Hadron-Hadron Interactions from Lattice QCD

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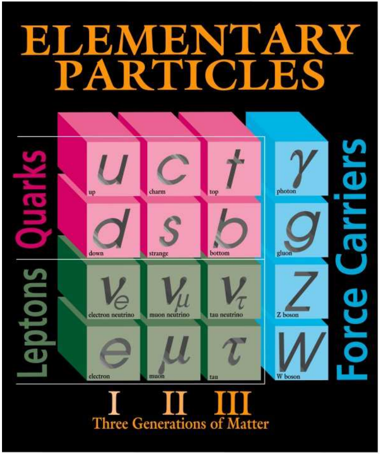
Motivation: The Theory of Strong Interactions

- Quantum Chromodynamics
  "theory of strong interactions"
- interaction of quarks and gluons
- strongly coupled at low energies
  $\rightarrow$ see previous talk
- not solvable analytically
- despite, astonishing simple action

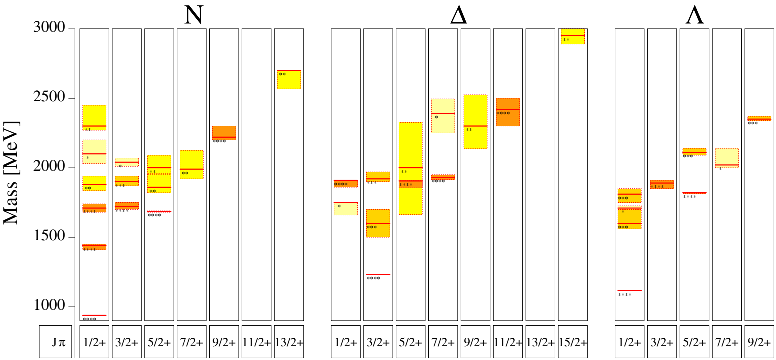


Fermilab 95-759

$$S[A_\mu, \bar{\psi}, \psi] = \int d^4x \left\{ \frac{1}{4} F_{\mu\nu}^2 + \bar{\psi}\left(\gamma_\mu D_\mu + m_q\right)\psi \right\} = S_{\mathrm{G}} + S_f$$

Motivation: Particle Zoo

QCD gives rise to a very rich particle spectrum, here nucleon, Δ and Λ



[PDG 2016, picture: B. Metsch]

- most states are resonances

$\Rightarrow$ first principles theoretical computation highly valuable

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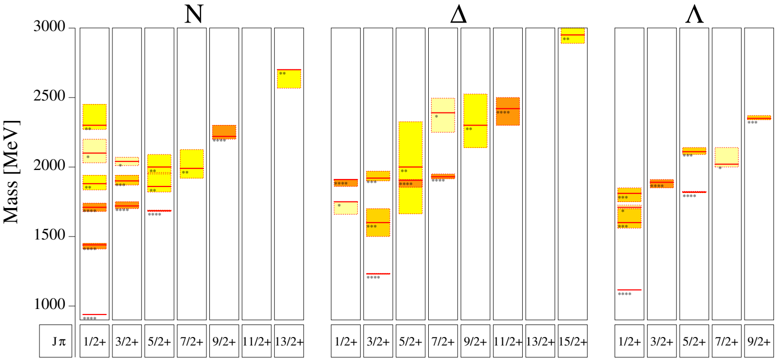
QCD gives rise to a very rich particle spectrum, here nucleon, Δ and Λ



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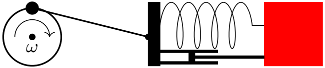
What is a resonance?

- consider a simple, driven damped harmonic oscillator



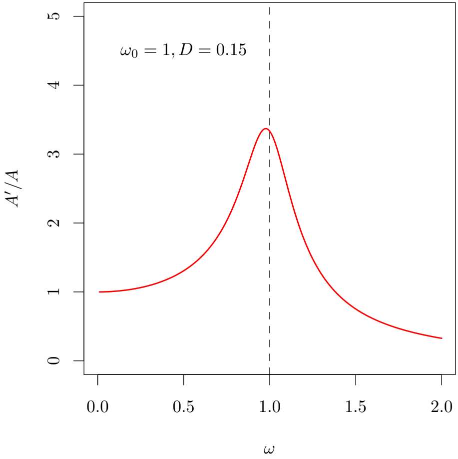
- equations of motion

$$\dot{x}^2 + 2D\omega_0\dot{x} + \omega^2 x = A\sin(\omega t)$$

- solution is known

$$x(t) = A'\sin(\omega t + \delta)$$

- for D small, a resonance occurs



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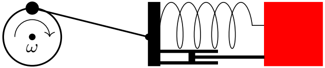

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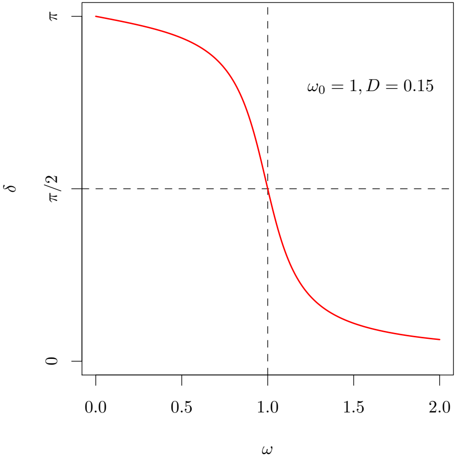

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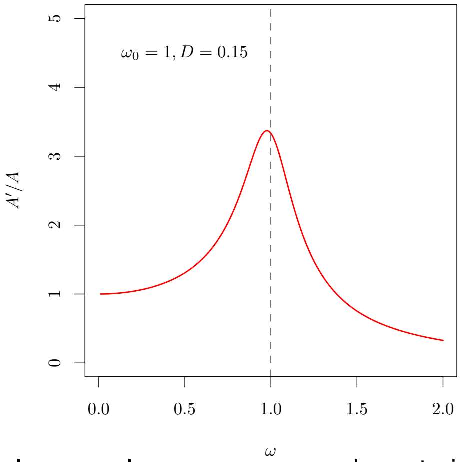
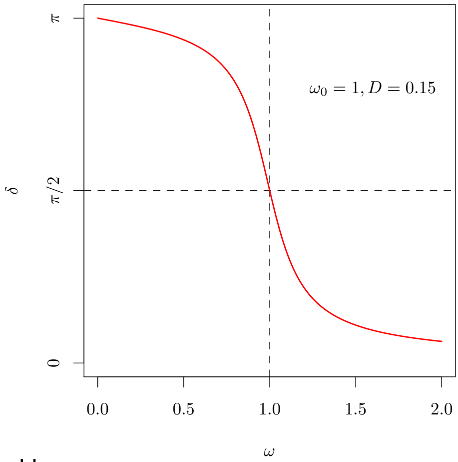


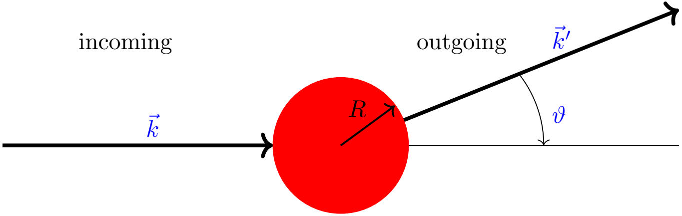


In general: resonances are characterised by

- resonance amplification in the amplitude ratio
- phase shift δ crosses $\pi/2$

Scattering of Particles

- consider interaction of finite range R, spherically symmetric



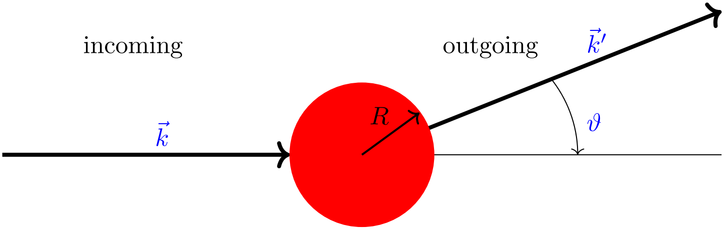
- incoming and outgoing waves differ by a phase shift
- scattering amplitude in the partial wave expansion

$$f_k(\theta) = -\frac{8\pi}{M}\sum_{\ell=0}^{\infty}(2\ell+1)\ f_\ell(k)\ P_\ell(\cos\theta)$$

with partial wave amplitude and phase shift δ_ℓ

$$f_\ell(k) = \frac{1}{k\cot\delta_\ell(k) - ik}$$

Scattering of Particles



- it actuallly suffices to know the phase shifts $\delta_\ell(k)$

- often, even a single partial wave is enough (due to symmetries)

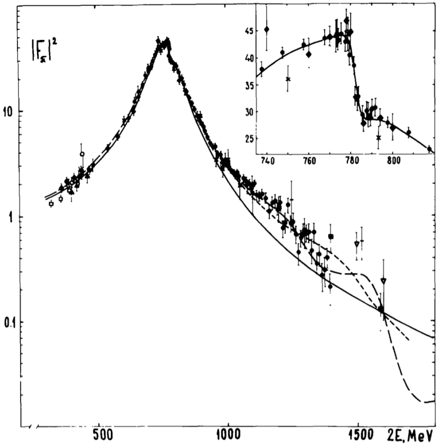
$\Rightarrow$ at small energies (small k) one can expand

$$k^{2\ell+1}\cot\delta_\ell \;=\; \frac{1}{a_\ell} + \frac{r}{2}k^2 + \ldots$$

- a_ℓ scattering length, r effective range

Example: ρ Resonance

- ρ: lowest QCD resonance
- in $\pi\pi$ channel with $I = 1$
- experimentally well measured
- clear signal in the amplitude



[Barkov et al., Nucl.Phys. B256 (1985)]

Example: ρ Resonance

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- in $\pi\pi$ channel with $I = 1$
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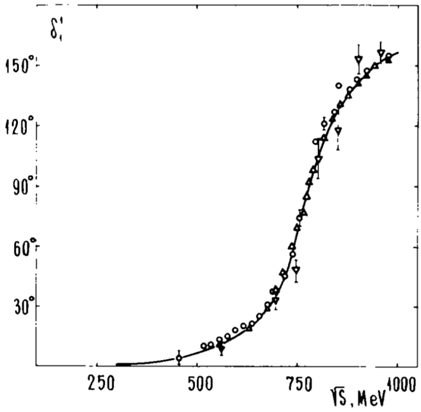
- clear signal in the amplitude
- and nice phase shift



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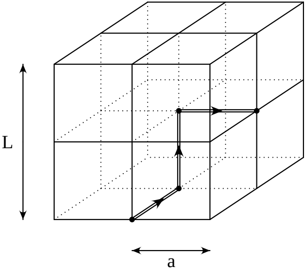
Lattice Regularisation

- work in Euclidean space-time
- lattice regularisation: discretise space-time
  - hyper-cubic $L^3 \times T$-lattice with lattice spacing a

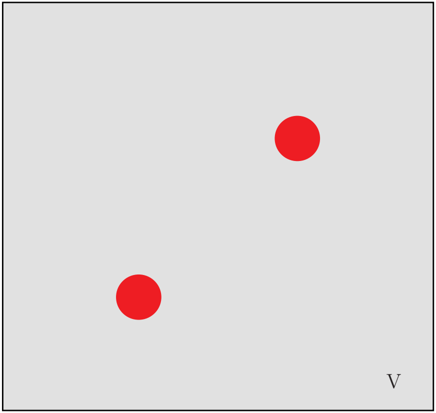
  $\Rightarrow$ momentum cut-off: $k_{\mathrm{max}} \propto 1/a$
  - derivatives $\Rightarrow$ finite differences
  - integrals $\Rightarrow$ sums
  - gauge potentials A_μ in $G_{\mu\nu}$ $\Rightarrow$ link matrices U_μ ('')



- finite volume: quantised energy levels
- showstopper: particle interactions cannot be studied directly

[Maiani and Testa, (1990)]

instead: use finite volume as vehicle...



- for $V \to \infty$:

$\Rightarrow$ interaction probability very low

$\Rightarrow$ $E_{2p}(p=0) = 2M_{1p}$

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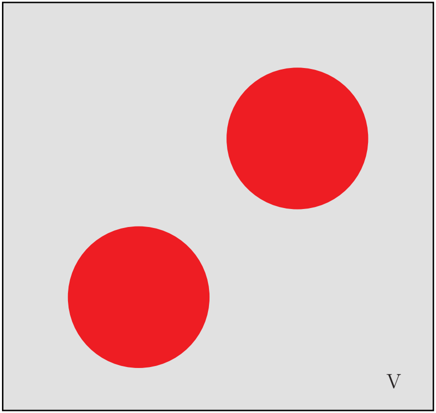

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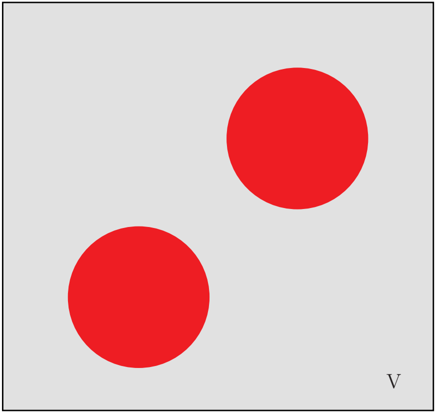

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- Lüscher: correction in $1/V$ related to scattering properties!

[Lüscher, 1986]

Uncertainties

- Euclidean space-time $\Rightarrow$ Monte Carlo Methods
  $\Rightarrow$ statistical errors

- and systematic errors:
  - lattice spacing effects $\Rightarrow$ continuum limit, lattice spacing $a \to 0$,
    $\Rightarrow$ remove leading order lattice artefacts
  - finite size effects $\Rightarrow$ thermodynamic limit, physical volume $L^3 \to \infty$,
    $\Rightarrow$ use chiral effective field theories.
  - chiral effects $\Rightarrow$ chiral limit, $M_{\mathrm{PS}} \to M_\pi\,, \quad M_\pi^2 \propto m_\ell$,
    $\Rightarrow$ use chiral effective field theories.
    or simulate directly at the physical point!

Example: ϕ^4 Theory

Example: Complex ϕ^4 Theory

- complex ϕ^4 theory as toy model
- lattice action

$$S = \sum_x \Big(-\kappa \sum_\mu (\varphi_x^\star \varphi_{x+\mu} + cc) + \lambda(|\varphi_x|^2 - 1)^2 + |\varphi_x|^2 \Big)$$

- perform threshold expansion

$$k^{2\ell+1} \cot \delta_\ell \;=\; \frac{1}{a_\ell} + \frac{r}{2} k^2 + \ldots$$

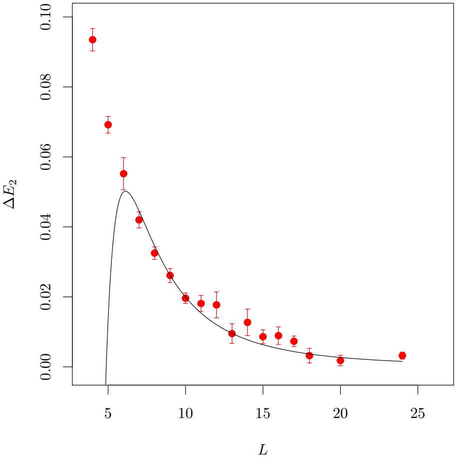
- then, the finite volume dependence reads

[Lüscher, 1986]

$$\delta E_2 = E_2 - 2E_1 = -\frac{4\pi a_0}{mL^3} \left(1 + c_1 \frac{a_0}{L} + c_2 \left(\frac{a_0}{L}\right)^2 + \frac{2\pi r a_0^2}{m^2 L^3} + \ldots \right)$$

Example: Complex ϕ^4 Theory

- can study arbitrary volumes
- for chosen parameter: repulsive
- depending on fit range sensitive to a_0 or r
- for too small L description breaks down



$\Rightarrow$ ΔE_2 gives access to a_0 and r

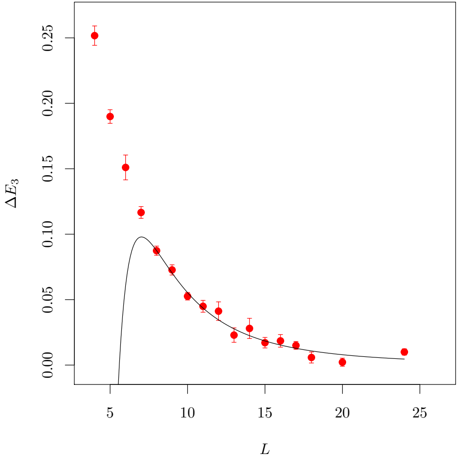
Example: Complex ϕ^4 Theory

- three particle formula

$$\Delta E_3 = E_3 - 3E_1 = \frac{12\pi a_0}{mL^3}\left(1 + \ldots + \left(\frac{a_0}{\pi L}\right)^3\left(A + c_L \log\frac{mL}{2\pi}\right)\right)$$

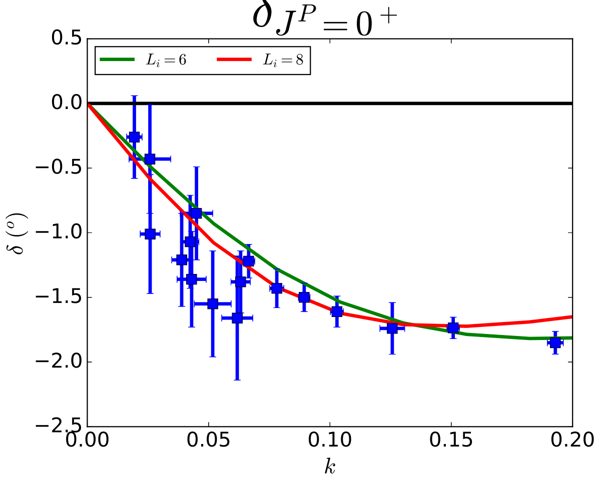
[see e.g. Sharpe 2017]

- A and c_L encode three body interaction
- data well described
- a_0, r input from ΔE_2
- clear evidence for non-zero three particle interaction!



Example: Complex ϕ^4 Theory

- every volume translates into one scattering momentum



$\pi - \pi$ Scattering with $I = 2$

$\pi - \pi$ Scattering for $I = 2$

- weakly repulsive channel
- very interesting check of chiral perturbation theory
- at small momenta $k \to 0$ use effective range expansion

$$k^{2\ell+1} \cot \delta_\ell \;=\; \frac{1}{a_\ell} + \mathcal{O}(k^2)$$

  scattering length a_ℓ

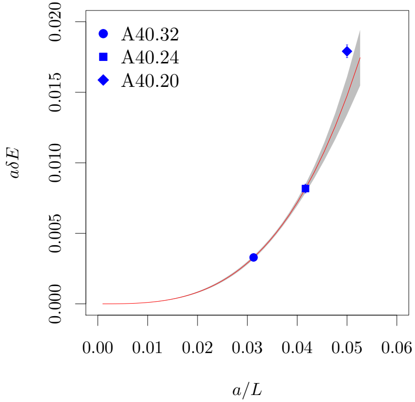
- only S-waves ($\ell = 0$) contribute (to a good approximation)
- results from experiment plus Roy equations available

$\Rightarrow$ benchmark quantity for lattice QCD

Lüscher formula (known constants c_i)

$$\delta E = E_{2p} - 2E_{1p} = -\frac{4\pi a_0}{M_\pi L^3}\left(1 + c_1 \frac{a_0}{L} + c_2 \frac{a_0^2}{L^2}\right) + \mathcal{O}(L^{-6}) \,,$$

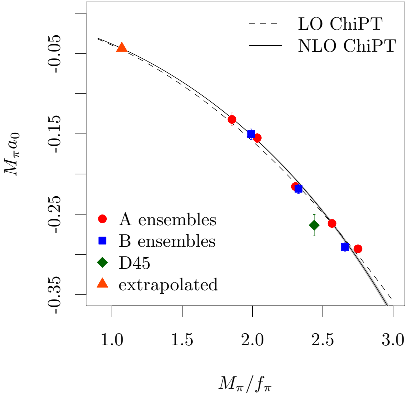
- valid, if other FS corrections small
- three ensembles with identical parameters but L
- smallest L deviates a few sigma
- smallest L too small
- all other ensembles have comparably larger L-values

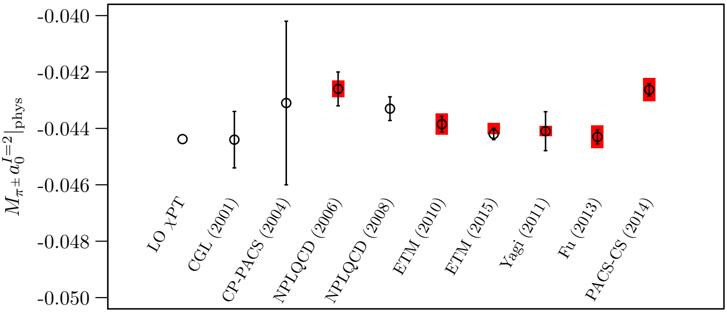


- ChiPT formula at NLO [Beane et al, (2005,2007)]

$$M_\pi a_0 = -\frac{M_\pi^2}{8\pi f_\pi^2}\left\{1 + \frac{M_\pi^2}{16\pi^2 f_\pi^2}\left[3\ln\frac{M_\pi^2}{f_\pi^2} - 1 - \ell_{\pi\pi}^{I=2}(\mu_R = f_{\pi,\mathrm{phys}})\right]\right\}$$

- functional form highly constraining
- surprisingly small deviations from LO ChiPT
- lattice artefacts small (in fact $\mathcal{O}(a^2 m_q)$)
- see JHEP 1509 (2015) 109





- result:

$$M_\pi a_0^{I=2} \;=\; -0.0442(2)_{\mathrm{stat}}\left({}^{+4}_{-0}\right)_{\mathrm{sys}}\,, \qquad \ell_{\pi\pi}^{I=2} \;=\; 3.79(0.61)_{\mathrm{stat}}\left({}^{+1.34}_{-0.11}\right)_{\mathrm{sys}}$$

[ETMC, Helmes, CU, et al, (2015)]

$\pi - K$ Scattering

Elastic Scattering of Strange Mesons

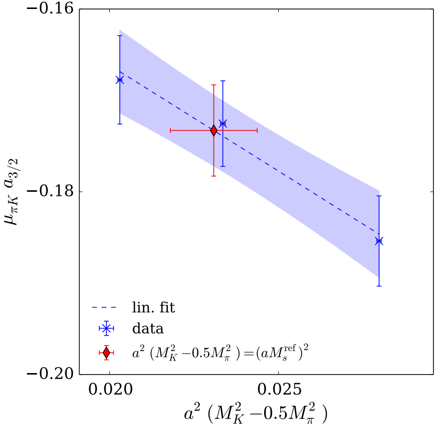
- now replace one of the pions by a kaon
- two isospin channels: $I = 1/2$ and $I = 3/2$
- $I = 1/2$ similar to $I = 0\ \pi - \pi$
  $I = 3/2$ similar to $I = 2\ \pi - \pi$
- DIRAC determined difference a_0^- from τ_{1S} of πK atoms
  [DIRAC, Phys. Rev. D 96, 052002 (2017)]
- with isospin odd scattering length $a_0^- = \frac{1}{3}(a_0^{1/2} - a_0^{3/2})$
- so far only lattice data for one lattice spacing available in literature

Strange Quark Mass Tuning

- value of sea strange quark mass up to 10% off
- corrected for by varying the valence strange quark mass

⇒ small unknown systematic uncertainty

- interpolate linearly in $M_K^2 - 0.5 M_\pi^2$
- input: M_K, M_π and lattice spacing
- now work at fixed strange quark mass value



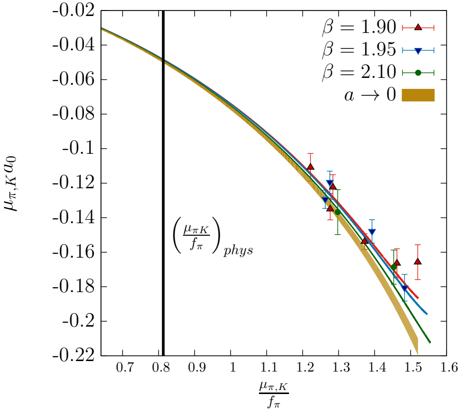
- $\mu_{\pi K}\, a_0$ known from χ-pt at NLO:

$$\mu_{\pi K}\, a_0^{3/2} = \frac{\mu_{\pi K}^2}{4\pi f_\pi^2}\left\{\frac{32 M_\pi M_K}{f_\pi^2} L_{\pi K}(\Lambda_\chi) - 1 - \frac{16 M_\pi^2}{f_\pi^2} L_5(\Lambda_\chi) + \frac{1}{16\pi^2 f_\pi^2}\chi_{\text{NLO}}^{3/2}(\Lambda_\chi, M_\pi, M_K, M_\eta)\right\}$$

- $\mu_{\pi K}$ reduced mass of $\pi - K$ system
- $\chi_{\text{NLO}}^{3/2}$ involves chiral logarithms.
- two LECs: L_5 and $L_{\pi K}$
- difficult to disentangle

$\Rightarrow$ use prior for $L_5 = 5.41(3) \cdot 10^{-3}$

[HPQCD, (2013)]



Comparison to Experiment

- recall, DIRAC experiment measures only a^-

$$a_0^{1/2} = a^+ + 2a^- \,, \qquad a_0^{3/2} = a^+ - a^-$$

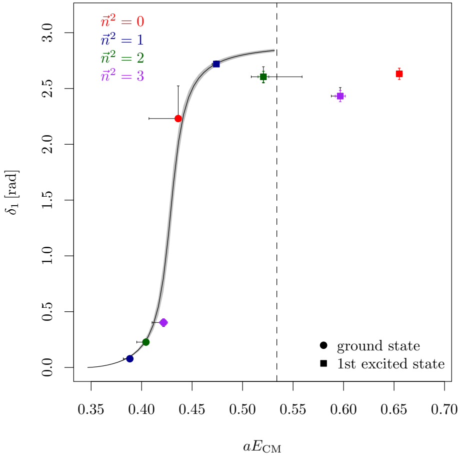
- $a^\pm$ can both be expanded in ChPT
- once one knows L_5 and $L_{\pi K}$, one can compute $a^\pm$ (and $a_0^{1/2}$)
- we obtain

	$(M_\pi a_0^{1/2})^{\text{phys}}$	$(M_\pi a_0^{3/2})$	$M_\pi a_0^-$
This Work	$0.165(1)$	$-0.059(1)$	$0.0744(2)$
NPLQCD	$0.173(2)$	$-0.057(2)$	$0.0773(10)$
DIRAC	-	-	$0.072^{(+31)}_{(-20)}$

$\pi - \pi$ Scattering with $I = 1$: the ρ resonance

The ρ Resonance from Lattice QCD (preliminary)

- phase shift δ_1 as a function of scattering energy
- here: single ensemble
- unphysically large pion mass
- clear resonance signature
- could determine mass and width



- the core of our computation is the Dirac kernel
- highly symmetric and sparse matrix stencil

$$[M_{eo}\psi_o](x) = \sum_\mu \kappa_\mu \left(U_\mu(x)(1-\gamma_\mu)\psi_o(x+\hat\mu) + U^\dagger_\mu(x-\hat\mu)(1+\gamma_\mu)\psi_o(x-\hat\mu)\right)\Big]$$

- μ runs over x, y, z, t directions
- x runs over space-time volume
- kernel ill condinioned, needs to be inverted very often using an iterative solver like CG (or multi-grid)
- code tuning is highly critical for us!
- Juqueen is and isn't a beautiful machine at the same time!

Numerics for Lattice QCD

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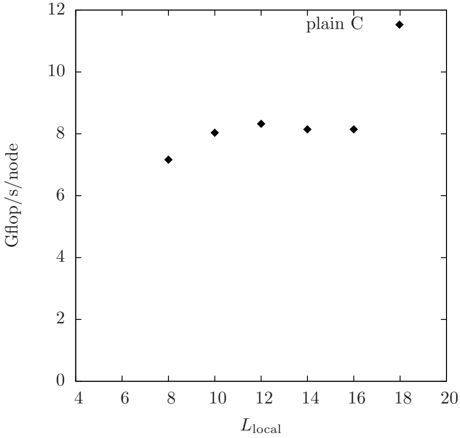
kernel performance tuning for BG/Q

- plain C is not acceptable



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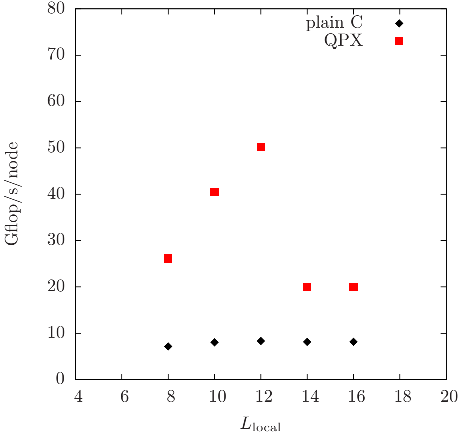

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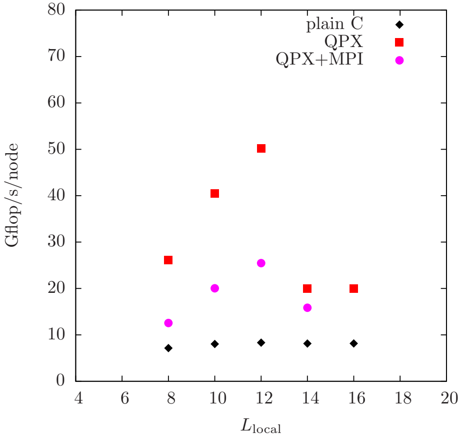

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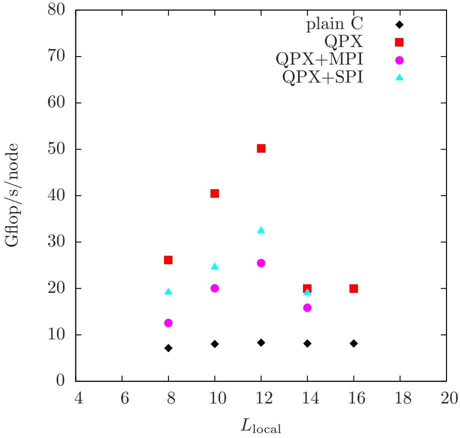
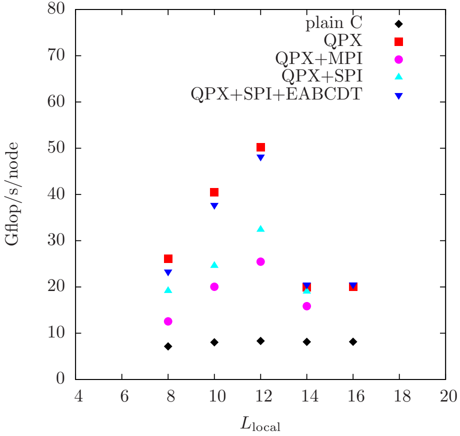
- use low level communication (SPI)



kernel performance tuning for BG/Q

- plain C is not acceptable
- explore vector unit (QPX)
- MPI hits badly
- use low level communication (SPI)
- and get mapping right



⇒ almost no communication overhead and 25% of Peak!

Summary

- very precise $N_f = 2+1+1$ lQCD results for $I = 2$ $\pi - \pi$ scattering
- continuum extrapolated results for $\pi - K$ scattering with $I = 3/2$
- using ChPT we also access $\pi - K$ with $I = 1/2$
- finalising analysis for $\pi - \pi$ with $I = 1$ (ρ resonance)
- currently studying $\pi - N$ scattering at physical pion mass (Δ resonance)

Outlook

- compute the binding energy of, say, oxygen directly from Quantum Chromodynamics?

$\Rightarrow$ clearly, a long way to go

- there are many challenges to deal with

- among others:
  - binding energy tiny compared to mass of the nucleus
  - very large volumes needed
  - enormous number of contractions

- resources at JSC will be crucial!

Thanks to ...

- the lattice QCD group in Bonn:
  C. Helmes, C. Jost, B. Knippschild, B. Kostrzewa, L. Liu, M. Oehm, K. Ottnad, M. Petschlies, F. Pittler, F. Romero Lopez, M. Ueding, M. Werner
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- the DFG funding this project in the Sino-German CRC 110
- the ETM collaboration
- ... and for your attention!