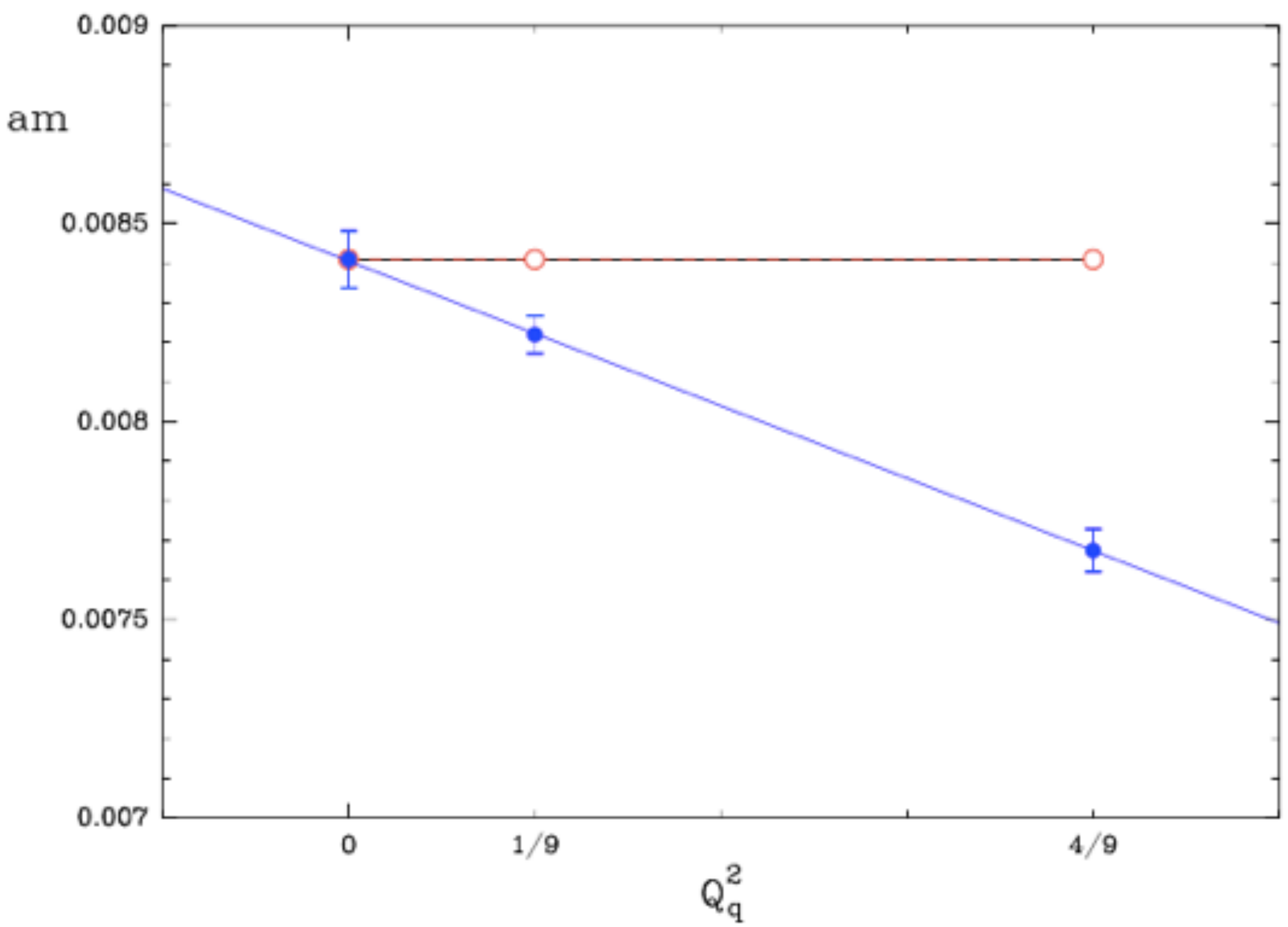
Lines are not quite parallel

- kappa-symmetric & kappa-critical for different charges

“Bare” quark masses ⇒ Dashen mass

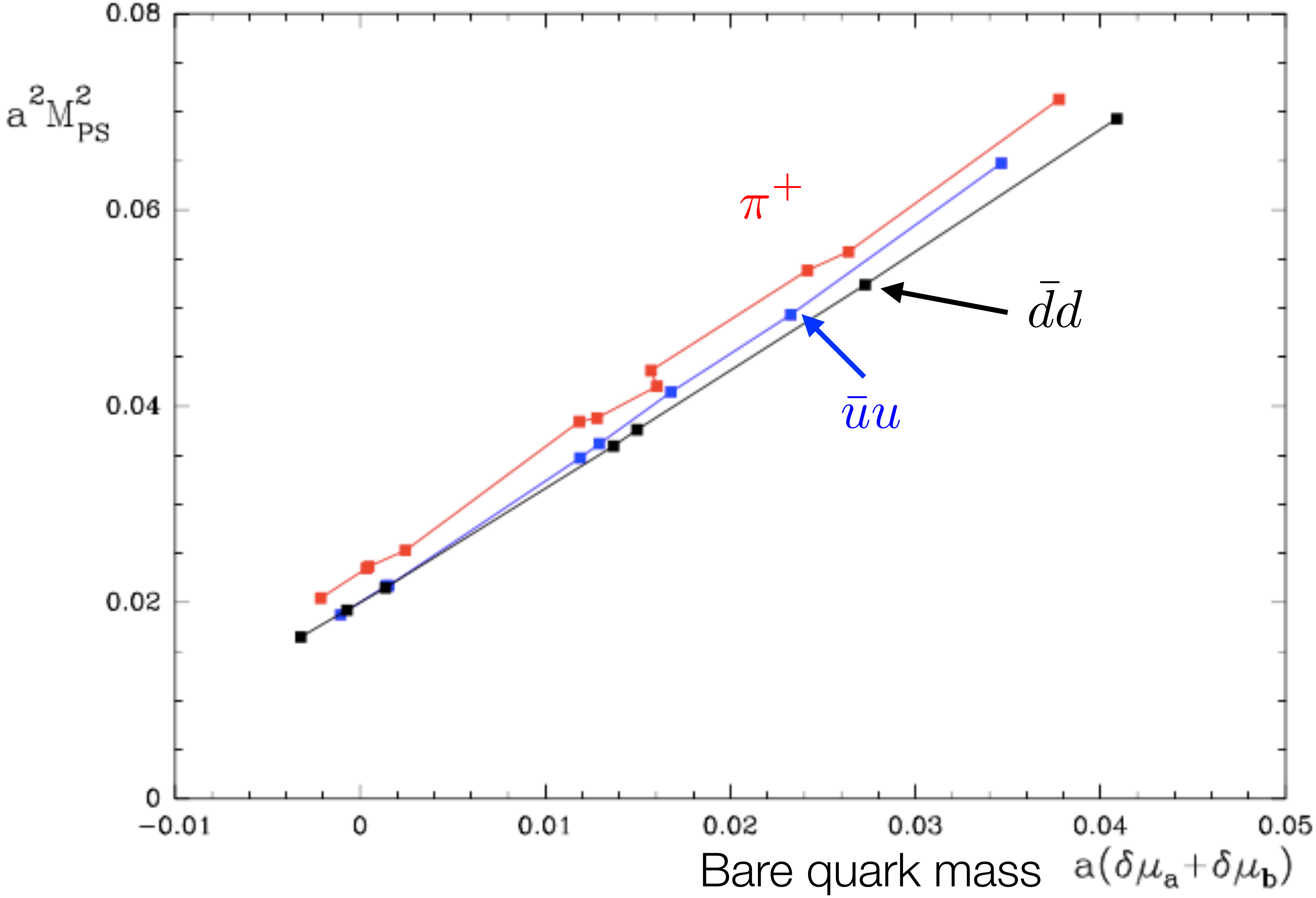
Bare mass $$am_q^{sym} = \frac{1}{2\kappa_q^{sym}} - \frac{1}{2\kappa_q^c}$$

- Small charge dependence of bare quark mass at symmetric point
  - Multiplicative factor to get to universal quark mass at symmetric point



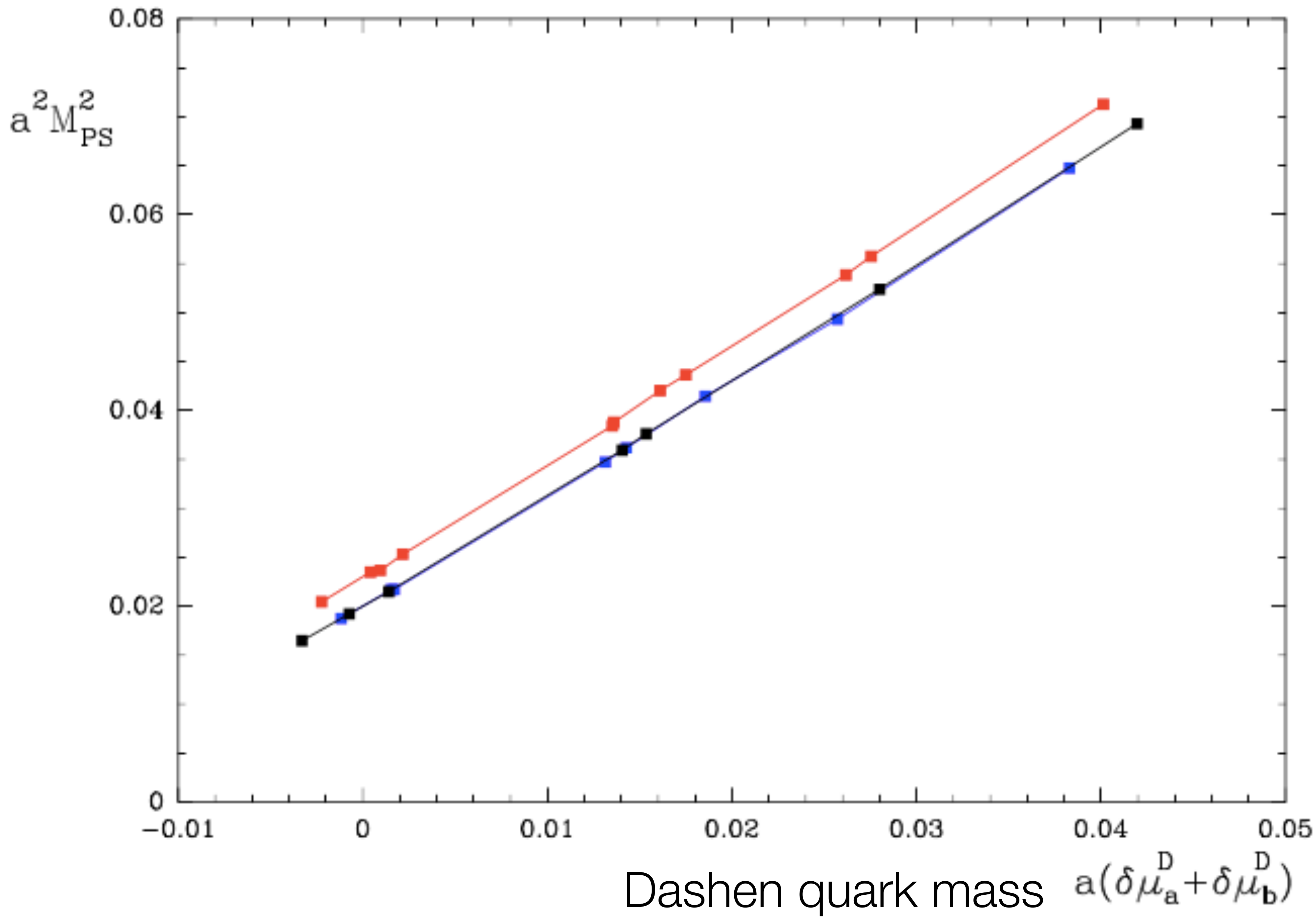
Dashen mass

$$\delta\mu_q^D = (1 + KQ_q^2 e^2)\delta\mu_q$$



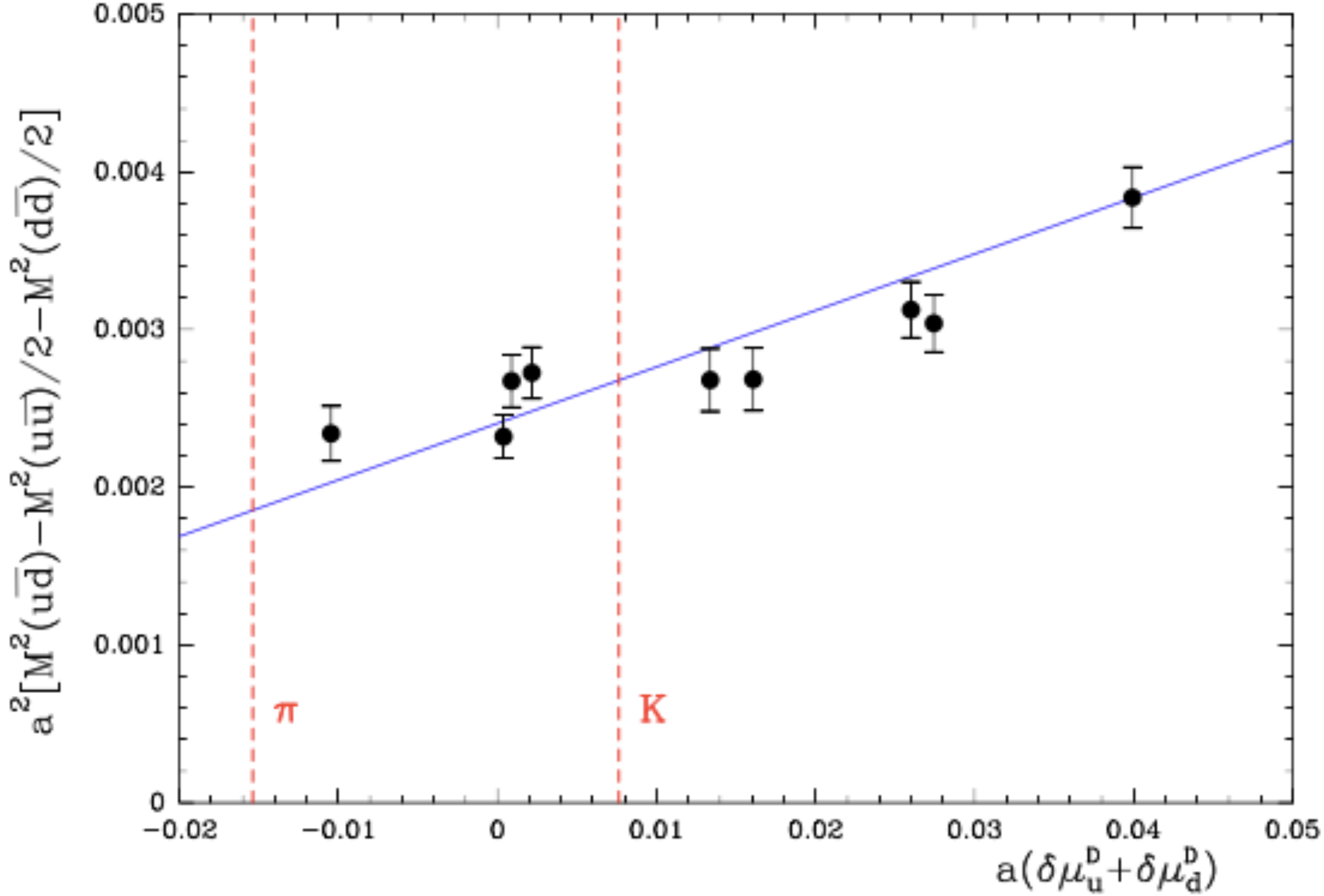
Pseudoscalar masses

Neutral mesons on different lines.
“Scatter” of charged pion:
dependence on $\delta m_u - \delta m_d$



Pseudoscalar masses

Neutral mesons on uniform curve. Removed “scatter” of charged mesons.



Violation of Dashen theorem

Clear mass dependence on electromagnetic self-energy

SU(3) Expansion

- In Dashen scheme, we absorb the QED contributions to the neutral pseudoscalar mesons into the quark self-energy

- Substantial simplification of expansion formula:

$$
\begin{aligned}
M^2(a\bar{b}) \;\; = \;\; & M^2 + \alpha(\delta\mu_a^D + \delta\mu_b^D) + \beta_0 \tfrac{1}{6}(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) \\
& + \beta_1((\delta\mu_a^D)^2 + (\delta\mu_b^D)^2) + \beta_2(\delta\mu_a^D - \delta\mu_b^D)^2 + \beta_2^{EM}(e_a - e_b)^2 \\
& + \gamma_2^{EM}(e_a - e_b)^2(\delta\mu_a^D + \delta\mu_b^D) + \gamma_3^{EM}(e_a^2 - e_b^2)(\delta\mu_a^D - \delta\mu_b^D) \, .
\end{aligned}
$$

  - Neutral mesons have no EM contribution:

$$
\begin{aligned}
M_{neut}^2(a\bar{b}) \;\; = \;\; & M^2 + \alpha(\delta\mu_a^D + \delta\mu_b^D) + \beta_0 \tfrac{1}{6}(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) \\
& + \beta_1 \left((\delta\mu_a^D)^2 + (\delta\mu_b^D)^2\right) + \beta_2 \left(\delta\mu_a^D - \delta\mu_b^D\right)^2
\end{aligned}
$$

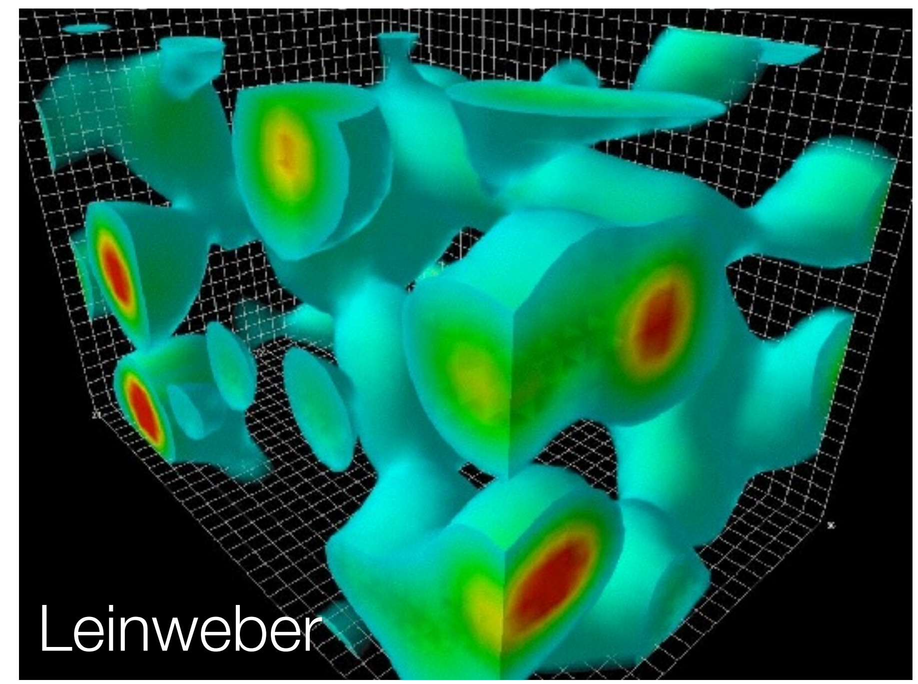
Finite volume effects?

Electromagnetism in lattice QCD

- The strong force (QCD) is finite-ranged
  - Finite-volume effects are "easily" controlled:

$$\text{eg.} \quad [m(L) - m(\infty)] \sim e^{-m_\pi L}$$

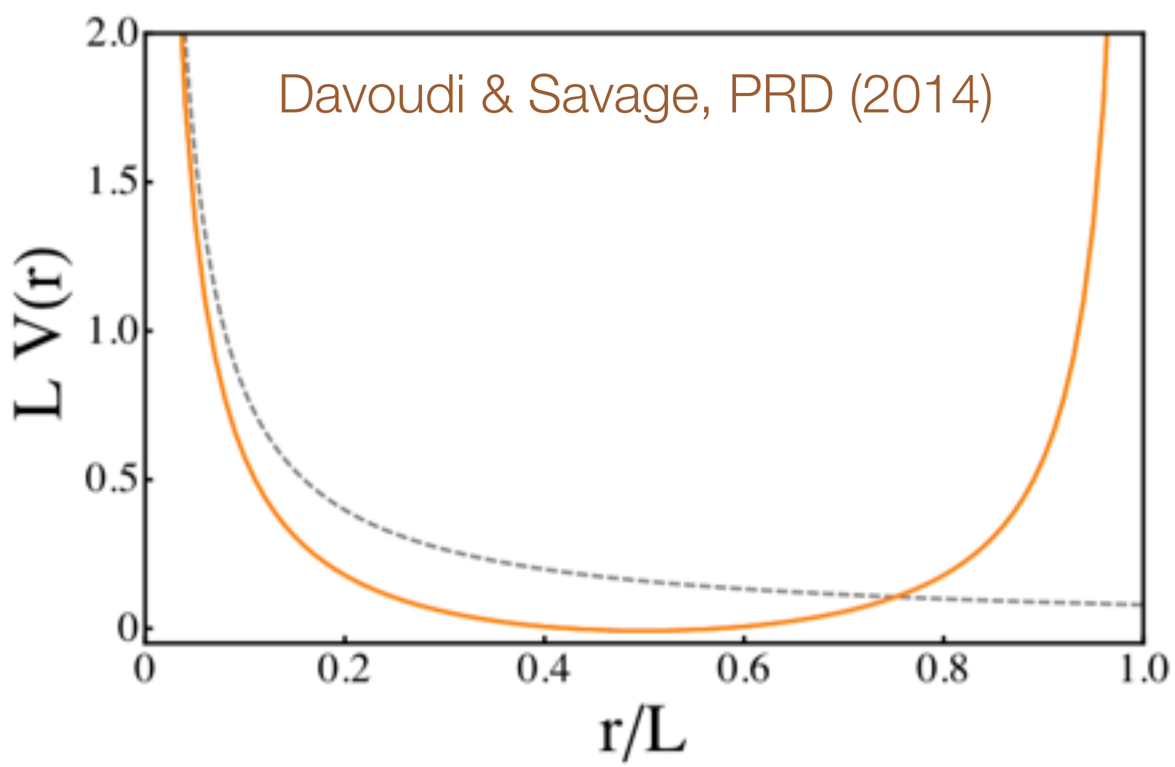
  - With a large enough box, volume artefacts can (almost) be ignored



- Photon is massless
  - Electromagnetic interactions are long ranging
  - Power-law corrections in the box size

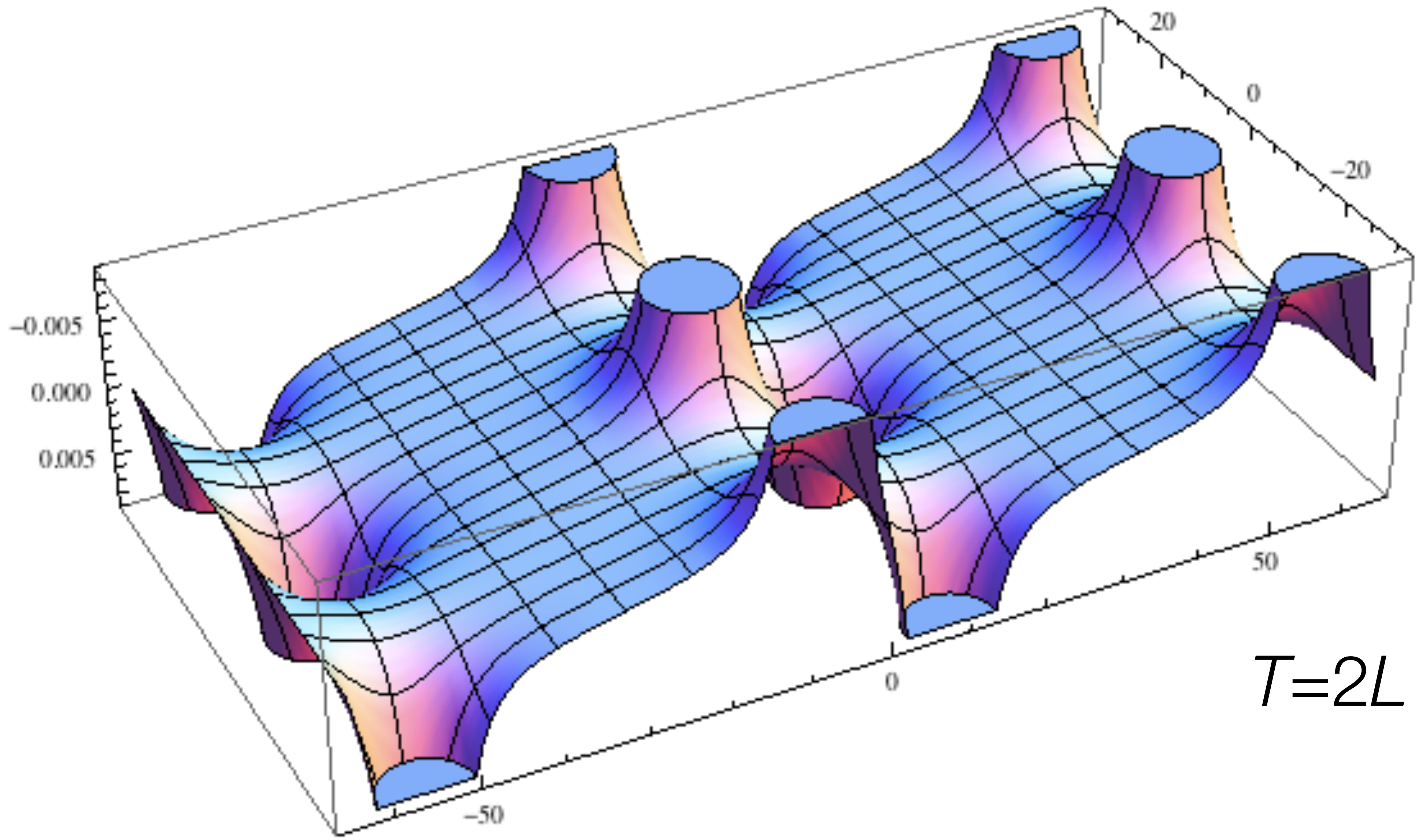
QED and the finite volume

- Expect finite volume artefacts to make a substantial contribution to lattice systematics



Periodic BCs:
Distortion of Coulomb potential
(on-axis displayed)

- At large enough volumes, expect that the long-ranging "Coulomb" effects will decouple from internal dynamics of hadrons
  - Ideally suited to description in terms of Effective Field Theory (EFT)



“4-D” Coulomb potential

Single point “source” and “sink”

Warm-up exercise

- Energy density of a classical uniform charge density subject to cubic periodic boundary conditions

Finite-volume corrections

$$U^{\text{sphere}}(Q,R,\mathrm{L}) = \frac{3}{5}\frac{Q^2}{4\pi R} + \frac{Q^2}{8\pi \mathrm{L}}c_1 + \frac{Q^2}{10\mathrm{L}}\left(\frac{R}{\mathrm{L}}\right)^2 + \cdots$$

Total field energy of uniformly charged sphere

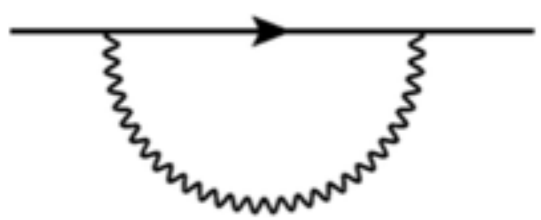
Leading term just depends on charge!

Geometric constant:
$c_1 \simeq -2.83729$

Construct EFT: Scalar Non-Rel. QED

$$\mathcal{L}_\phi = \phi^\dagger \left[iD_0 + \frac{|\mathbf{D}|^2}{2m_\phi} + \frac{|\mathbf{D}|^4}{8m_\phi^3} + \frac{e\langle r^2\rangle_\phi}{6} \boldsymbol{\nabla}\cdot\mathbf{E} + 2\pi\tilde{\alpha}_E^{(\phi)}|\mathbf{E}|^2 + 2\pi\tilde{\beta}_M^{(\phi)}|\mathbf{B}|^2 + iec_M \frac{\{D^i, (\boldsymbol{\nabla}\times\mathbf{B})^i\}}{8m_\phi^3} + \cdots \right]\phi \,,$$

- Leading-order FV correction (charge)



$$\delta m_\phi^{(\mathrm{LO})} = \frac{\alpha Q^2}{2\pi L}\sum_{\vec{n}\neq\vec{0}} \frac{1}{|\vec{n}|^2} = \frac{\alpha Q^2}{2L} c_1$$

Divergent sum: regularisation implied (FV effects independent of UV cutoff)

Davoudi & Savage, PRD (2014)

Construct EFT: Scalar Non-Rel. QED

$$\mathcal{L}_\phi = \phi^\dagger \left[iD_0 + \frac{|\mathbf{D}|^2}{2m_\phi} + \frac{|\mathbf{D}|^4}{8m_\phi^3} + \frac{e\langle r^2\rangle_\phi}{6} \boldsymbol{\nabla}\cdot\mathbf{E} + 2\pi\tilde{\alpha}_E^{(\phi)}|\mathbf{E}|^2 + 2\pi\tilde{\beta}_M^{(\phi)}|\mathbf{B}|^2 + iec_M \frac{\{D^i, (\boldsymbol{\nabla}\times\mathbf{B})^i\}}{8m_\phi^3} + \cdots \right]\phi\,,$$

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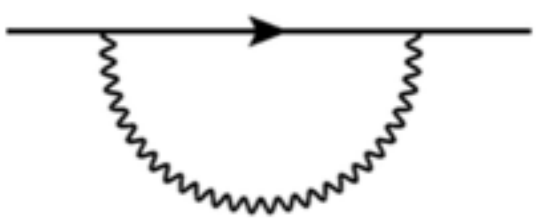
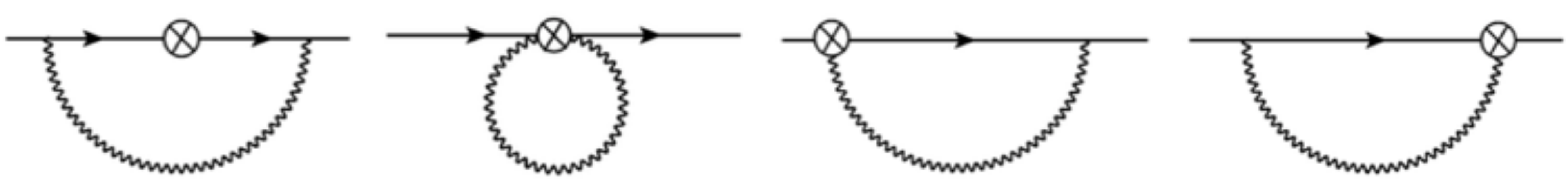


$$\delta m_\phi^{(\mathrm{LO})} = \frac{\alpha Q^2}{2\pi L}\sum_{\vec{n}\neq\vec{0}}\frac{1}{|\vec{n}|^2} = \frac{\alpha Q^2}{2L}c_1$$

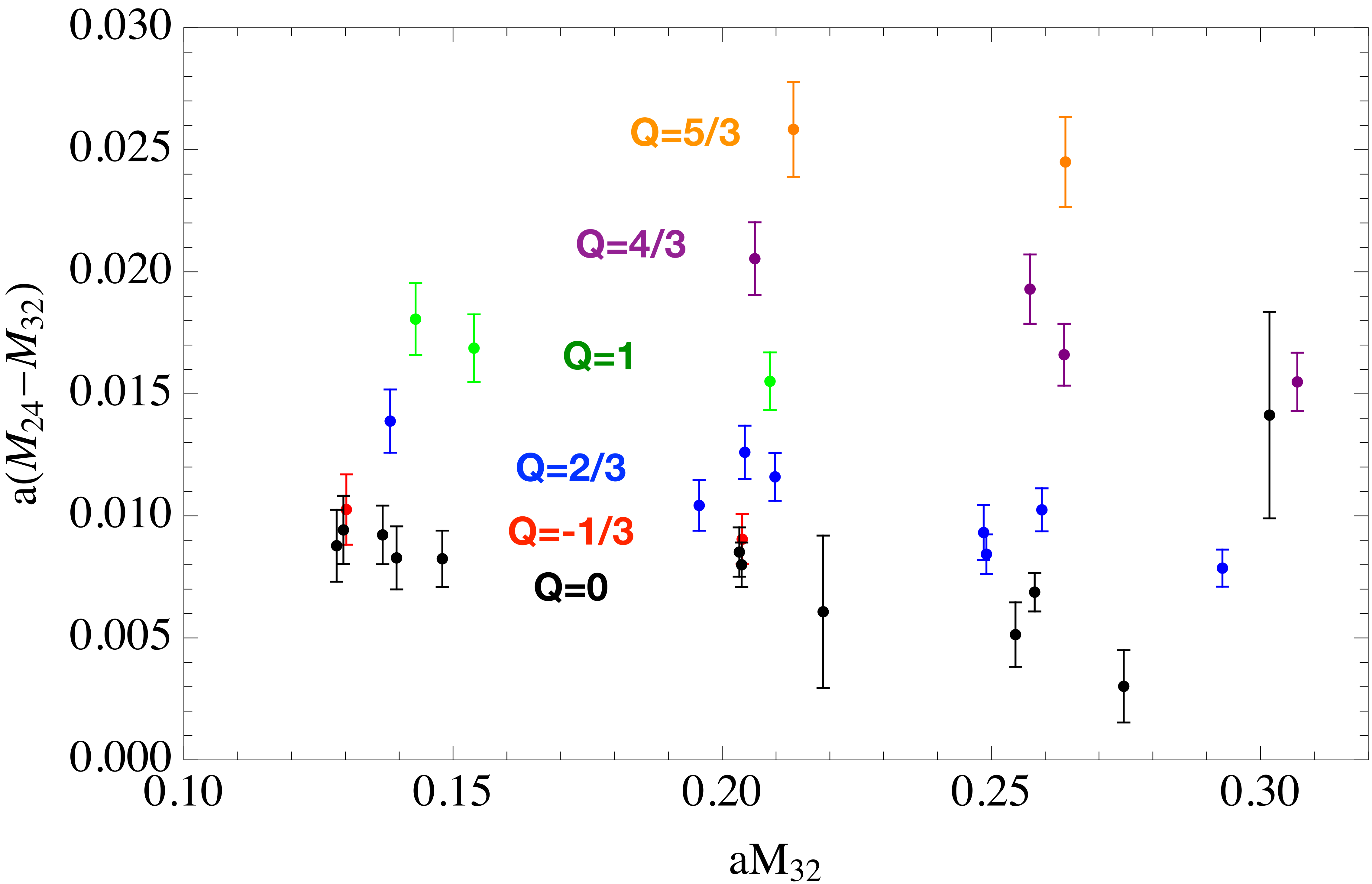
- Next-leading-order (kinetic energy operator)



$$\delta m_\phi^{(\mathrm{NLO})} = \frac{\alpha Q^2}{m_\phi L}\sum_{\vec{n}\neq\vec{0}}\frac{1}{|\vec{n}|} = \frac{\alpha Q^2}{m_\phi L^2}c_1$$

LO and NLO corrections are negative!

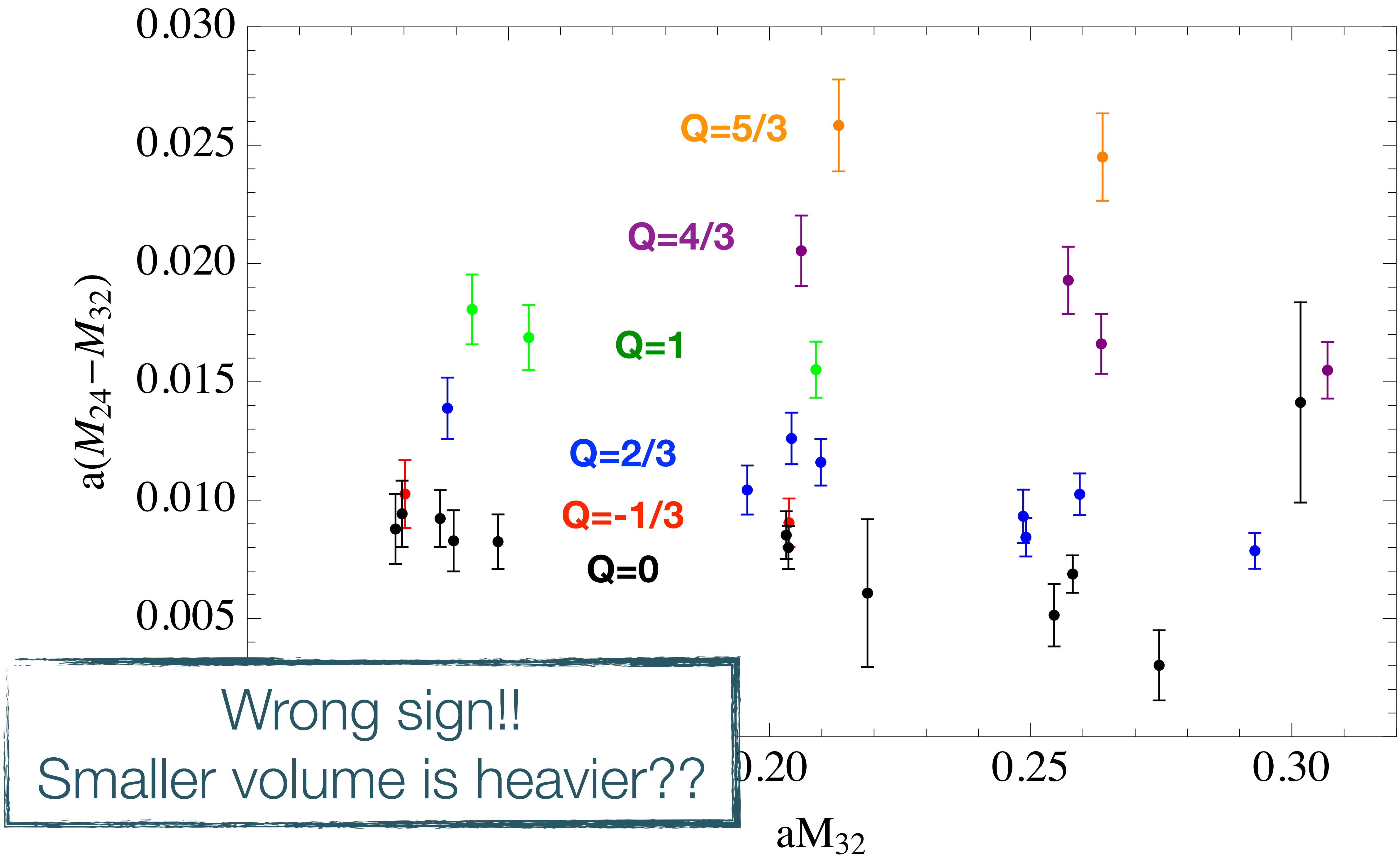
$$\boxed{\text{Energy of Coulomb cloud is suppressed by boundary conditions}}$$



PQ Simulations

[*u*, *d*, *n* (Q=0) & *w* (Q=+4/3) quarks)

24^3 and 32^3 lattices:
Colour coded by net charge



PQ Simulations

[*u*, *d*, *n* (Q=0) & *w* (Q=+4/3) quarks]

24^3 and 32^3 lattices:
Colour coded by net charge

Finite-volume effects not as anticipated

- My first question:
  - “How good is the non-relativistic approximation for a lattice pion?”
  - Consider lattice “energy” of recoil pion:

$$E_\pi = \sqrt{m_\pi^2 + \vec{k}^2} = \sqrt{m_\pi^2 + \vec{n}^2 \left(\frac{2\pi}{L}\right)^2}$$

$$m_\pi L \sim 4 \;\Rightarrow\; \frac{2\pi}{L} > m_\pi$$

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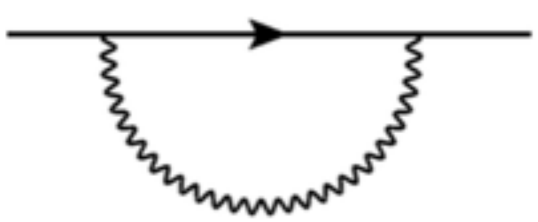
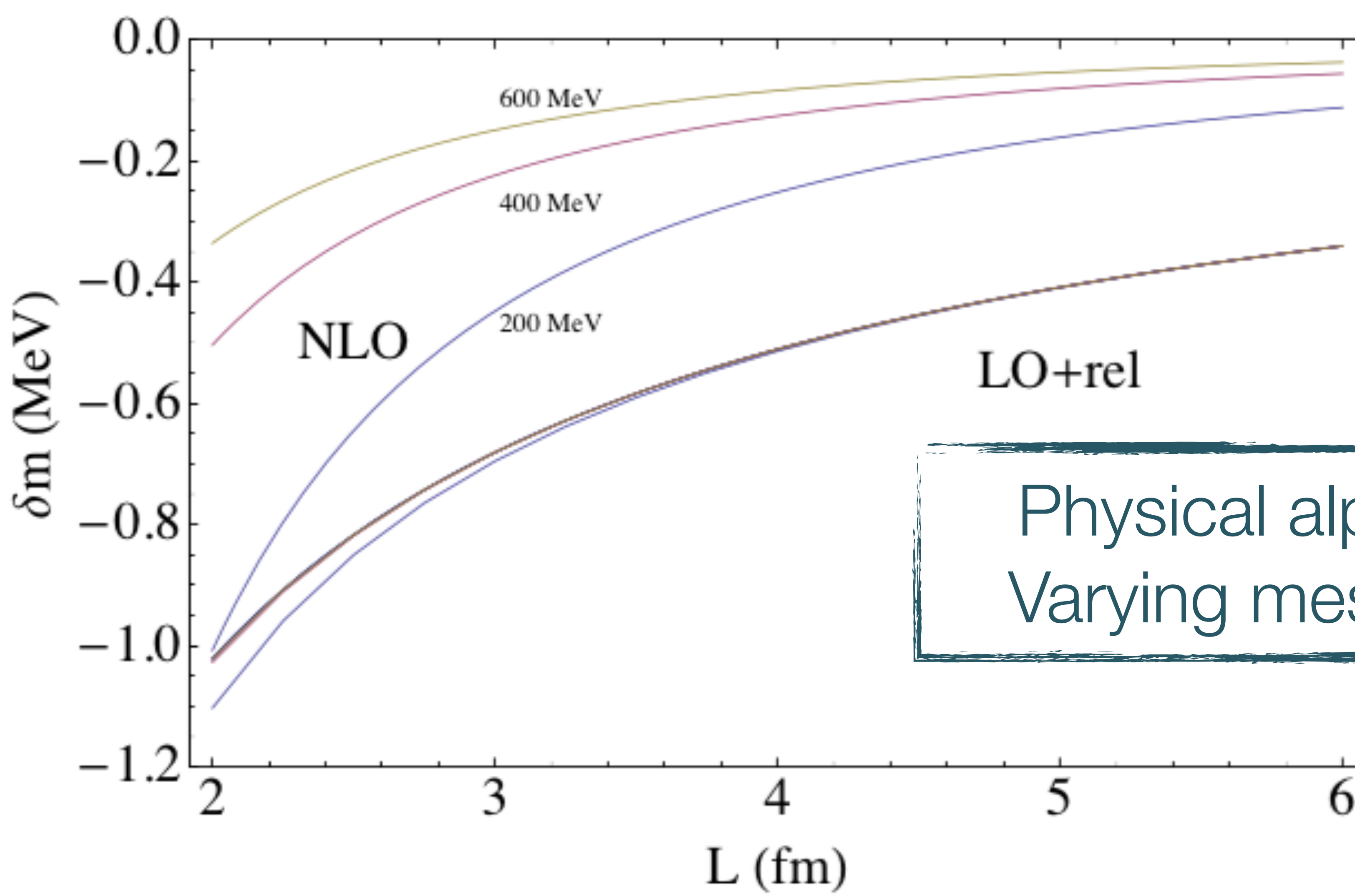
Relativistic pion propagator



$$-i\Sigma(p^2 = m^2) = \frac{\alpha}{4\pi^3} \int d^4k \frac{3k^2 - 4p.k - 4m^2}{(k^2 + i\epsilon)(k^2 - 2p.k + i\epsilon)}$$

Relativistic loop

- Recover LO and NLO result of NRQED (as expected)



Physical alpha_QED
Varying meson mass

Relativistic loop

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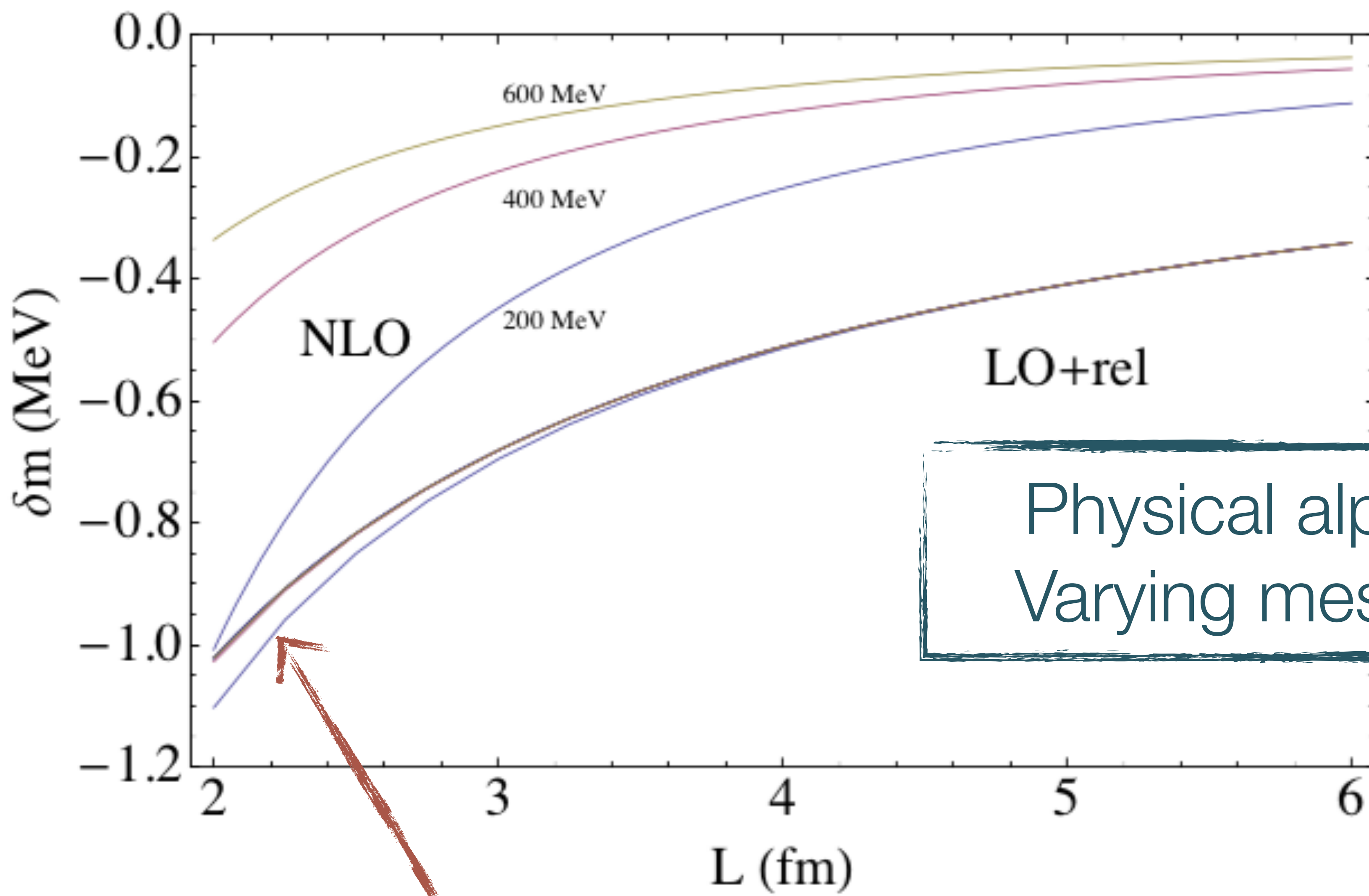


Physical alpha_QED
Varying meson mass

Relativistic pion only visible for very light mass
*m*L ~ 2*

A subtle detail I didn't address in the photon self energy:

The finite sum does not include the zero momentum term

$$\delta m_{\phi}^{(\mathrm{LO})} = \frac{\alpha Q^2}{2\pi L} \sum_{\vec{n} \neq \vec{0}} \frac{1}{|\vec{n}|^2} = \frac{\alpha Q^2}{2L} c_1$$

Zero mode contribution

- Naive application of perturbation theory would yield infinite correction for zero-momentum contribution
    - In the infinite space, phase space eliminates singularity
- Zero mode in box can be legitimately eliminated by appropriate gauge-fixing condition
    - Simplest method:

$$\sum_x A_\mu(x) = 0, \text{ for all } \mu$$

    - Hayakawa & Uno (2008):

$$\sum_{\vec{x}} A_\mu(t, \vec{x}) = 0, \text{ for all } \mu \text{ and } t$$

$$\Rightarrow \text{ Fourier mode: } \tilde{A}_\mu(t, \vec{0}) = 0$$

Zero mode contribution

- With small zero-momentum modes eliminated, no need to include their field fluctuations in perturbative expansion

- Imposing zero mode condition at the outset is non-trivial
  - Difficult to implement directly in generation of gauge fields (non-local constraint)
  - Gauge fixing is necessary to study correlation functions of charged particles
    - *OUR* Gauge fixing is implemented **after** field generation

Gauge fixing

- QCDSF-UKQCD-CSSM Simulations: Landau gauge fixing

$$\partial . A^{\mathrm{GF}} = 0$$

$$A_\mu(x) \to A_\mu^{\mathrm{GF}}(x) = A_\mu(x) + \partial_\mu \Lambda(x)$$

  - As in continuum this does not eliminate all gauge-like degrees of freedom
    Consider:
    $$A_\mu^{\mathrm{GF}}(x) \to A_\mu^{\mathrm{GF}'} = A_\mu^{\mathrm{GF}}(x) + \partial_\mu \Lambda'(x); \quad \partial^2 \Lambda'(x) = 0$$

- Consider second transformation on fermion field:

$$\psi(x) \to \psi'(x) = \exp[-iQ\Lambda'(x)]\psi(x)$$

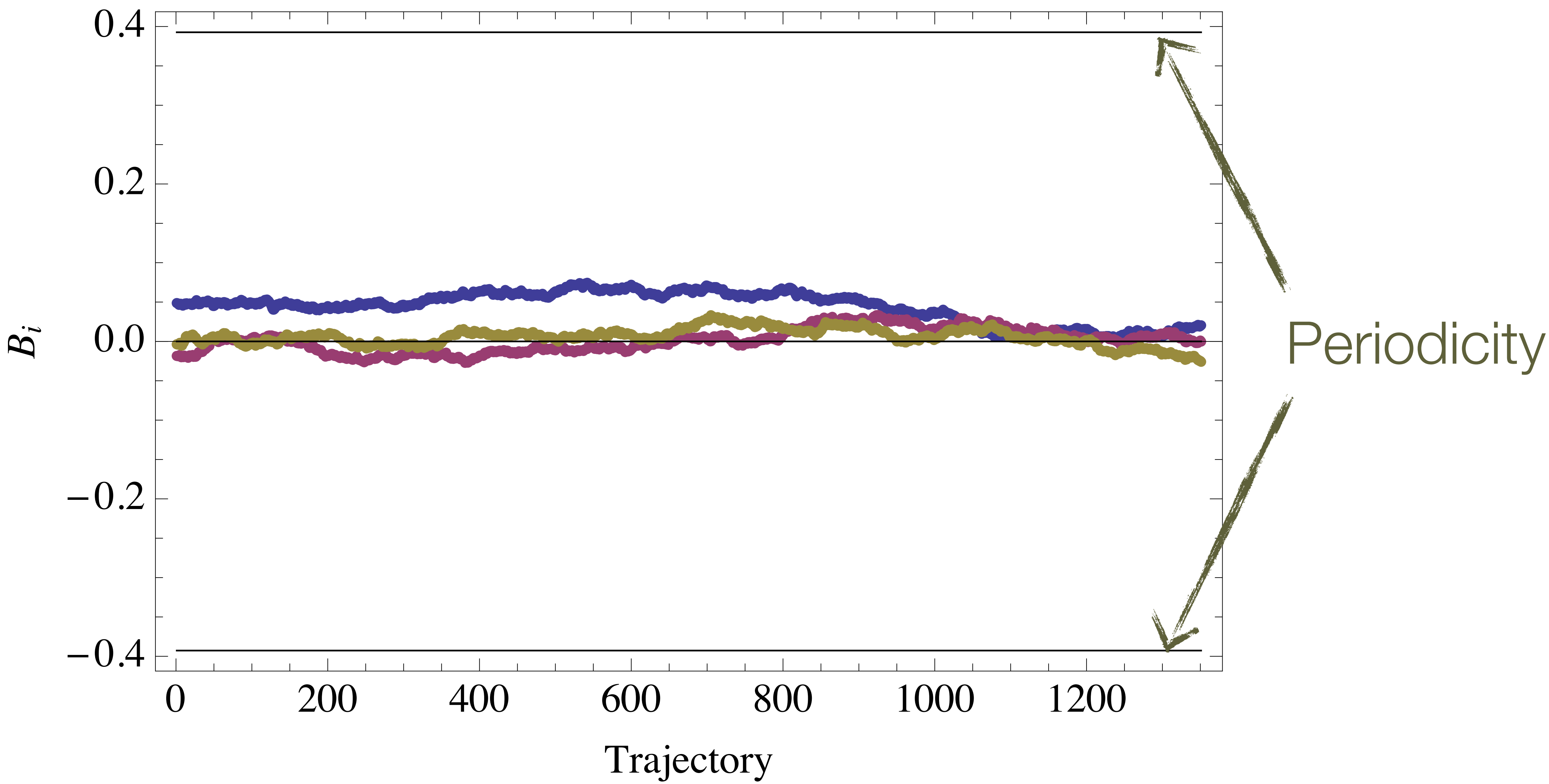
  - To maintain fermion field periodicity we must take
    $$Q\Lambda'(x) = \sum_\mu \frac{2\pi}{L_\mu} n_\mu x_\mu, \quad n_\mu \text{ integer}$$

- This gauge-field redundancy can be eliminated by adding multiples of $2\pi/QL_\mu$ to A_μ such that:

$$-\frac{\pi}{QL_\mu} < B_\mu \leq \frac{\pi}{QL_\mu}; \quad \text{for } B_\mu \equiv \frac{1}{V}\sum_x A_\mu(x)$$

Gauge fixing

- Boundary quantisation condition is such that arbitrary gauge transformation does not leave action invariant
  - Imposing a GF condition that eliminates zero modes exactly destroys the importance sampling of the action
  - And it means the valence quarks are partially quenched (they feel a different U(1) field as compared to the sea quarks)
  - [Numerical effects may be small, but I am unaware of supporting evidence]



Spatial zero modes: B_i

Importance sampling holds zero modes near origin

Influence of zero modes on hadron correlator

- Can’t use standard perturbation theory (as we discussed earlier)
- Must incorporate the zero modes in the quadratic (in the charged fields) part of the action
    - Hence we modify the propagators
    - Analog of doing degenerate perturbation theory in QM

Influence of zero modes on hadron correlator

- Consider equation of motion for charged scalar field

$$D^\mu(D_\mu\phi) + m^2\phi = 0$$

$$\partial^2\phi + ie(\partial.A)\phi + 2ieA^\mu\partial_\mu\phi - e^2A^\mu A_\mu\phi + m^2\phi = 0$$

  - Take just constant field and write in Fourier space:

$$(-k^2 - 2eB^\mu k_\mu - e^2B^2 + m^2)\tilde{\phi}(k) = 0$$

  - Transformed to Euclidean space

$$D_E^B(x-y) = \int \frac{d^4k_E}{(2\pi)^4}\frac{1}{(k_E+eB_E)^2+m^2}e^{ik_E.(x-y)}.$$

  - Which has poles given by

$$k_4 = \pm i\sqrt{m^2+(\vec{k}+e\vec{B})^2} - eB_4$$

and hence a Euclidean time evolution governed by

$$e^{-t\sqrt{m^2+(e\vec{B})^2}}e^{-ieB_4t}.$$

Just the same as twisted BCs that have been studied extensively in the literature.
eg. Sachrajda & Villadoro, Tiburzi et al., Bijnens et al.

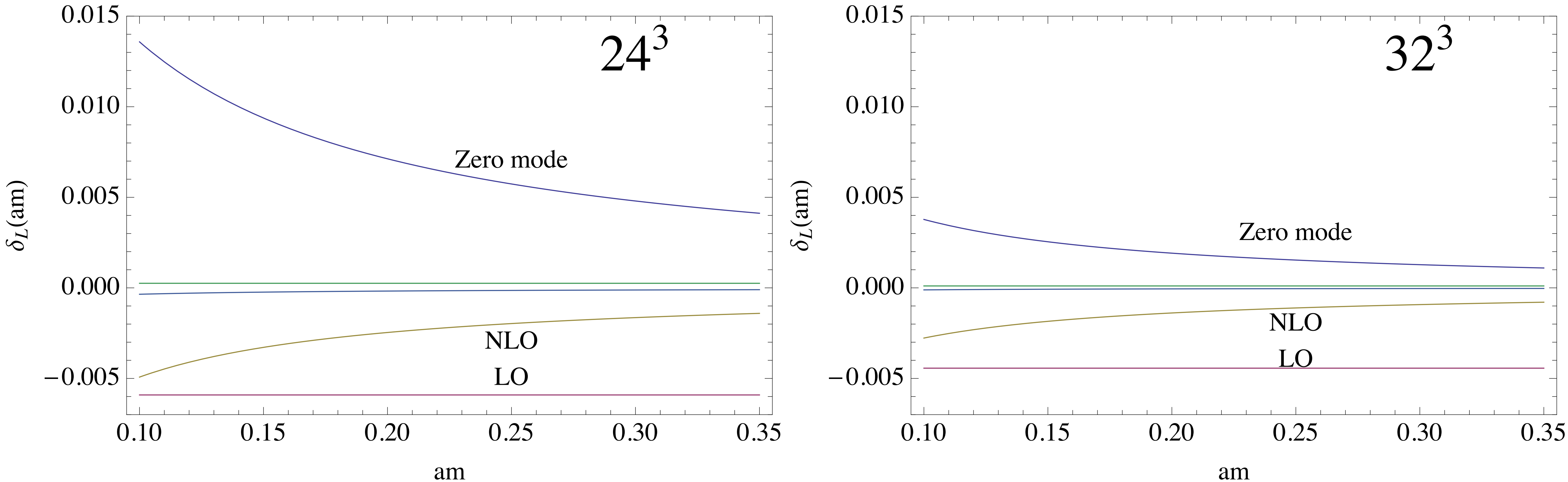
Zero mode energy shift

- The influence complex phase from the temporal B is tiny

- Ground state energy of a single particle shifted from rest mass

$$E = \sqrt{m^2 + Q^2(e\vec{B})^2} \simeq m + Q^2 \frac{(e\vec{B})^2}{2m}$$

- Contributes in addition to FV effects already discussed



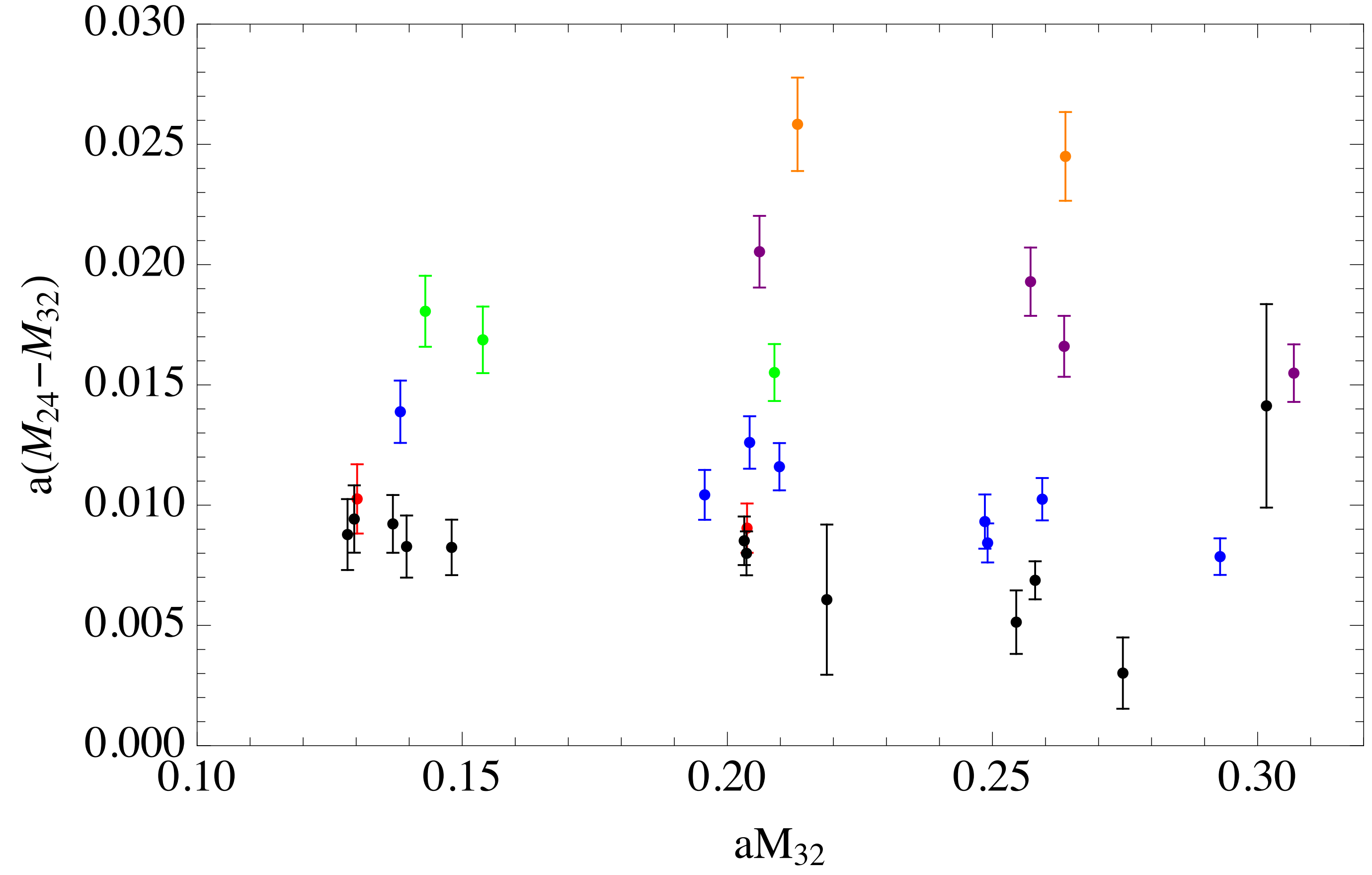
Unit charge meson

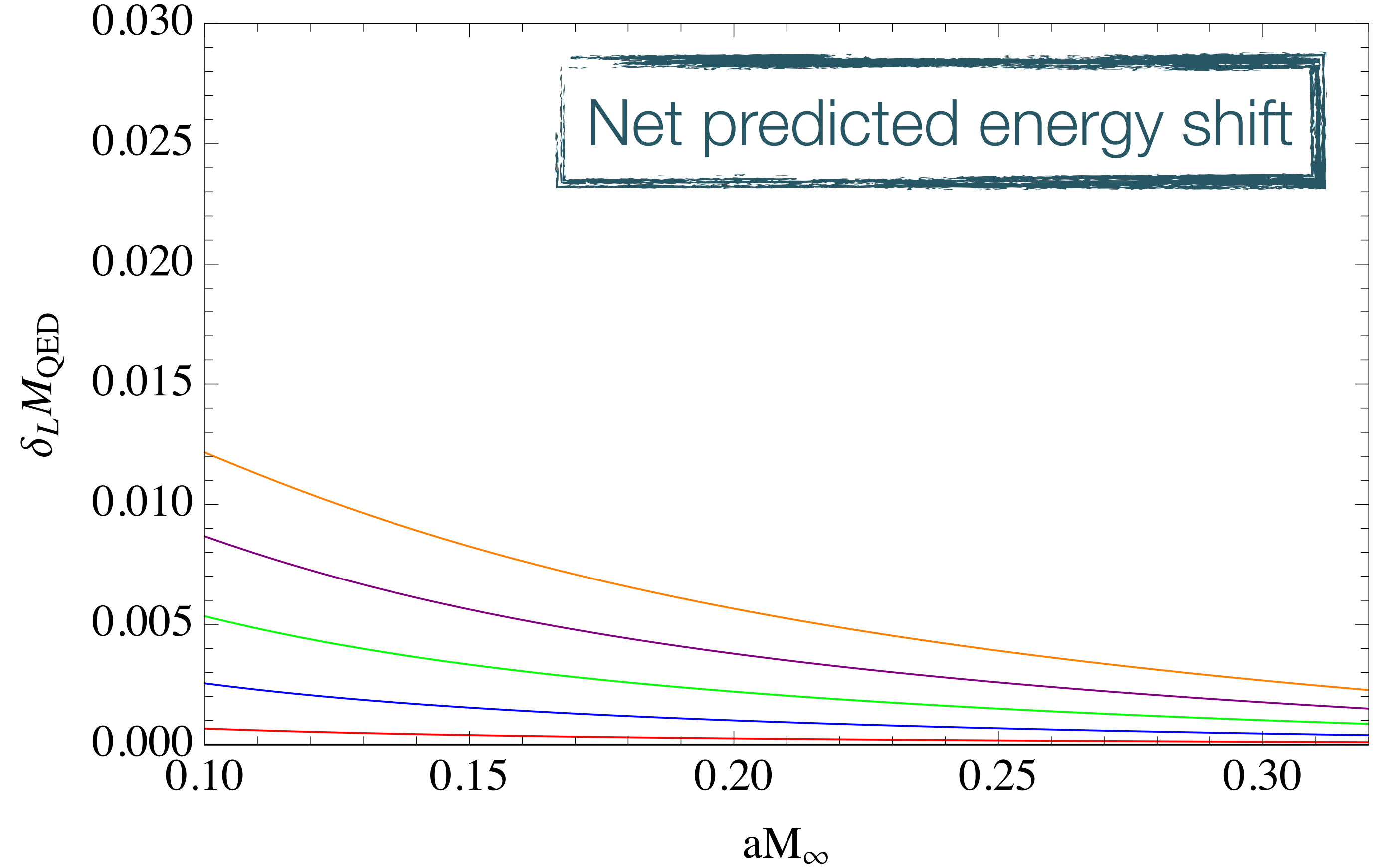
$\alpha = 0.1$

Finite-volume energy shift

Zero mode is dominant correction for 24^3: Opposite sign!

Finite-volume corrections, w/B

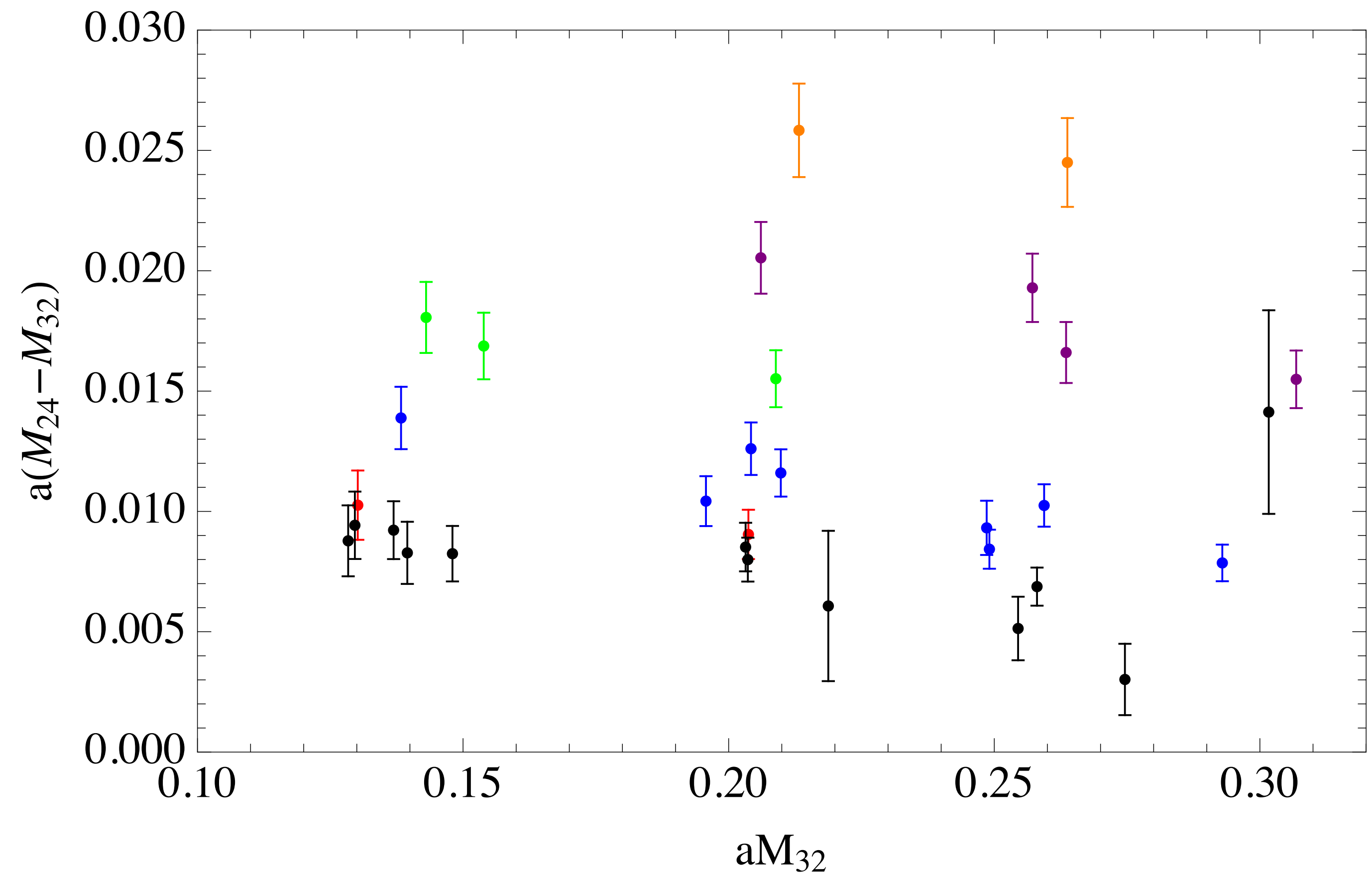


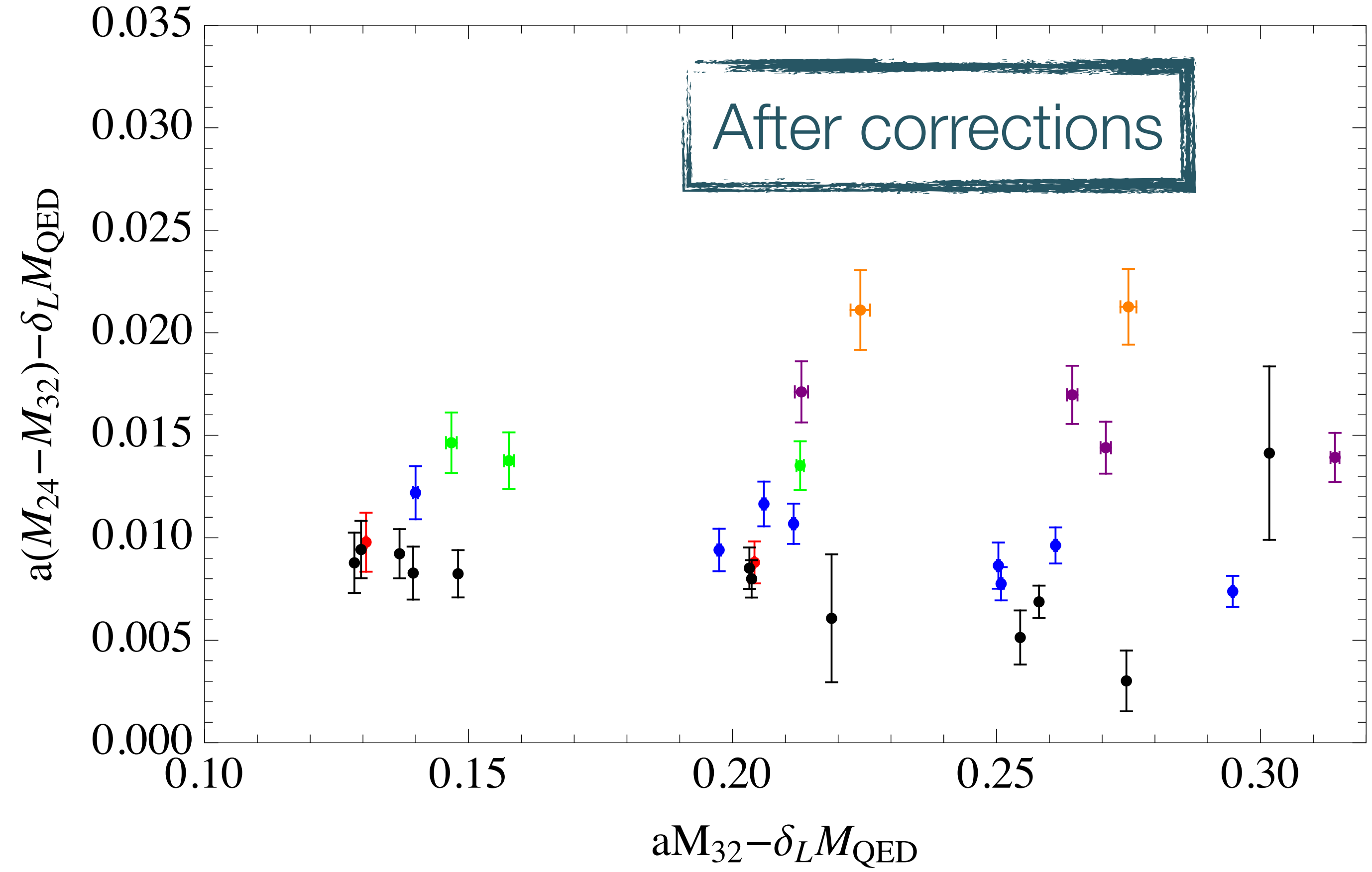


Finite-volume corrections, w/B

Zero modes are predicting the correct sign

But perhaps not the whole story

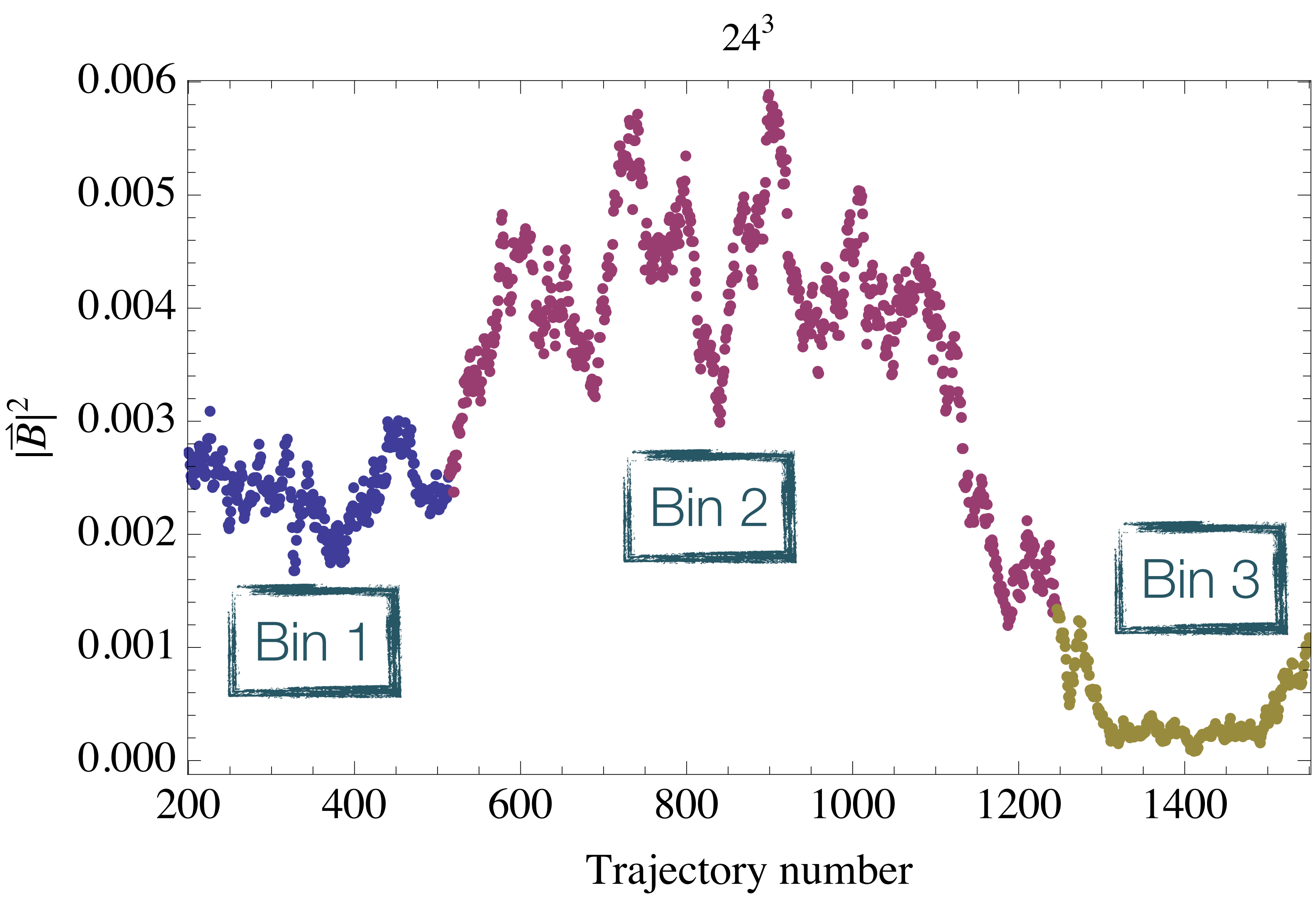




B-field correlations

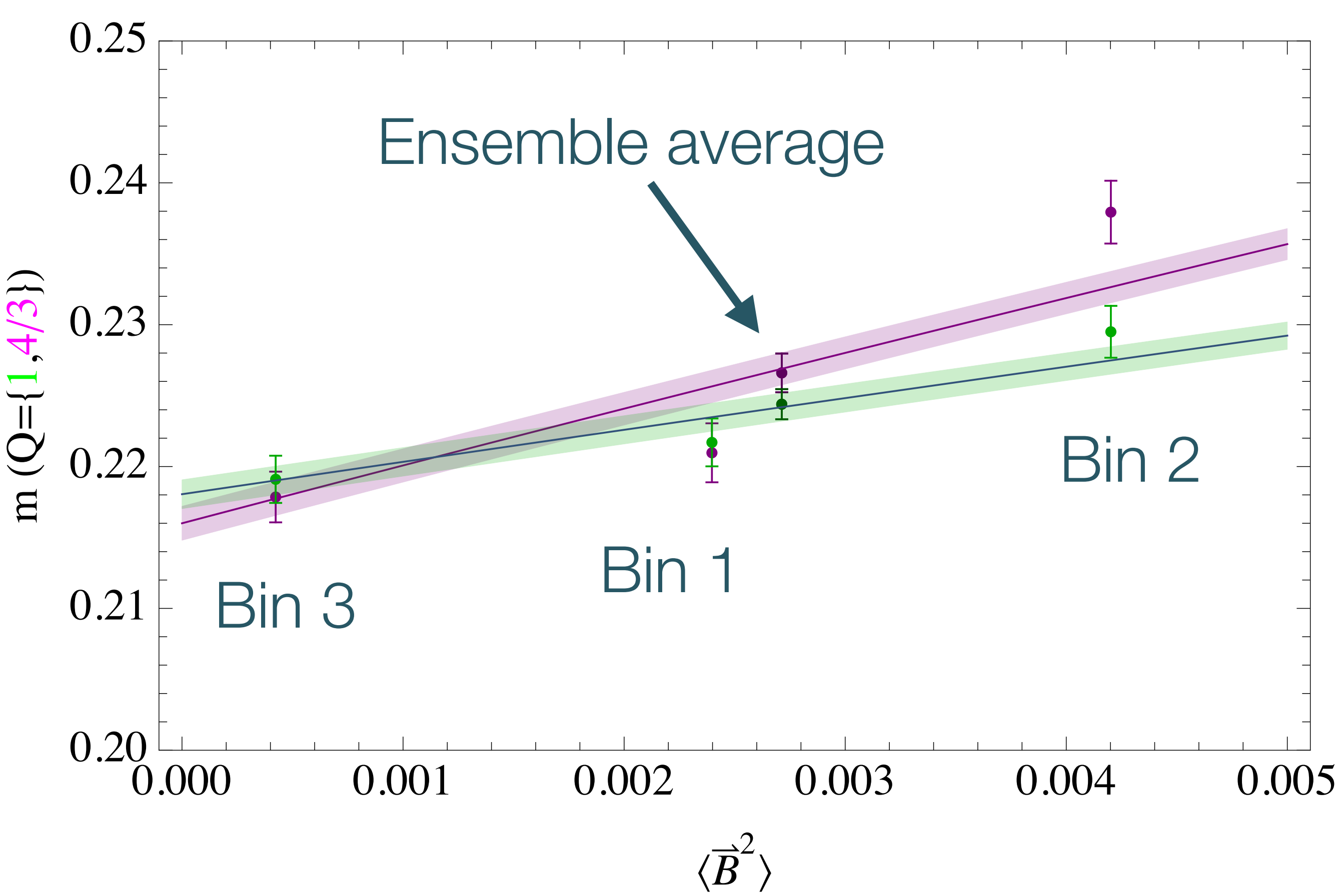
- Just to confirm the B-field correction, let's consider the variation on the same trajectory (24^3 lattice)

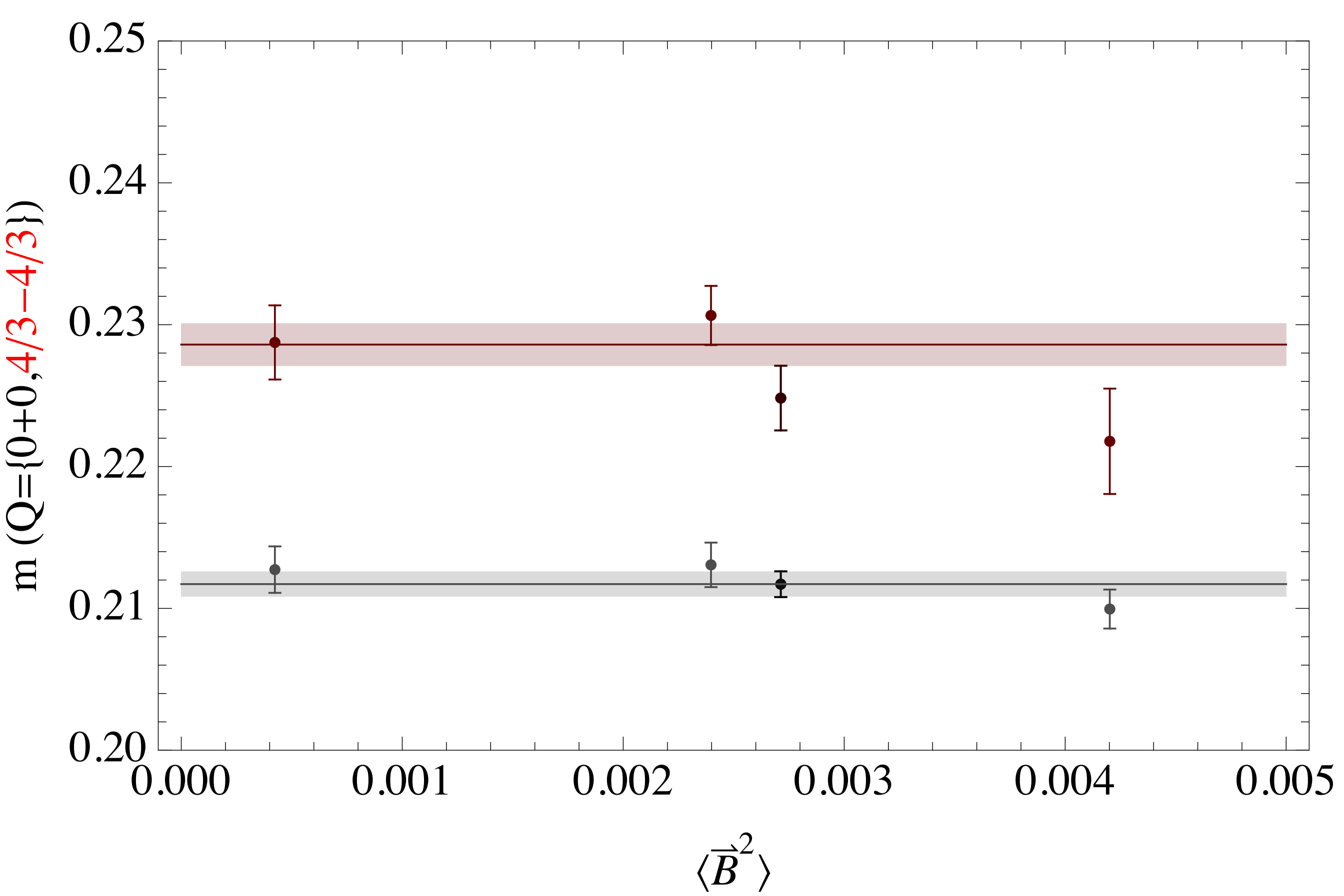
- B^2 moves slowly in HMC time, consider energy on binned intervals



B-field correlations

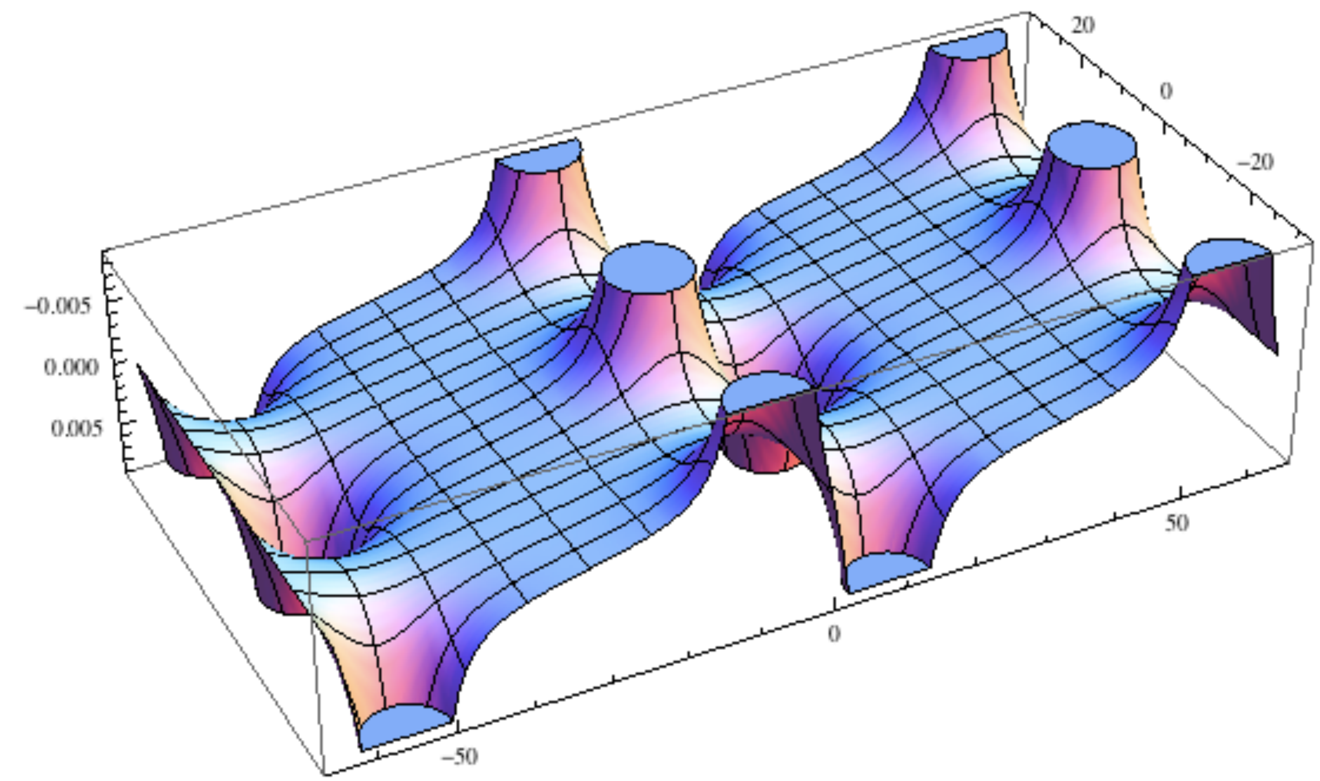
- Slopes are predicted (not a fit; ensemble avg. not included in fit)
- Charged particles clearly showing predicted trend
  Neutral mesons essentially flat (also as expected)

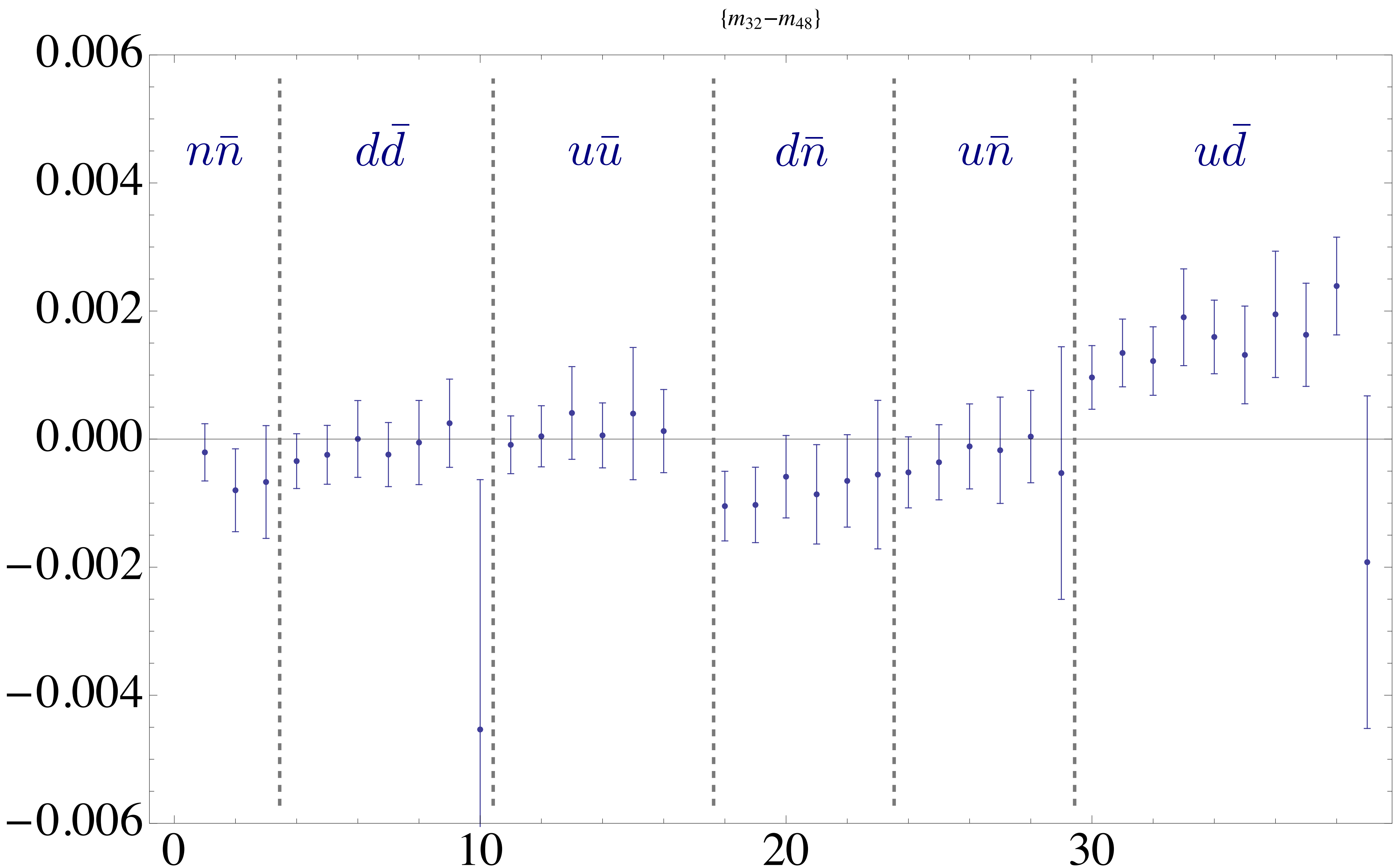




Volume effects

- Small volume 24^3; still significant finite volume corrections
- Focus main results on larger 32^3 & 48^3

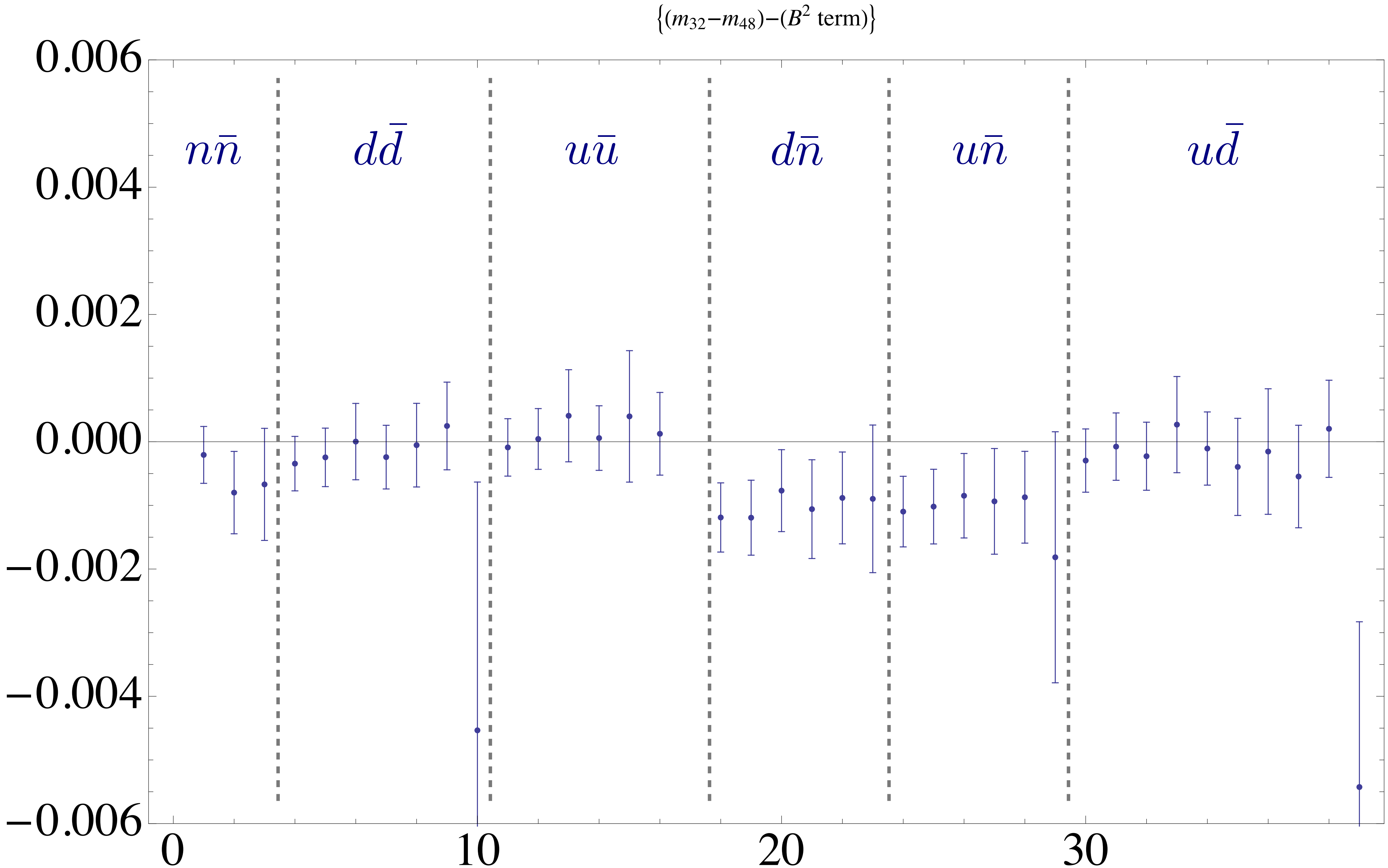




Lattice results

Finite volume effects

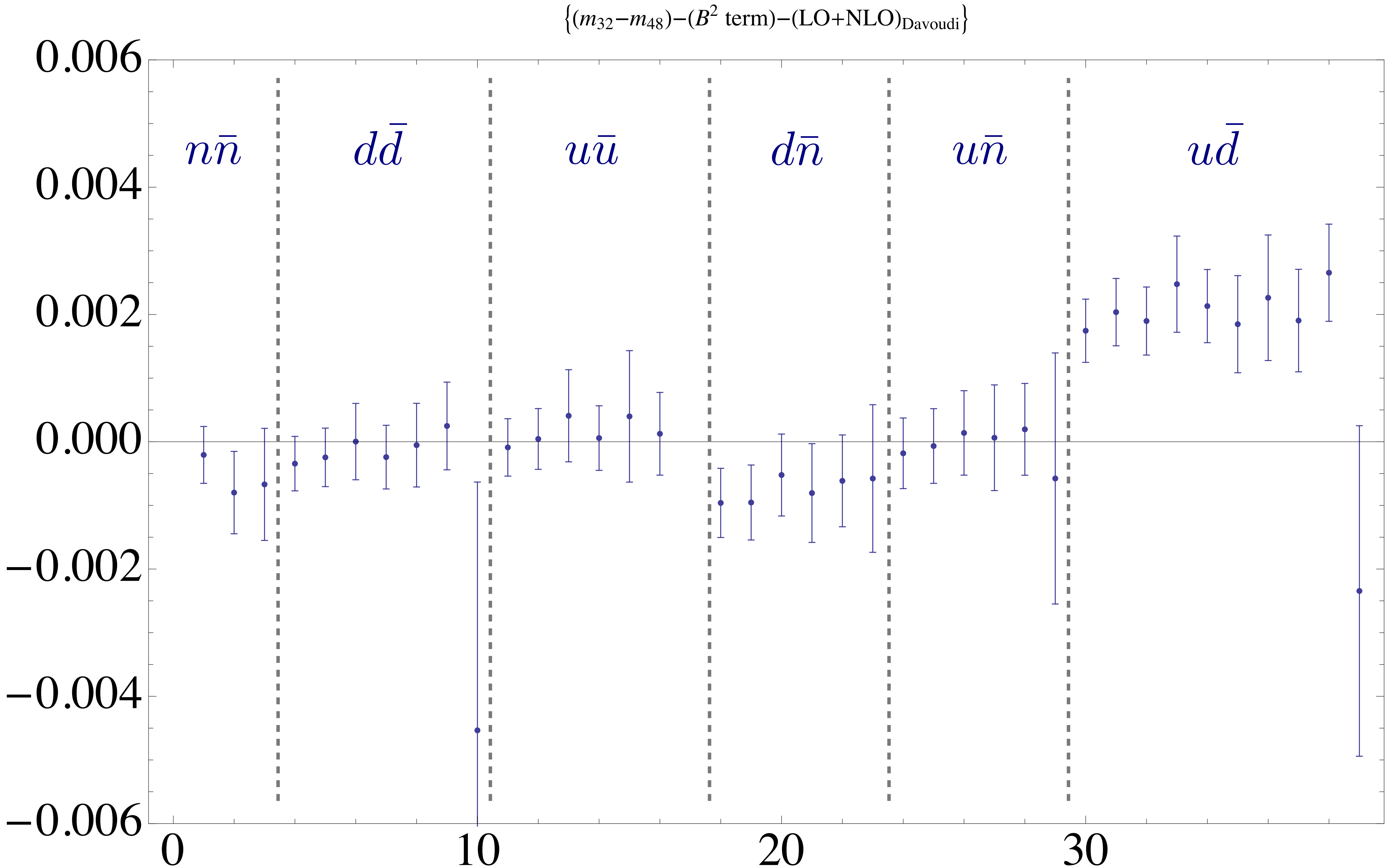
Mass differences: 32^3 - 48^3



Corrected for B term

Finite volume effects

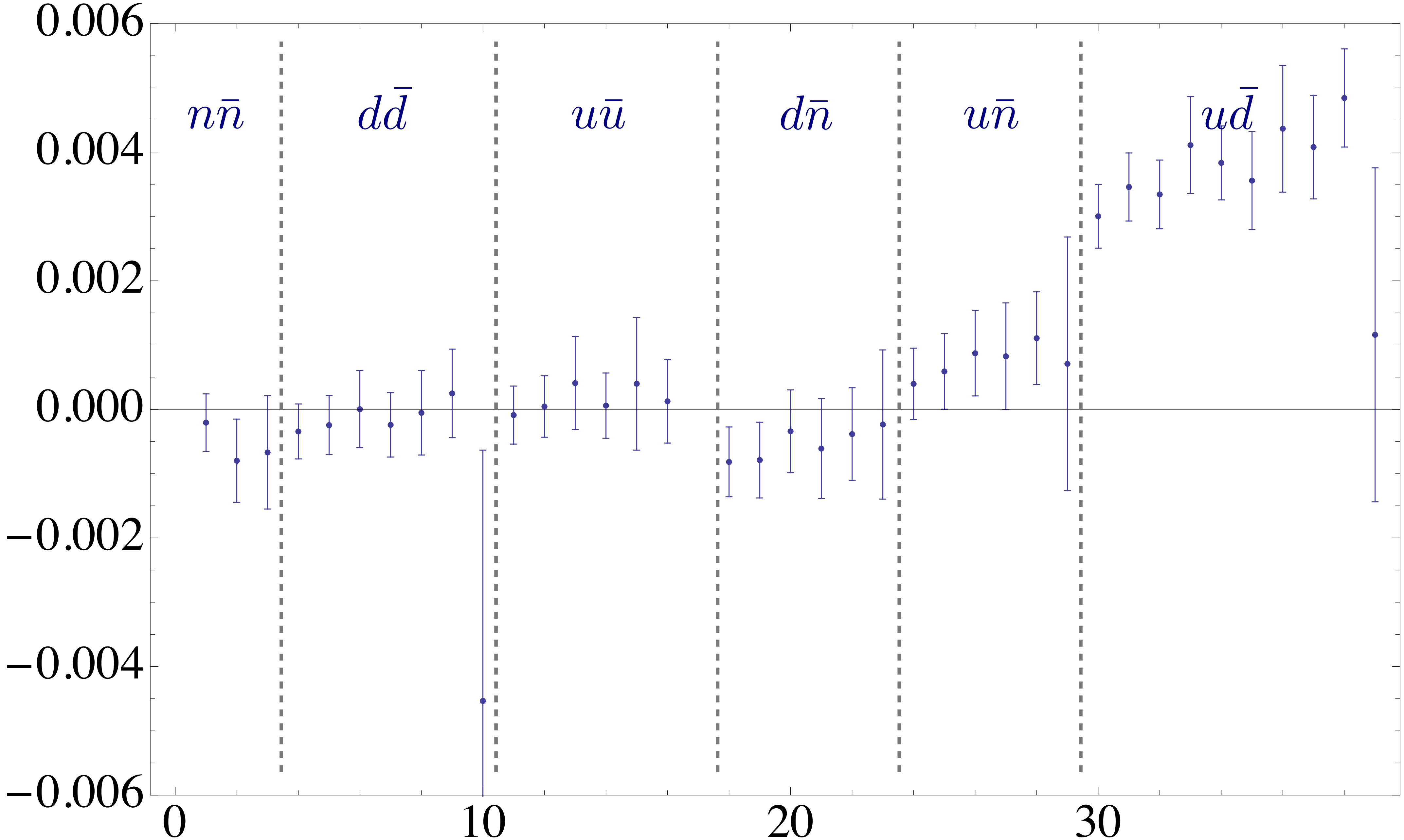
Mass differences: 32^3 - 48^3



Corrected for B term w/ LO+NLO

Finite volume effects

Mass differences: 32^3 - 48^3



Corrected for LO+NLO *only*

Finite volume effects

Mass differences: 32^3 - 48^3

Results

- Include B-term correction only
- Analysis of 32^3 and 48^3 independently
- Kappa-sym tuning

flavour	$32^3 \times 64$	$48^3 \times 96$	simulation
n	0.1208142(14)	0.1208135(9)	
d, s	0.1217026(5)	0.1217032(3)	0.121713
u	0.1243838(10)	0.1243824(6)	0.124362

- Symmetric point: $X_N/X_\pi = 2.79(3), \quad [X_N/X_\pi]^{\text{exp.}} = 2.81$

Results

- Physical point determination. Constrain to experimental masses:

$$\begin{aligned} M_{\pi^0} &= 134.977 \text{ MeV}, \\ M_{K^0} &= 497.614 \text{ MeV}, \\ M_{K^+} &= 493.677 \text{ MeV} \end{aligned}$$

- Physical point, and lattice scale:

	$32^3 \times 64$	$48^3 \times 96$
$a\delta m_u^\star$	$-0.00834(8)$	$-0.00791(4)$
$a\delta m_d^\star$	$-0.00776(7)$	$-0.00740(4)$
$a\delta m_s^\star$	$0.01610(15)$	$0.01531(8)$
a^{-1}/GeV	$2.89(5)$	$2.91(3)$

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a^{-1}/GeV	$2.89(5)$	$2.91(3)$

Sum = 0

Results

- Prediction for the charged pion mass (MeV):

	$32^3 \times 64$	$48^3 \times 96$	Real World
M_{π^+}	140.3(5)	139.6(2)	139.570
$M_{\pi^+} - M_{\pi^0}$	5.3(5)	4.6(2)	4.594

Epsilon parameters

- Violation of Dashen theorem, e.g.

$$\Delta^{\gamma}_{K^+} - \Delta^{\gamma}_{K^0} - \Delta^{\gamma}_{\pi^+} + \Delta^{\gamma}_{\pi^0} = \epsilon \Delta_{\pi}$$

- Very simple in Dashen scheme:

$$\epsilon^D_{\pi^0} = 0, \qquad \epsilon^D_{K^0} = 0, \qquad \epsilon^D_{\pi^+} = 1\,,$$

$$\epsilon^D = \frac{M^2_\gamma(K^+)}{M^2_\gamma(\pi^+)} - 1 = \epsilon^D_{K^+} - 1$$

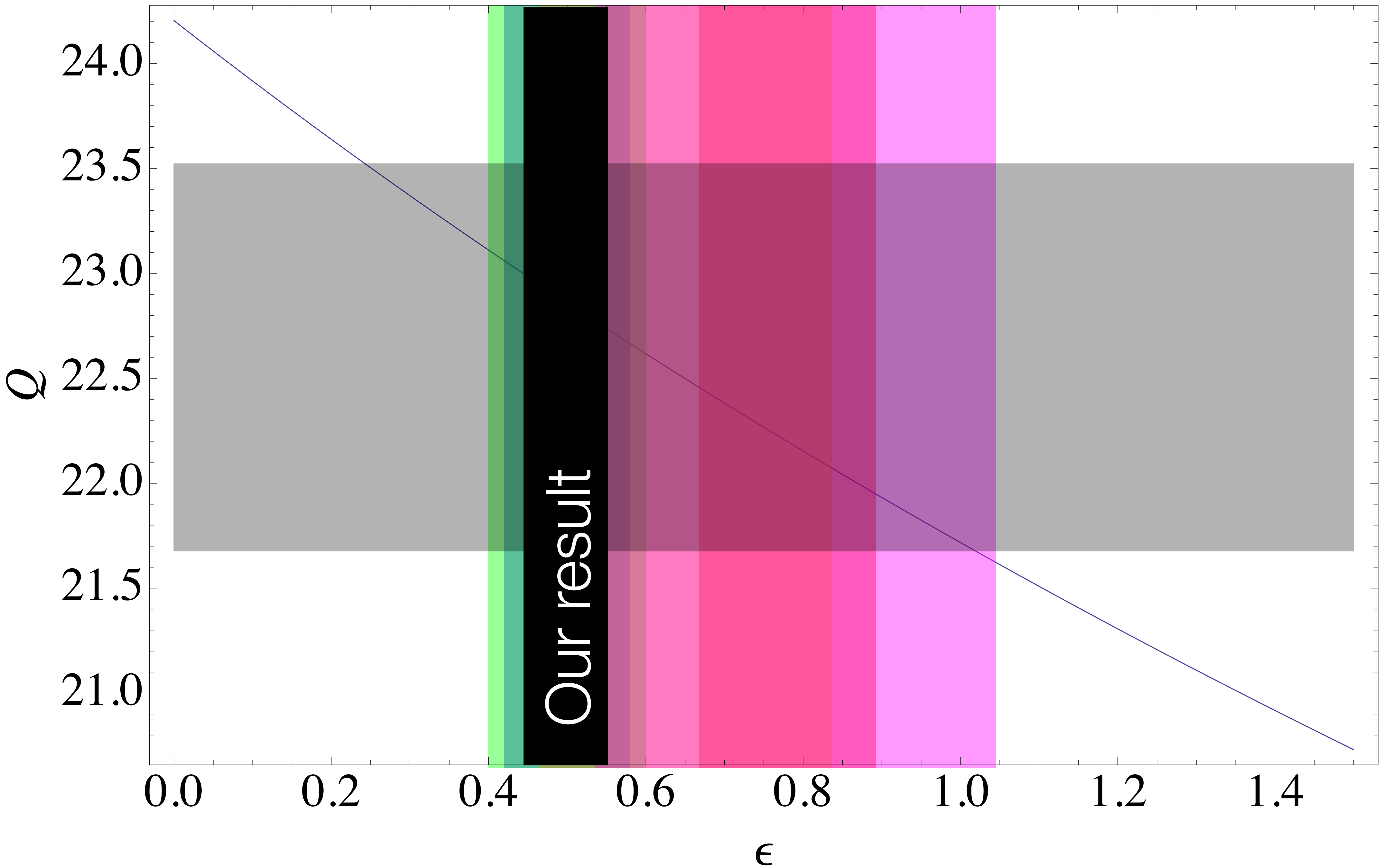
$$\begin{aligned} \epsilon^D &= 0.38(10) \qquad & 32^3 \times 64\,, \\ \epsilon^D &= 0.49(5) \qquad & 48^3 \times 96\,, \end{aligned}$$

Changing schemes

- Prescription for transforming results to MS-bar

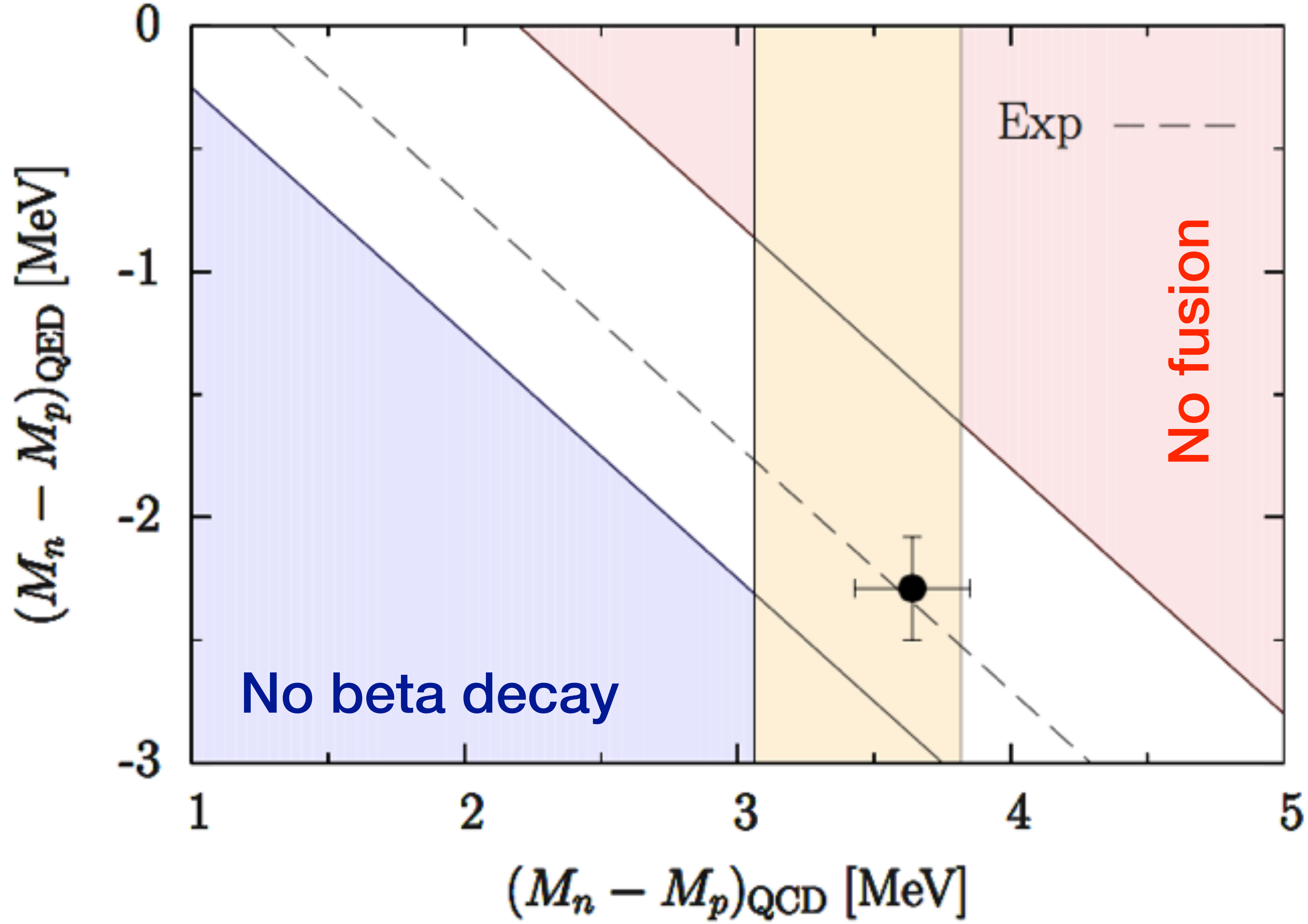
- MS-bar epsilon parameters:

$$\begin{aligned}
\epsilon_{\pi^0} &= -\alpha_{EM}\Upsilon^{D\to\overline{MS}}\tfrac{1}{2}\left[\tfrac{4}{9}M^2(u\bar{u})+\tfrac{1}{9}M^2(d\bar{d})\right]/\Delta_\pi = 0.03\pm 0.02\,,\\
\epsilon_{\pi^+} &= \epsilon^D_{\pi^+}-\alpha_{EM}\Upsilon^{D\to\overline{MS}}\tfrac{1}{2}\left[\tfrac{4}{9}M^2(u\bar{u})+\tfrac{1}{9}M^2(d\bar{d})\right]/\Delta_\pi = 1.03\pm 0.02\,,\\
\epsilon_{K^0} &= -\alpha_{EM}\Upsilon^{D\to\overline{MS}}\tfrac{1}{2}\left[\tfrac{1}{9}M^2(d\bar{d})+\tfrac{1}{9}M^2(s\bar{s})\right]/\Delta_\pi = 0.2\pm 0.1\,,\\
\epsilon_{K^+} &= \epsilon^D_{K^+}-\alpha_{EM}\Upsilon^{D\to\overline{MS}}\tfrac{1}{2}\left[\tfrac{4}{9}M^2(u\bar{u})+\tfrac{1}{9}M^2(s\bar{s})\right]/\Delta_\pi = 1.7\pm 0.1\,,\\
\epsilon &= \epsilon^D-\alpha_{EM}\Upsilon^{D\to\overline{MS}}\tfrac{1}{2}\left[\tfrac{4}{9}M^2(u\bar{u})-\tfrac{1}{9}M^2(d\bar{d})\right]/\Delta_\pi = 0.50\pm 0.06\,.
\end{aligned}$$



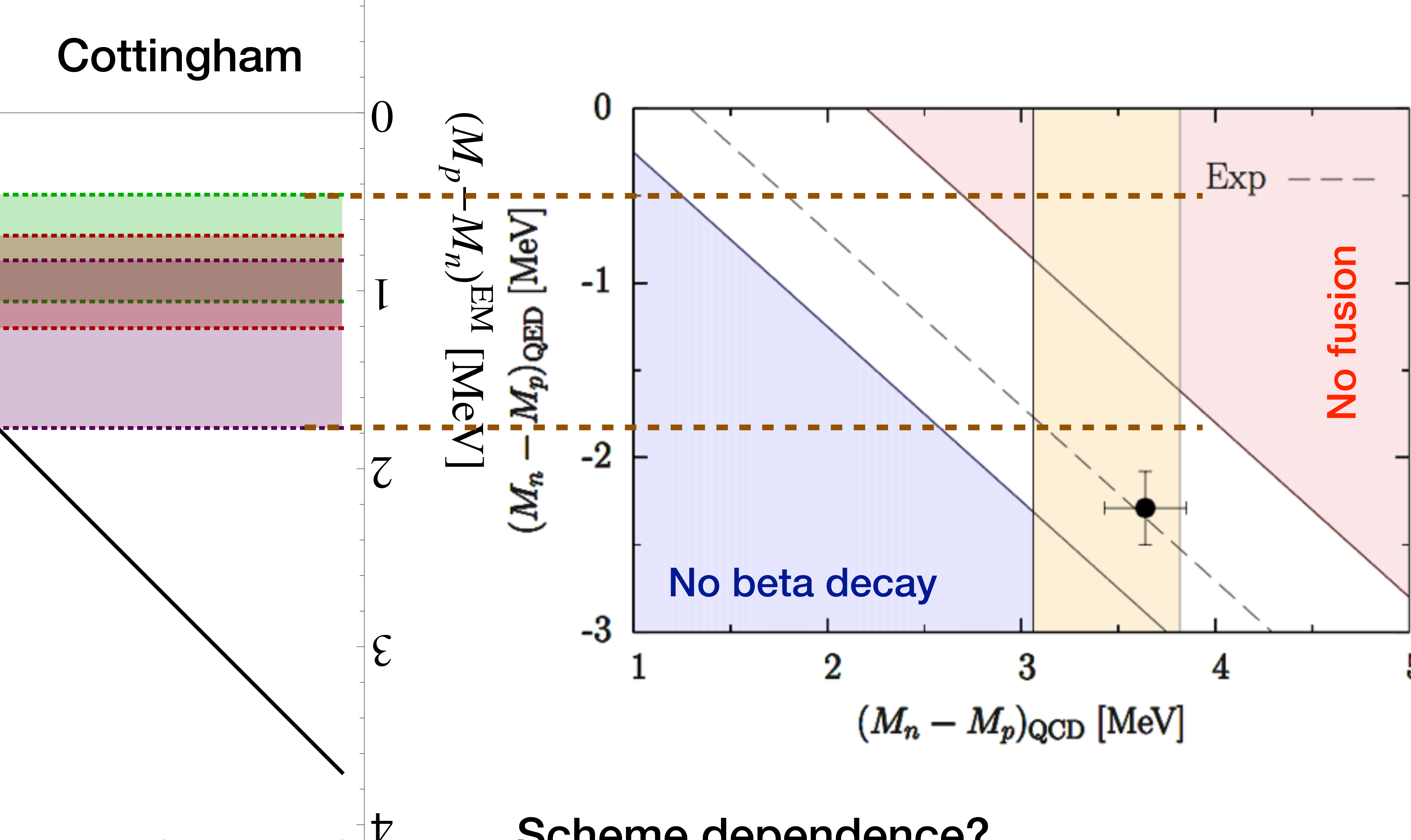
Q parameter

Lower end of other estimates



Scheme dependence?

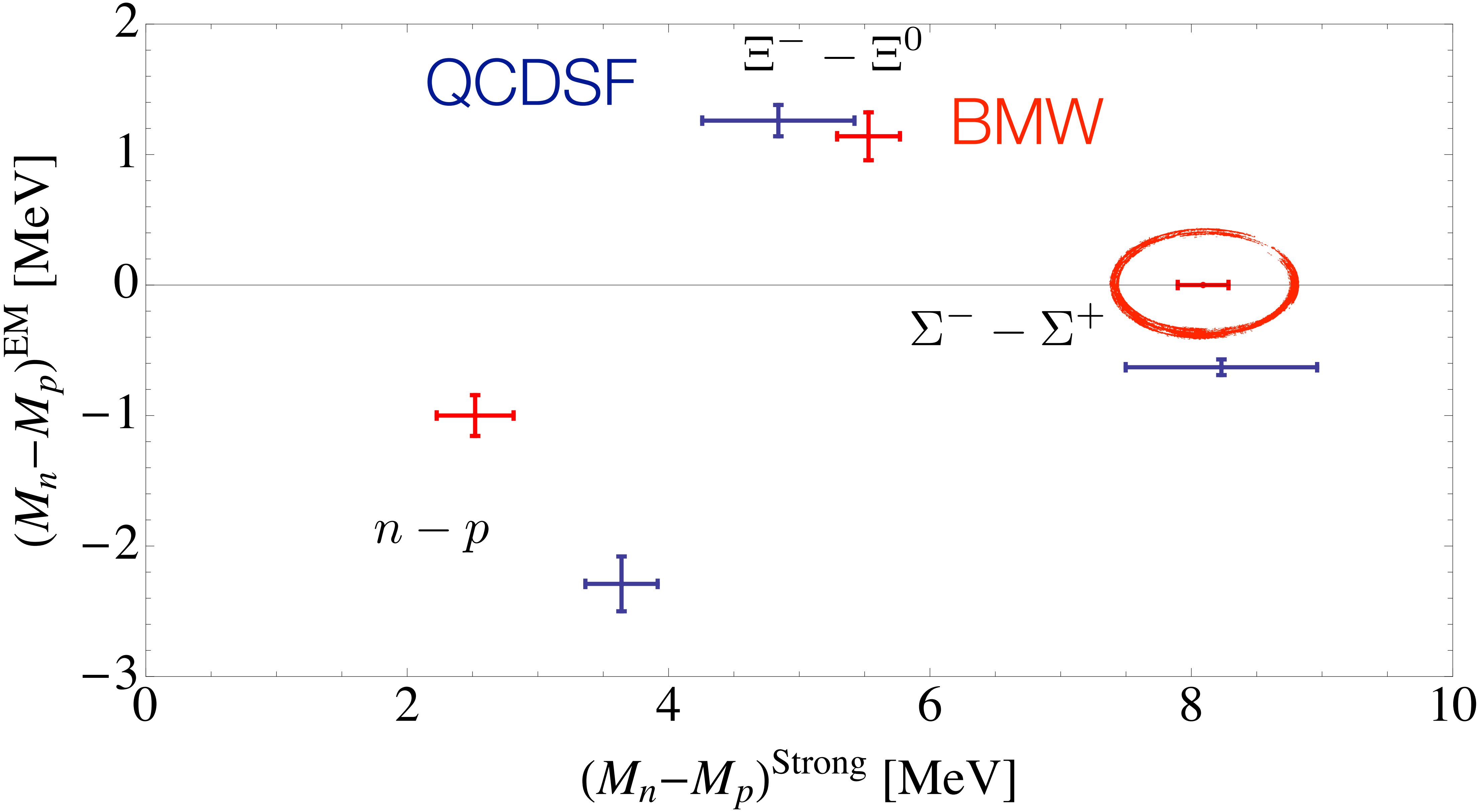
Proton–Neutron | EM–Strong separation



Scheme dependence?

Proton–Neutron

EM–Strong separation



Proton–Neutron

Comparison with BMW

Final remarks

- Incorporate QED into scheme to study SU(3) symmetry-breaking patterns
- Dashen scheme ideally suited for studying lattice spectrum
- Unexpected behaviour in finite-volume effects
    - Treatment of zero modes crucial
- Estimates for epsilon parameters
- EM–strong separation in proton–neutron splitting