lattice QCD (and some of its applications)

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lattice QCD

what is it ?

what can you do with it ?

what can't you do with it ?

quantum chromodynamics

gauge field theory of quarks (fermions) and gluons (vector gauge fields) with SU(3) 'color' symmetry

qcd lagrangian

$$\mathcal{L} = \bar{\psi}\big(i\gamma^\mu D_\mu - m\big)\psi - \tfrac{1}{2}\mathrm{tr}\big(F_{\mu\nu}F^{\mu\nu}\big)$$

gauge covariant derivative

$$D_\mu = \partial_\mu + igA_\mu$$

field strength tensor

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig\big[A_\mu, A_\nu\big]$$

qcd fields

color index $i = 1\ldots 3$

quark field $\psi^i_\alpha(x)$

Dirac spin index $\alpha = 1\ldots 4$

traceless matrix in color

gluon field $A^{ij}_\mu(x)$

Lorentz vector

$$= \sum_{a=1\ldots 8} A^a_\mu(x)\, t^a_{ij}$$

expansion in SU(3) generators

$$t^a = \tfrac{1}{2}\lambda^a$$

$$\big[t^a, t^b\big] = if^{abc}t^c$$

$$\mathrm{tr}\big(t^a t^b\big) = \tfrac{1}{2}\delta^{ab}$$

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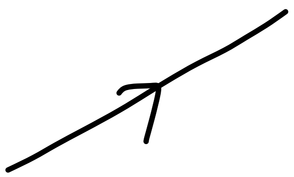
qcd ingredients

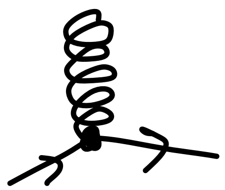
relativistic fermions

$$\bar{\psi}\big(i\gamma^\mu\partial_\mu - m\big)\psi$$



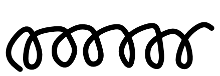
color vector current

$$g\,\big(\bar{\psi}\gamma^\mu t^a\psi\big)\,A^a_\mu$$



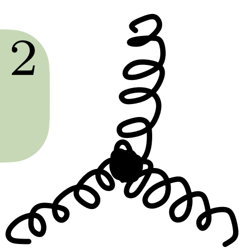
massless gluons

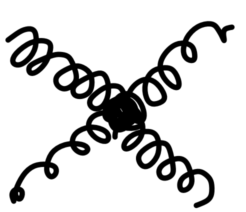
$$\big(\partial_\mu A_\nu - \partial_\mu A_\nu\big)^2$$



gluon self-interactions

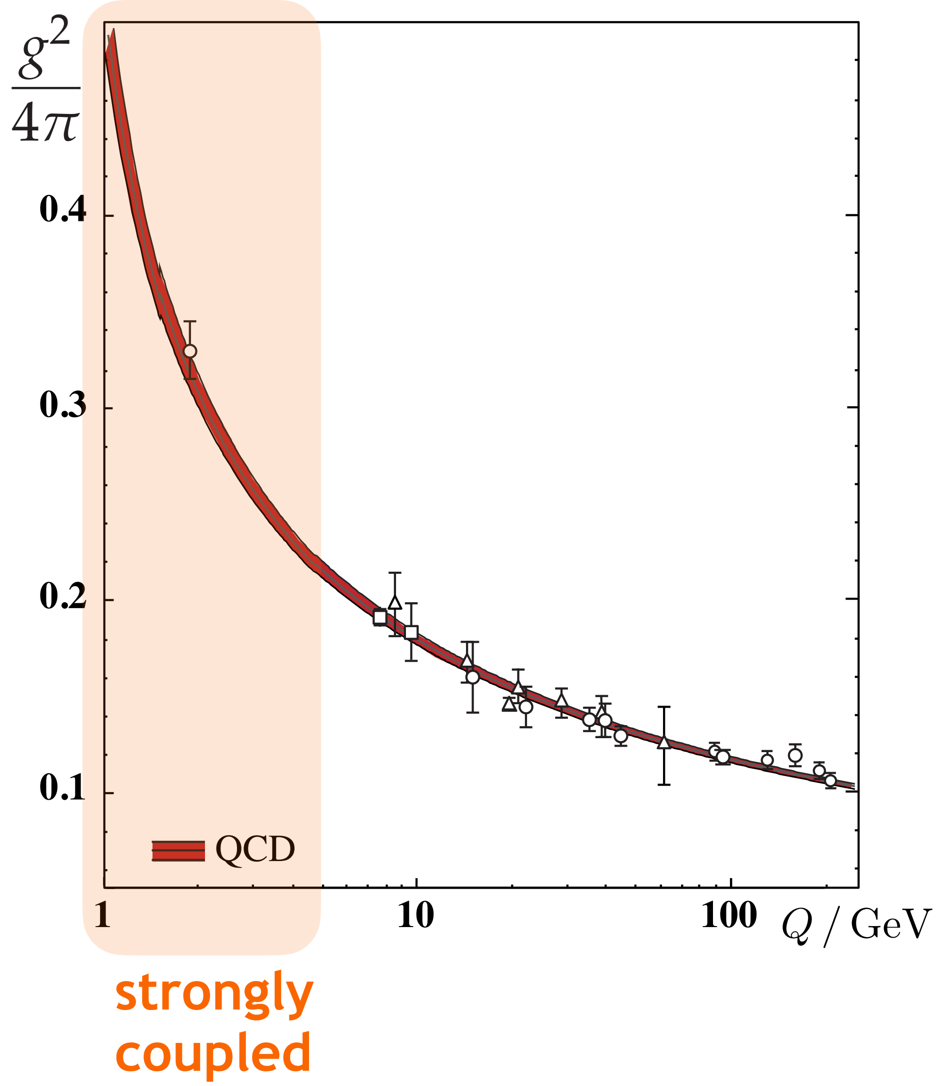
$$g[A,A]\partial A,\; g^2\big([A,A]\big)^2$$





strong QCD — beyond perturbation theory

qcd coupling



many observed hadron phenomena require physics beyond perturbation theory

binding of quarks and gluons into hadrons

expected chiral symmetry not present in hadron spectrum

confinement

and many more …

we need a first-principles non-perturbative calculational tool …

lattice QCD is a systematically improvable approximate non-perturbative approach to QCD

path integrals in quantum mechanics

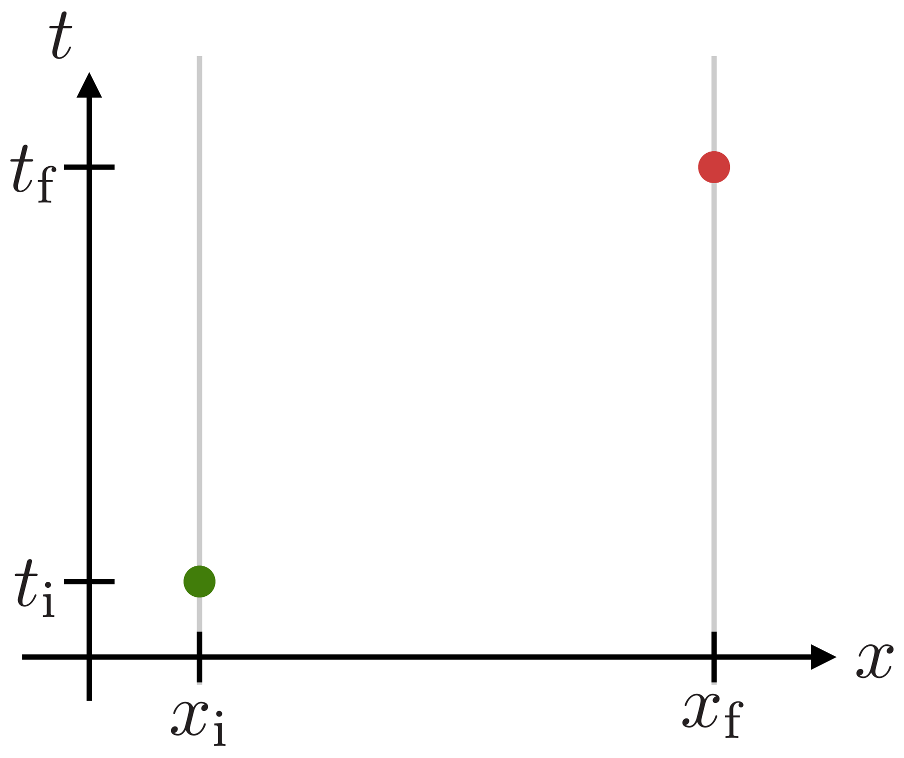
e.g. a free particle moving between a

definite initial position (x_i, t_i)

and a

definite final position (x_f, t_f)

space-time diagram



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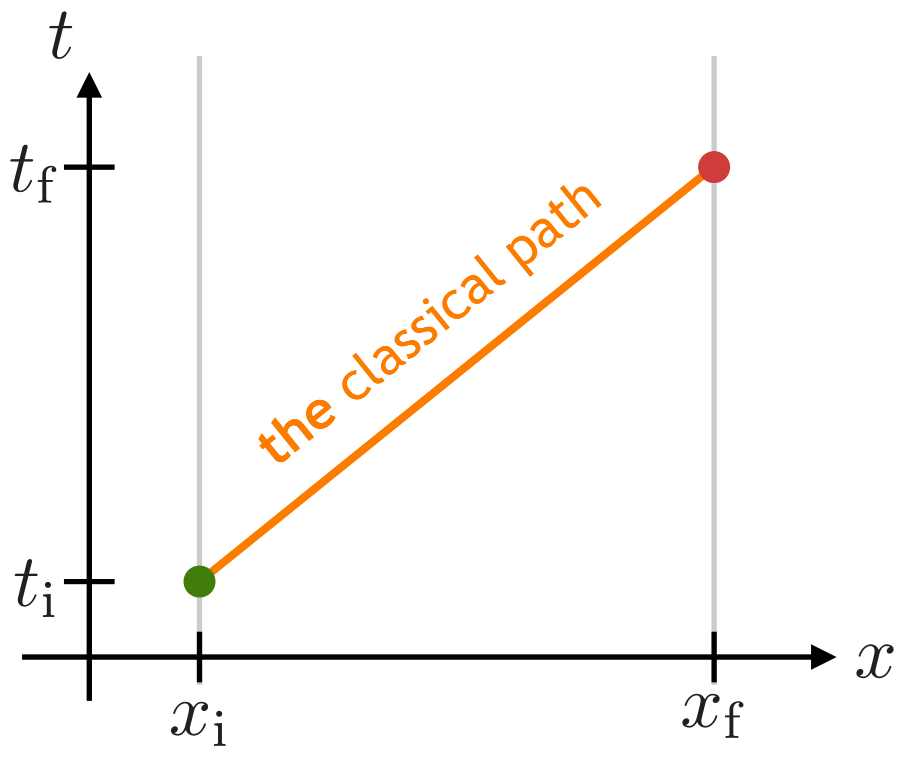

the **unique** classical path is the path of **minimum action**

the *action* $S\big[x(t)\big] = \int_{t_\mathrm{i}}^{t_\mathrm{f}} dt\, L(x, \dot{x})$

$$L_\mathrm{free} = \tfrac{1}{2} m \dot{x}^2$$

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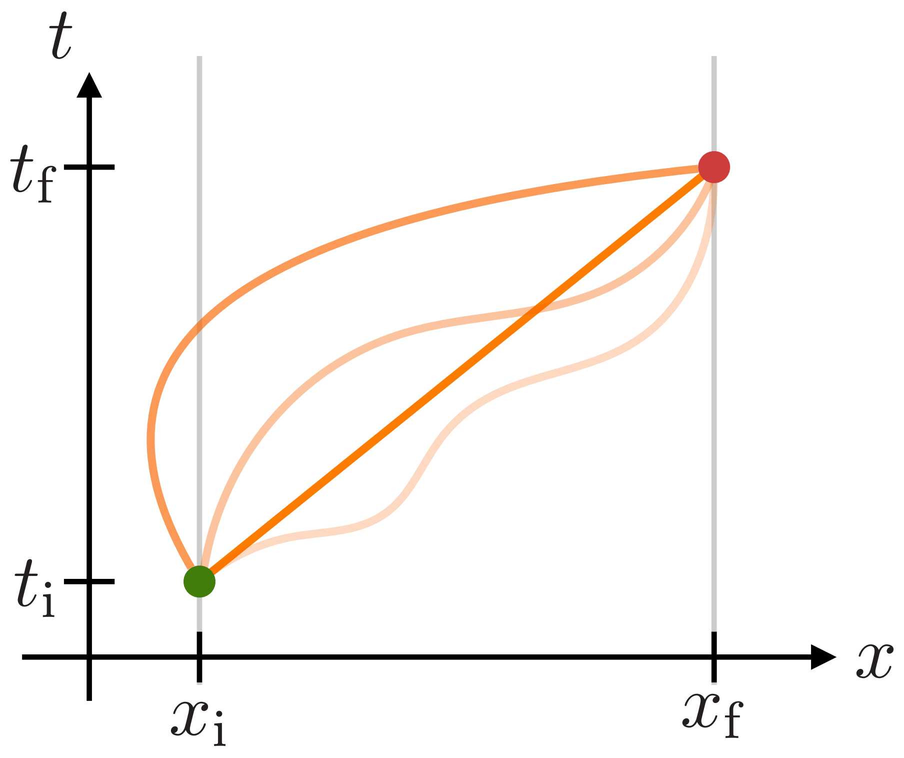

quantum mechanical amplitude

$$\langle x_\mathrm{f} | e^{-i\hat{H}(t_\mathrm{f}-t_\mathrm{i})} | x_\mathrm{i} \rangle$$

$$= \int \mathcal{D}x \, e^{-iS[x(t)]}$$

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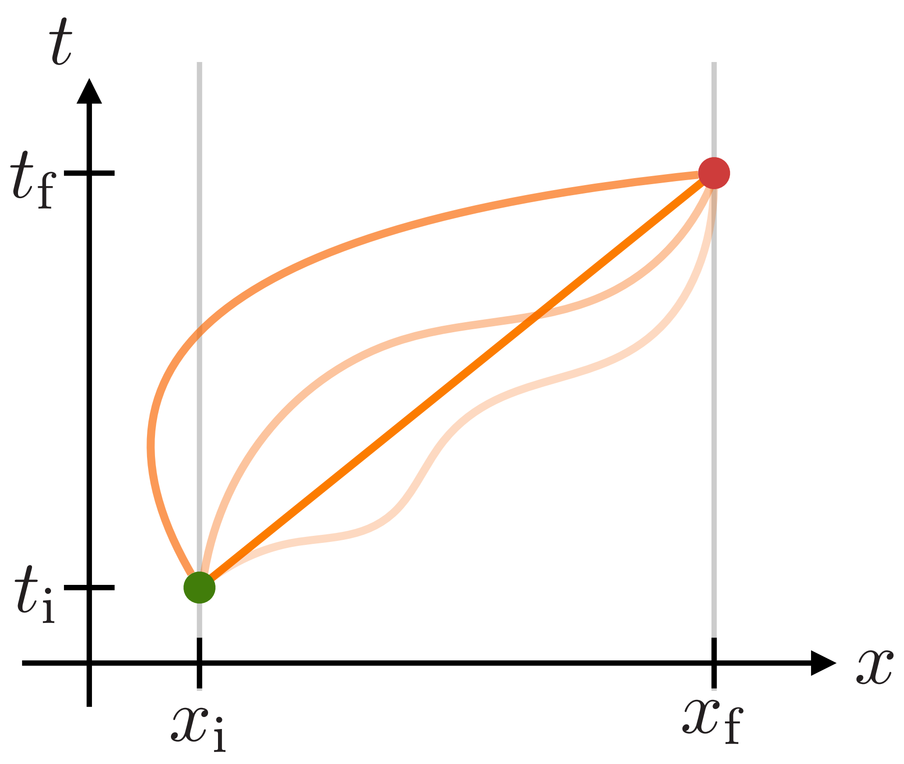

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"sum" over all paths

weighted by a phase set by the action

and conventional quantum mechanics follows ...

consider a real scalar field theory

$$\varphi(\mathbf{x}, t)$$

$$\mathcal{L} = \tfrac{1}{2}\partial_\mu \varphi \, \partial^\mu \varphi - \tfrac{1}{2} m^2 \varphi^2 + V[\varphi]$$

?

consider a real scalar field theory

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$$\mathcal{L} = \tfrac{1}{2}\partial_\mu \varphi\, \partial^\mu \varphi - \tfrac{1}{2} m^2 \varphi^2 + V\big[\varphi\big]$$

can define a path integral

$$Z = \int \mathcal{D}\varphi(x)\, e^{-iS[\varphi(x)]}$$

where the action is $S\big[\varphi(x)\big] = \int d^4x\, \mathcal{L}\big[\varphi(x)\big]$

"sum" over all
field configurations

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"sum" over all
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correlation functions can be expressed similarly

e.g. relationship between the field value at one space-time point
and the value at another space-time point

$$\big\langle 0 \big| \hat{\varphi}(y)\, \hat{\varphi}(z) \big| 0 \big\rangle = \frac{1}{Z}\int\mathcal{D}\varphi(x)\ \varphi(y)\,\varphi(z)\ e^{-iS[\varphi(x)]}$$

the spin vectors in a ferromagnet is a nice classical example

?

path integrals in quantum field theory

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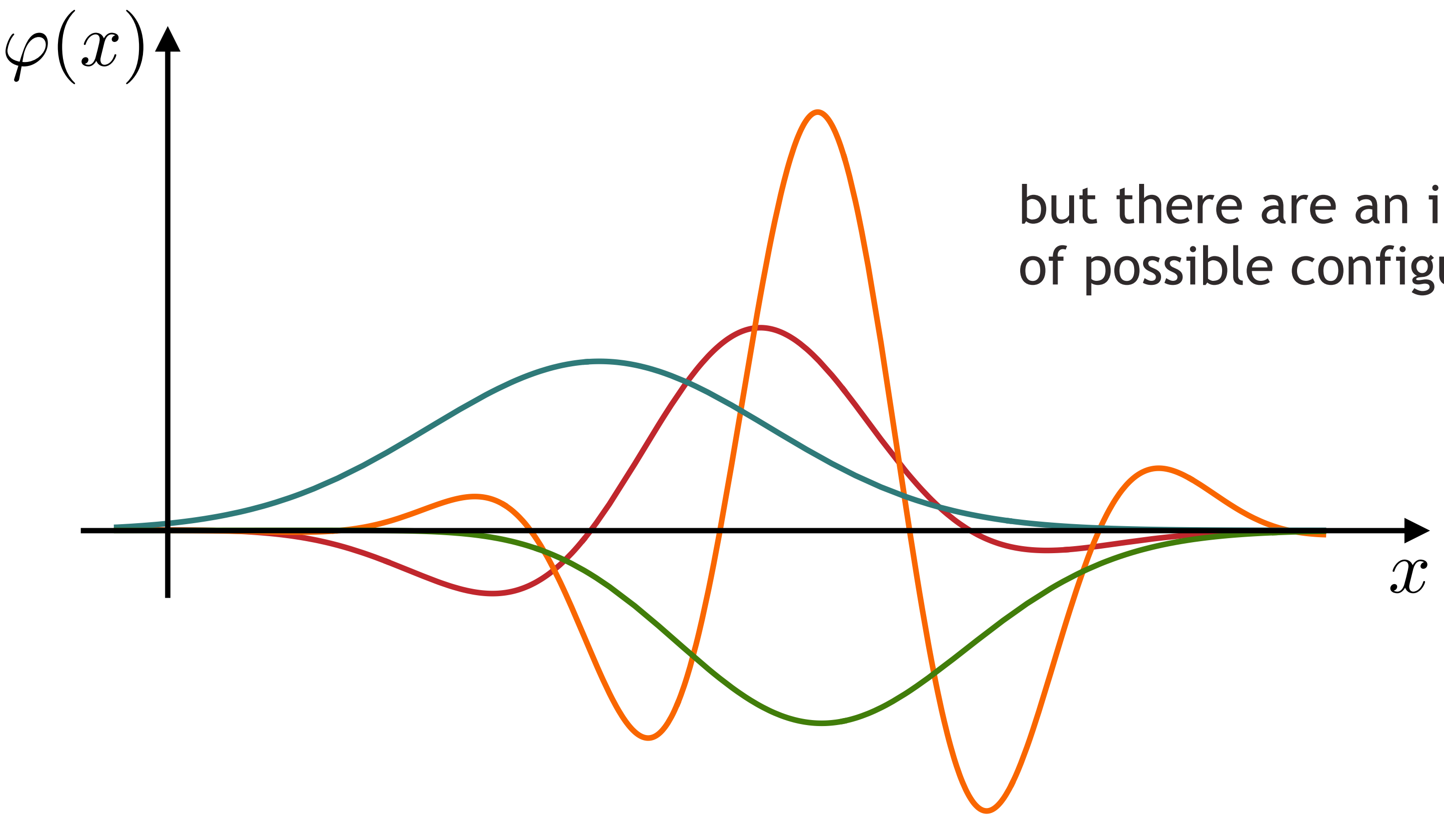
the spin vectors in a ferromagnet is a nice classical example

but practically how does one 'do' the integral $\int\mathcal{D}\varphi(x)$?

go to one dimension for simplicity of illustration

scalar field configurations



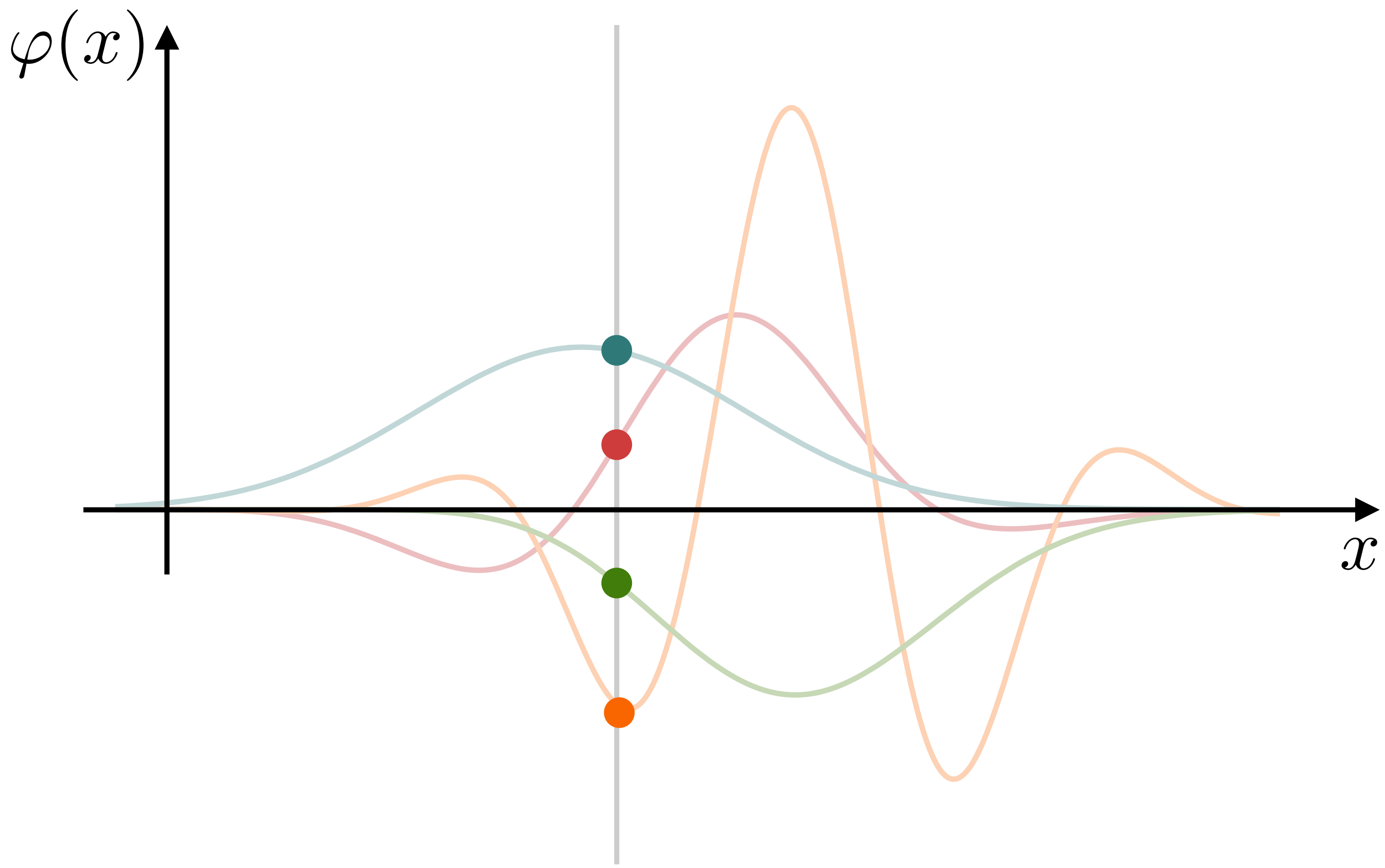
but there are an infinite number of possible configurations ...

discretize the space

$$\int \mathcal{D}\varphi(x) = \prod_x \int d\varphi_x = \int d\varphi_1 \int d\varphi_2 \int d\varphi_3 \cdots$$

an integral over all the values the field can take at x_2

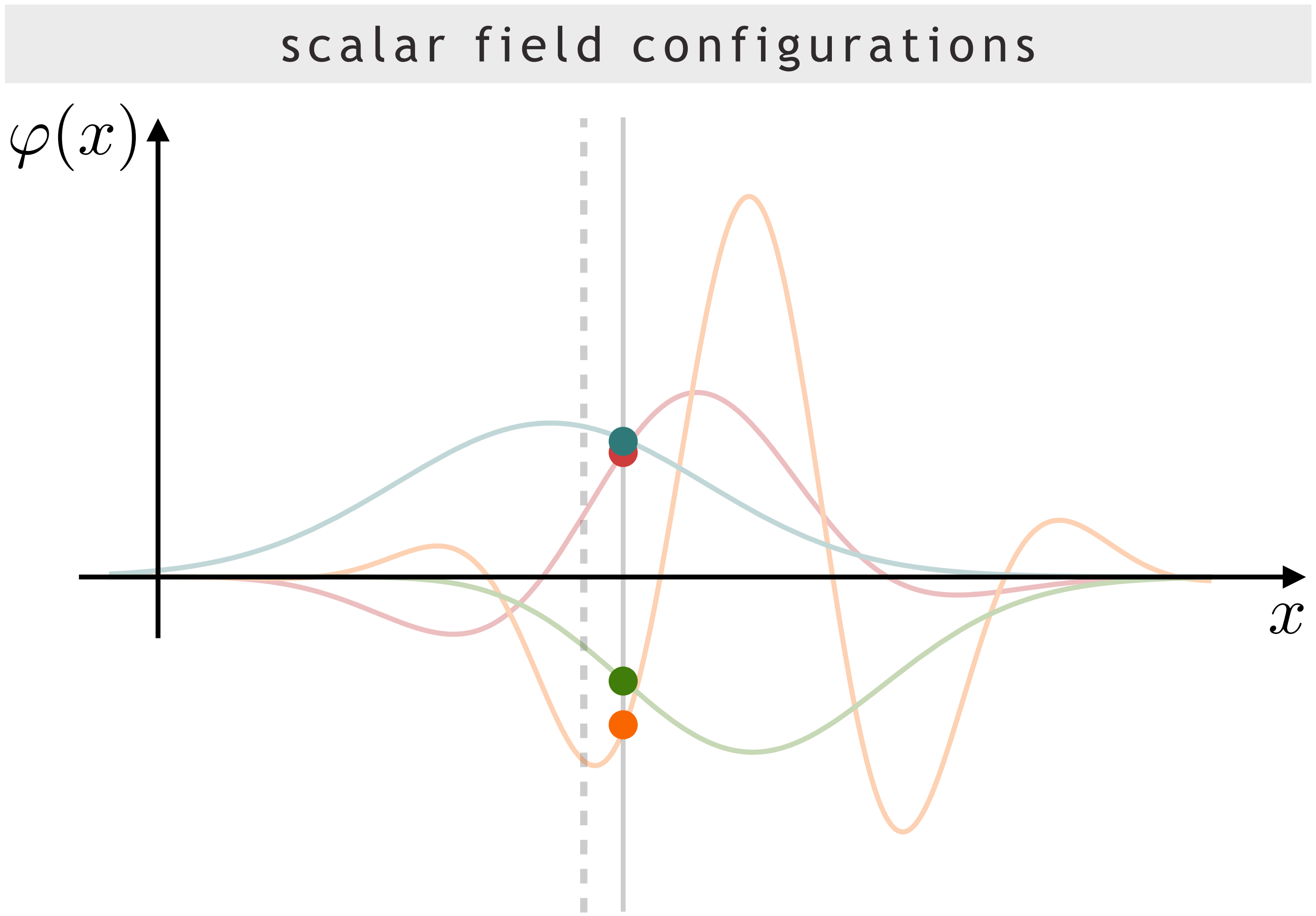
scalar field configurations



discretize the space

$$\int \mathcal{D}\varphi(x) = \prod_x \int d\varphi_x = \int d\varphi_1 \int d\varphi_2 \int d\varphi_3 \cdots$$

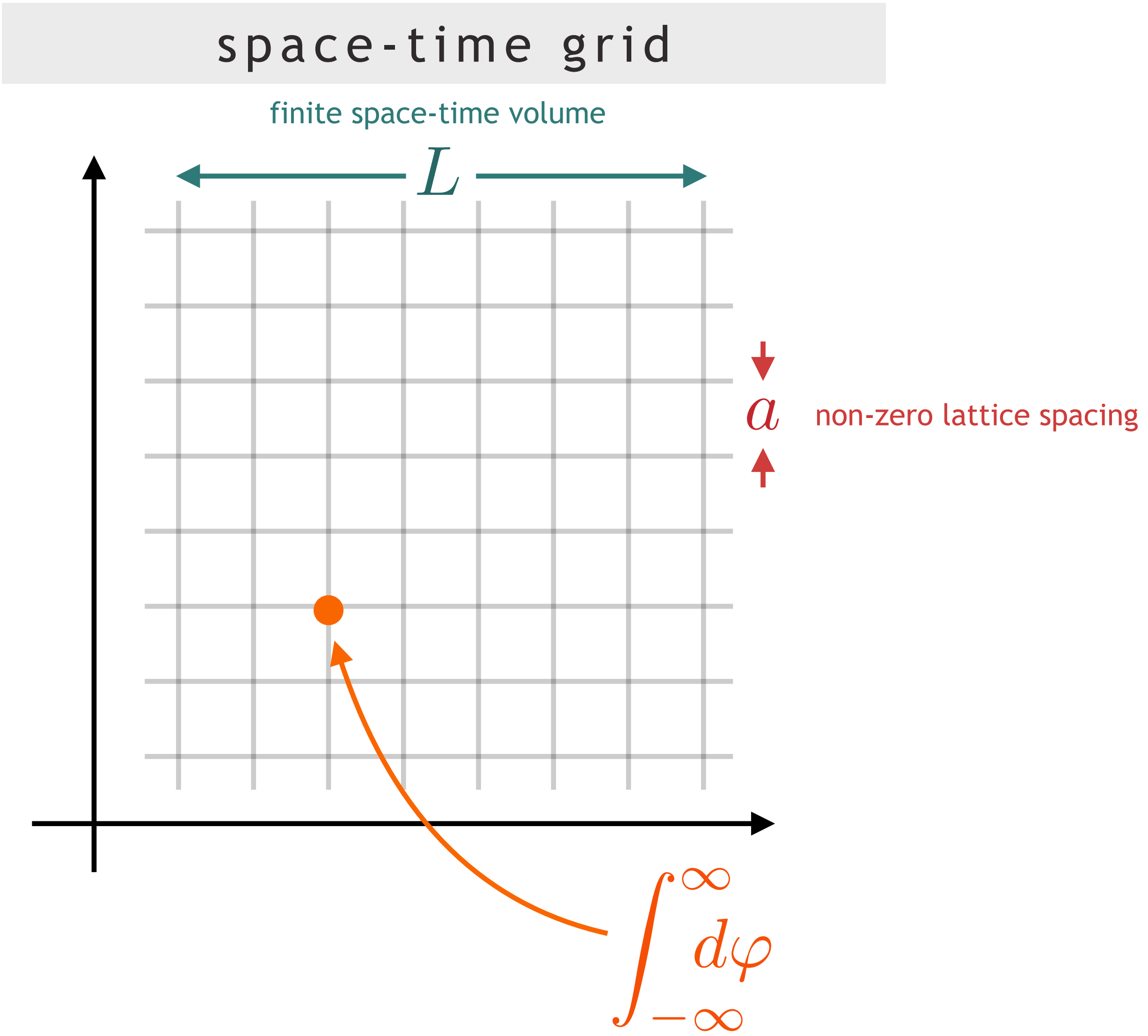
an integral over all the values the field can take at x_3



lattice quantum field theory

approach generally is to use a (hyper)cubic grid

$$\int \mathcal{D}\varphi(x) = \prod_x \int d\varphi_x$$



hiding it here,
but boundary conditions
are important

euclidean lattice quantum field theory

even with the grid, still not practical: $Z = \int \mathcal{D}\varphi(x)\, e^{-iS[\varphi(x)]}$

a **phase** is not ideal for averaging

make a variable transform $t \to -it$ then $-iS = -i \int d^3x\, dt\, \mathcal{L} \to -\int d^3x\, dt\, \mathcal{L}_\mathrm{E} = -S_\mathrm{E}$

euclidean path integral

$$Z_\mathrm{E} = \int \mathcal{D}\varphi(x)\, e^{-S_\mathrm{E}[\varphi(x)]}$$

a bounded real number
⇝ a probability ?

maybe this worries you ?

you can show that an infinitesimal rotation of time into the complex plane correctly generates the $+i\epsilon$ pieces needed in propagators

but if the theory has no singularities in the half-plane of the time variable, then doing a 90° rotation is equally justified

computational approach

euclidean path integral

$$Z_{\mathrm{E}} = \int \mathcal{D}\varphi(x)\, e^{-S_{\mathrm{E}}[\varphi(x)]}$$

probability for a field configuration $\varphi(x)$

⇒ **importance sampled Monte Carlo generation of field configurations**

obtain an **ensemble** of configurations $\{\varphi_x\}_{i=1\ldots N}$

[value of the field at each point on the grid] for some observable (vacuum matrix element)

$$\langle 0 | \, O[\hat{\varphi}] \, | 0 \rangle = \int \mathcal{D}\varphi \, O[\varphi] \, e^{-S_{\mathrm{E}}[\varphi]}$$

can now be estimated as an **average over the ensemble**

$$\langle 0 | \, O[\hat{\varphi}] \, | 0 \rangle \approx \overline{O} = \frac{1}{N} \sum_{i=1}^{N} O[\varphi^{(i)}]$$

plus get an **uncertainty estimate** from the variance

$$\sigma(O) = \sqrt{\tfrac{1}{N(N-1)} \sum_{i=1}^{N} \left(O[\varphi^{(i)}] - \overline{O} \right)^2}$$

ensemble mean and error

$$\langle 0 | \, O[\hat{\varphi}] \, | 0 \rangle \approx \overline{O} \pm \sigma(O)$$

QCD isn’t a scalar field theory,
how do you handle fermions and gauge fields ?

parallel transporters and gauge invariance

in the continuum theory,
consider a quark field pair separated by some distance

$q\bar{q}$ pair

the combination $\overline{\psi}^j(y)\,\delta_{ji}\,\psi^i(x)$ is not **gauge-invariant**

we can perform **different** local gauge transformations at locations ***x*** and ***y***

parallel transporters and gauge invariance

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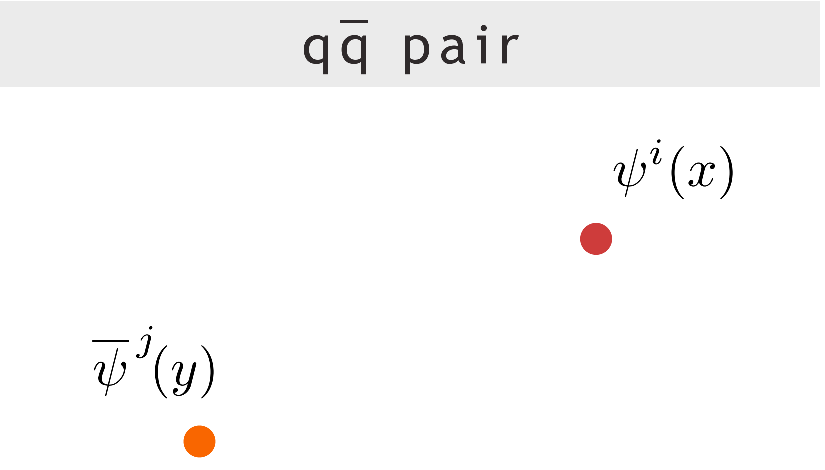

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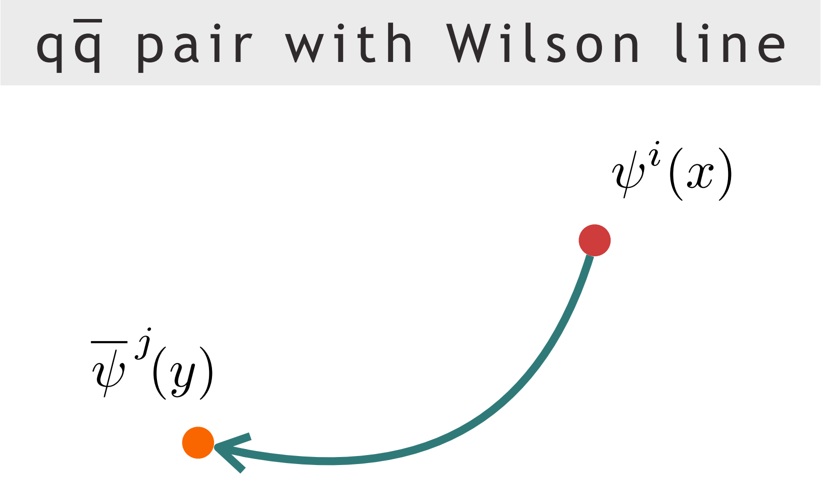
we can perform **different** local gauge transformations at locations ***x*** and ***y***

a **gauge-invariant** combination is $\overline{\psi}^j(y) \left[e^{ig \int_x^y dz_\mu A^\mu(z)} \right]_{ji} \psi^i(x)$

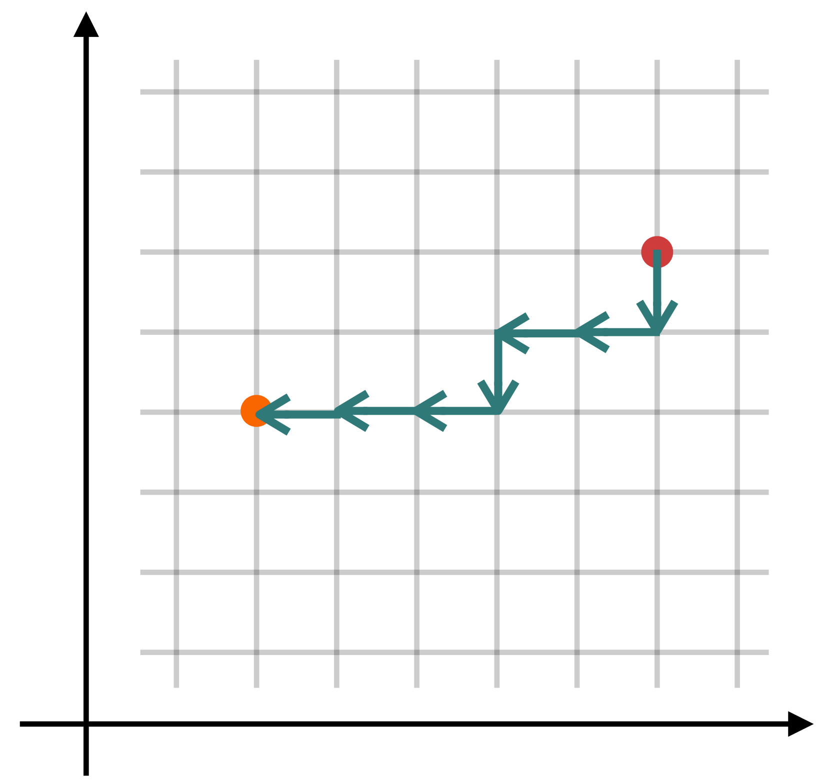
a **'Wilson line'** transports the color



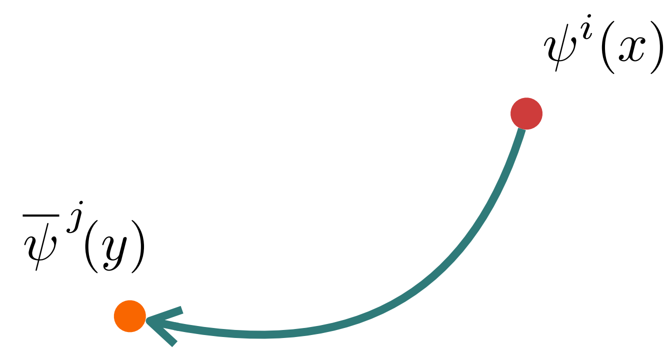
gauge ‘links’

on a lattice, make hops to neighboring sites

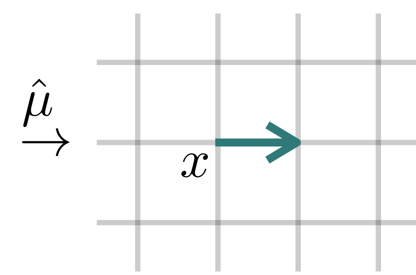
space-time grid



q$\bar{q}$ pair with Wilson line



shortest path between neighboring sites = a **‘link’**



$$\left[e^{igaA^{\mu}(x)}\right]_{ji}$$

$$U_{\mu}(x) = e^{igaA^{\mu}(x)}$$ SU(3) matrix on each **link** of the lattice

can construct a gauge-invariant **finite-difference** – approximation to a derivative ?

$$\overline{\psi}(x)\,\gamma_\mu\,U_\mu(x)\,\psi(x+\hat{\mu}a) - \overline{\psi}(x)\,\gamma_\mu\,U^\dagger_\mu(x-\hat{\mu}a)\,\psi(x-\hat{\mu}a)$$

c.f. $\frac{1}{2a}\big(f(x+a)-f(x-a)\big) \xrightarrow{a\to 0} \frac{df}{dx} + O(a^2)$

$$\xrightarrow{a\to 0} 2a\,\overline{\psi}\,\gamma_\mu\big(\partial_\mu + igA_\mu\big)\,\psi + \dots$$

and using constructions like these we can build **discretized actions**

Dirac matrix

e.g. $\int d^4x\,\overline{\psi}(\gamma_\mu D_\mu + m)\psi \quad \rightsquigarrow \quad \overline{\psi}^{\,i\alpha}_x\, M^{i\alpha,j\beta}_{x,y}[U]\,\psi^{j\beta}_y$

matrix in
color, spin, spacetime

N.B. **large** matrix, but **sparse**

e.g. for a $24^3\times128$ lattice, ~ 21M×21M

most of the elements are zero

(100 Pb !!!)

integrating out the quarks

a gauge-field 'configuration' is simple — it's an SU(3) matrix on each link

but what about a quark-field configuration? **fermion fields anticommute ⇒ Grassmann variables**

actually we can do the quark field integration exactly in the path integral:

$$\int \mathcal{D}\psi \mathcal{D}\overline{\psi} \mathcal{D}U \, e^{-S_{\mathrm{E}}[\psi, \overline{\psi}, U]} = \int \mathcal{D}U \, e^{-S^{\mathrm{g}}_{\mathrm{E}}[U]} \int \mathcal{D}\psi \mathcal{D}\overline{\psi} \, e^{-\overline{\psi} M[U] \psi}$$

$$= \det M[U]$$

$$= \int \mathcal{D}U \, \det M[U] \, e^{-S^{\mathrm{g}}_{\mathrm{E}}[U]}$$

interpret as the probability for configuration $U_\mu(x)$

a (gauge-variant) correlation function

$$\langle 0 | \hat{\psi}_x^{i\alpha} \, \hat{\overline{\psi}}_y^{j\beta} | 0 \rangle = \int \mathcal{D}\psi \mathcal{D}\overline{\psi} \mathcal{D}U \, \psi_x^{i\alpha} \, \overline{\psi}_y^{j\beta} \, e^{-S_{\mathrm{E}}[\psi, \overline{\psi}, U]}$$

correlation between
quark at *x*, color *i*, spin *α*
and
quark at *y*, color *j*, spin *β*

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$$= \int \mathcal{D}U \left[M^{-1}[U] \right]_{x,y}^{i\alpha, j\beta} \det M[U] \, e^{-S^\mathrm{g}_\mathrm{E}[U]}$$

probability

c.f. Wick's theorem

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compute
'quark propagator'
on each
configuration

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actually, don't do this
because it will average to zero

a meson correlation function

$$\langle 0 | \sum_{\vec{x}} \left(\overline{\psi}\gamma_5\psi\right)_{\vec{x},t} \left(\overline{\psi}\gamma_5\psi\right)_{\vec{0},0} | 0 \rangle$$

$\overline{\psi}\gamma_5\psi$ pseudoscalar quantum numbers

$\sum_{\vec{x}} f(\vec{x}) = \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} f(\vec{x})\Big|_{\vec{p}=\vec{0}}$ projection into zero momentum

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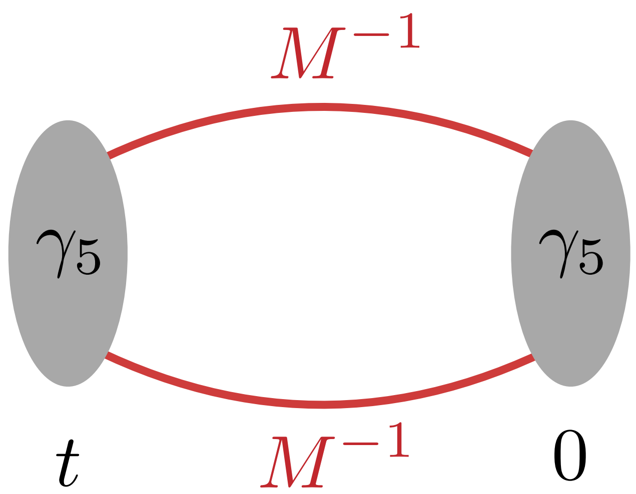

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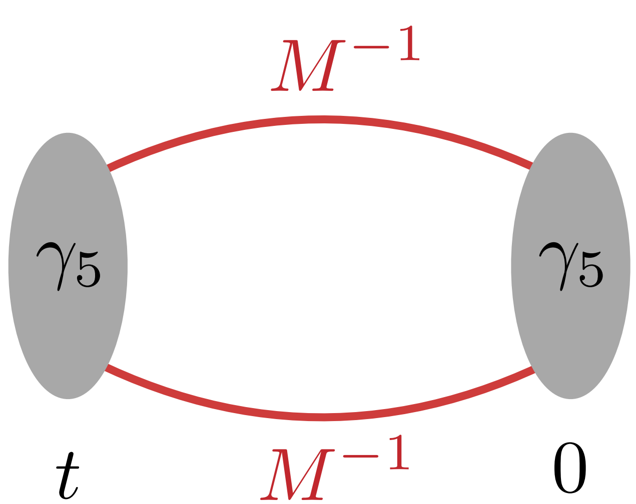

point – all propagator

$$\big[M[U]\big]_{\vec{y}t',\vec{x}t}\, \chi_{\vec{x}t} = \delta_{\vec{y},\vec{0}}\, \delta_{t',0}$$

sparse matrix — point source

$$\chi_{\vec{x}t} = \big[M^{-1}[U]\big]_{\vec{x}t,\vec{0}0}$$

point-all propagator

solving a sparse linear system: **A** · *x* = *b*

e.g. for a
$24^3 \times 128$ lattice,
~ 21M×12
(few Gb)

the lattice QCD workflow

select a discretization

'tune' the parameters

as in any treatment of QCD, minimal experimental input required
to set quark masses and the coupling/lattice spacing

generate 100s of
gauge-field configurations

serious parallel supercomputing

compute quark
propagators

serious computing
GPUs very useful

'contract' into
correlation functions

capacity computing
'bookkeeping' / memory management

•
•
•

PHYSICS ?

finite lattice spacing

acts as a UV cutoff $\Lambda \sim \frac{1}{a}$

appears as a scale $\hat{m} = am$

discretization errors $X(a) = X(0) + a\,\delta X_1 + \ldots$

extrapolate $a \to 0$

lattice systematics (much simplified)

finite lattice spacing

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discretization choice

all should agree in the *a*→0 limit

impact at finite *a* depends on observable

choose a discretization appropriate to your quantities

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finite lattice volume

need $L \gg \frac{1}{m_\pi}$

impacts multi-hadron systems
in an interesting way

**carefully understand QFT
in a finite volume**

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all should agree in the *a*→0 limit

impact at finite *a* depends on observable

choose a discretization appropriate to your quantities

quark mass choice

many calculations done with $m_{u,d} > m_{u,d}^{\text{phys}}$

use quark mass as a tool to understand QCD

lattice QCD — what can you do with it ?

hadron spectroscopy — masses of 'stable' hadrons

hadron structure — operator matrix-elements between hadron states

thermodynamics of QCD — put theory at finite temperature by reducing the periodic time extent

remove unwanted QCD effects — e.g. heavy-flavor decays for CP-violation, muon g-2 …

… and lots more …

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two-point correlation functions and the spectrum

consider $\langle 0 | \, \mathcal{O}_\mathrm{f}(t) \, \mathcal{O}_\mathrm{i}^\dagger(0) \, | 0 \rangle$

Euclidean time-evolution $\mathcal{O}(t) = e^{Ht} \, \mathcal{O}(0) \, e^{-Ht}$

$$= \langle 0 | \, \mathcal{O}_\mathrm{f}(0) \, e^{-Ht} \, \mathcal{O}_\mathrm{i}^\dagger(0) \, | 0 \rangle$$

two-point correlation functions and the spectrum

consider $\langle 0 | \, O_{\mathrm{f}}(t) \, O_{\mathrm{i}}^{\dagger}(0) \, | 0 \rangle$

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$$= \langle 0 | \, O_{\mathrm{f}}(0) \, e^{-Ht} \, O_{\mathrm{i}}^{\dagger}(0) \, | 0 \rangle$$

Hamiltonian has a complete set of eigenstates

$$H | \mathfrak{n} \rangle = E_{\mathfrak{n}} | \mathfrak{n} \rangle$$

$$1 = \sum_{\mathfrak{n}} | \mathfrak{n} \rangle \langle \mathfrak{n} |$$

(only discrete eigenstates ?)

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$$1 = \sum_{\mathfrak{n}} | \mathfrak{n} \rangle \langle \mathfrak{n} |$$

(only discrete eigenstates ?)

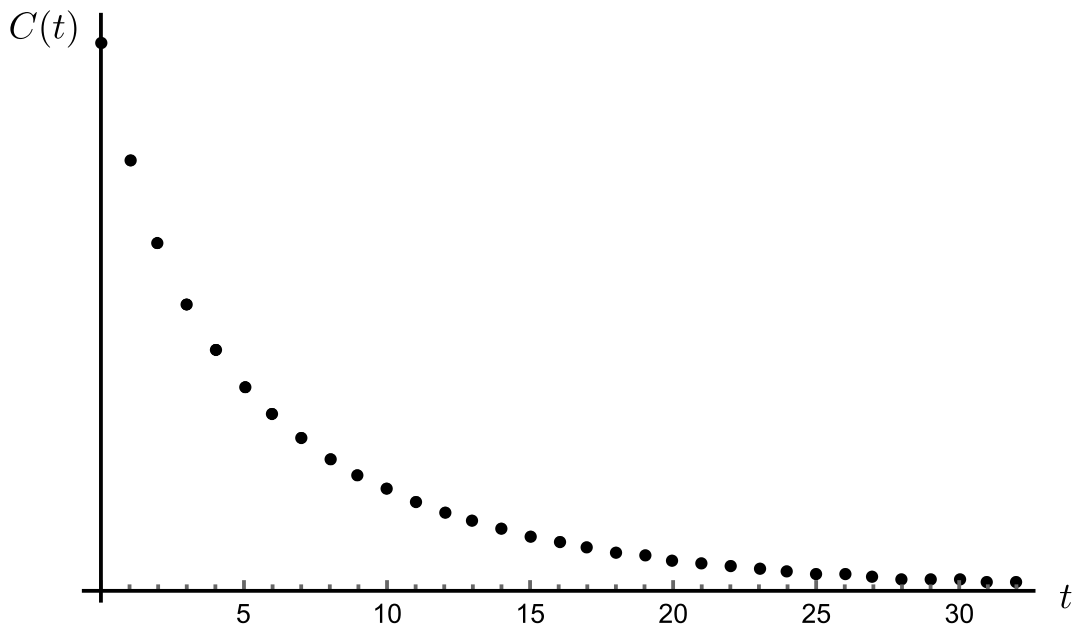
$$= \sum_{\mathfrak{n}} e^{-E_{\mathfrak{n}} t} \langle 0 | O_{\mathrm{f}}(0) | \mathfrak{n} \rangle \langle \mathfrak{n} | O_{\mathrm{i}}^{\dagger}(0) | 0 \rangle$$

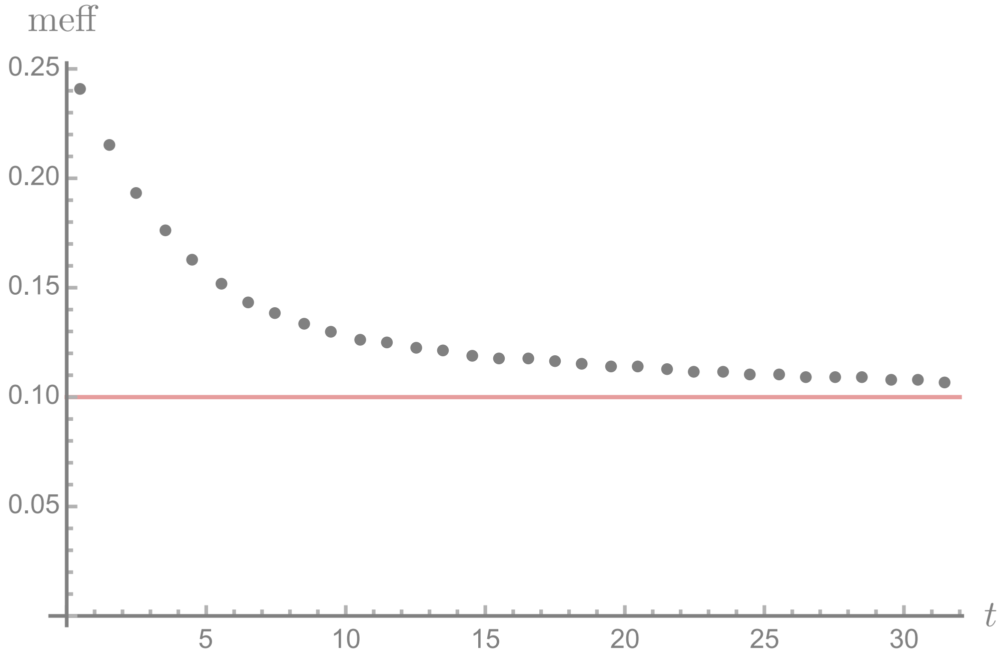
amplitude for $O_{\mathrm{i}}^{\dagger}$
to ‘interpolate’ state $| \mathfrak{n} \rangle$
from the vacuum

time dependence of two point correlation functions

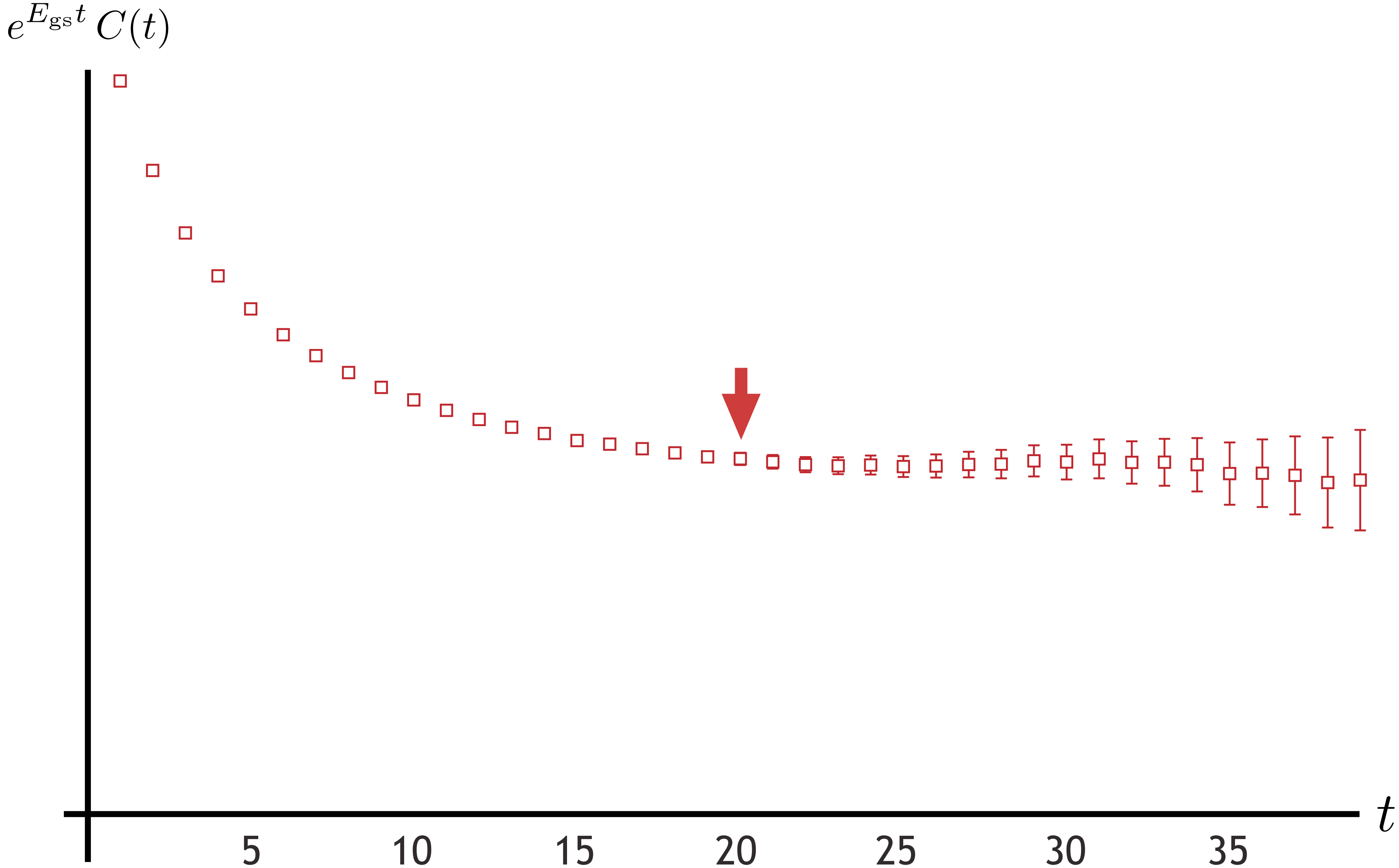
notice that as $t \to \infty$ $\qquad C(t) \to c \cdot e^{-E_{\rm gs} t}$

useful to define the 'effective mass' $\log\left[\frac{C(t)}{C(t+1)}\right]$



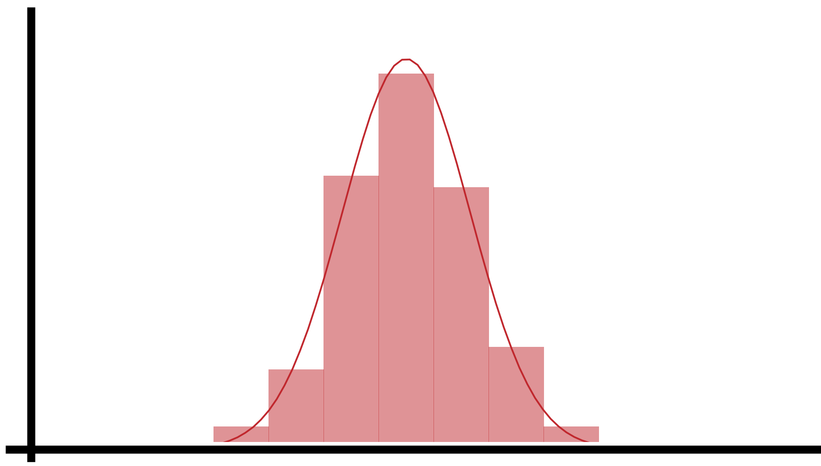


an actual lattice QCD two point correlation function

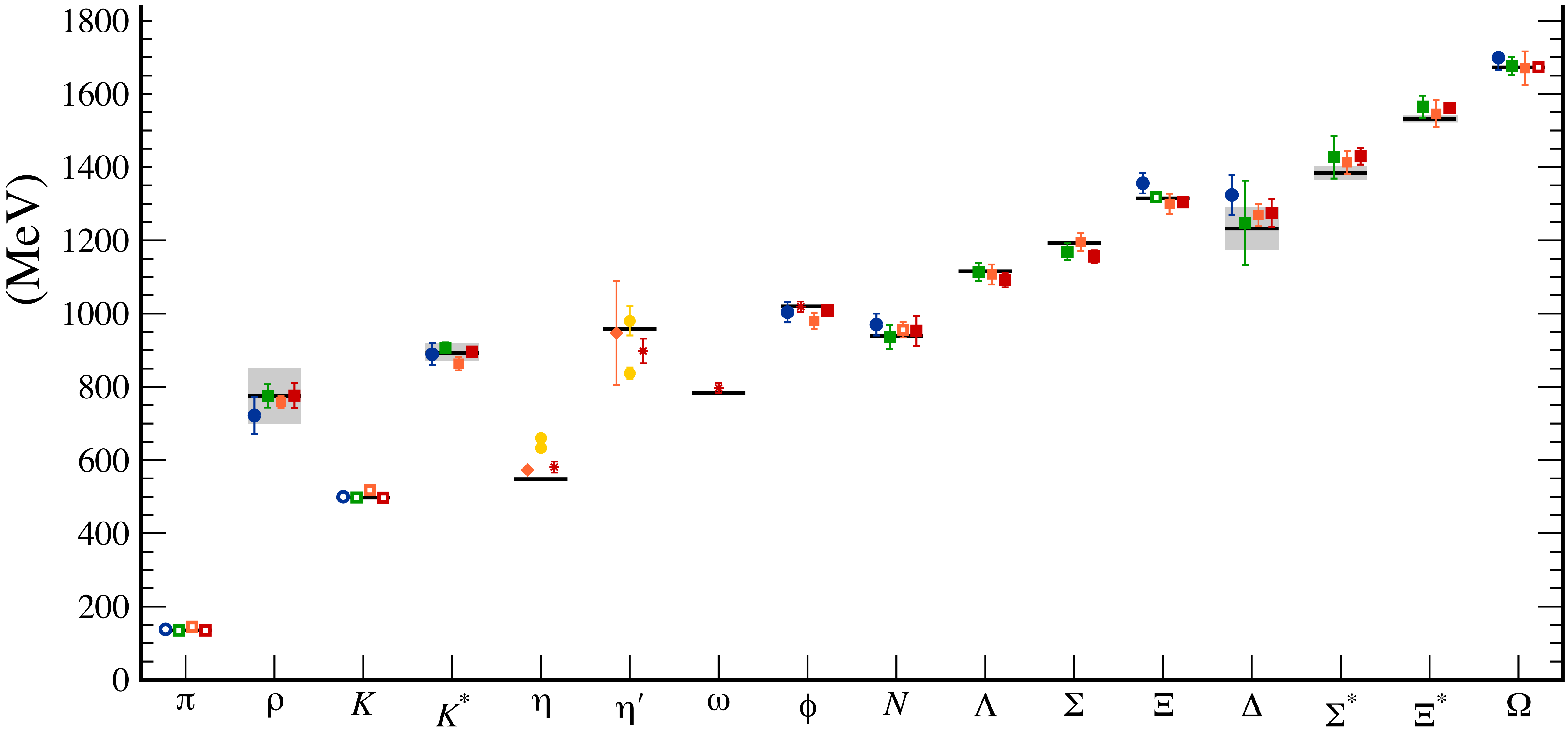


generally statistical noise increases with increasing t

ensemble distn



‘stable’ hadron spectrum



lattice QCD — what can you do with it ?

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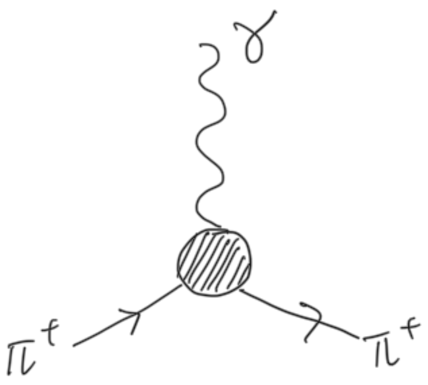
three-point correlation functions and matrix elements

e.g. the pion electromagnetic form-factor

$$\langle \pi^+(\vec{p}\,')\,|\,\overline{\psi}\gamma^\mu\psi(0)\,|\,\pi^+(\vec{p}\,)\rangle = (p+p')^\mu\, F_\pi(Q^2)$$



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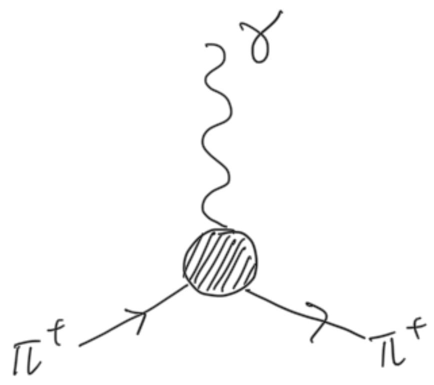

access through a three-point correlation function

$$\langle 0\,|\,\overline{\psi}\gamma_5\psi(\Delta t)\,\overline{\psi}\gamma^\mu\psi(t)\,\overline{\psi}\gamma_5\psi(0)\,|\,0\rangle$$

three-point correlation functions and matrix elements

e.g. the pion electromagnetic form-factor

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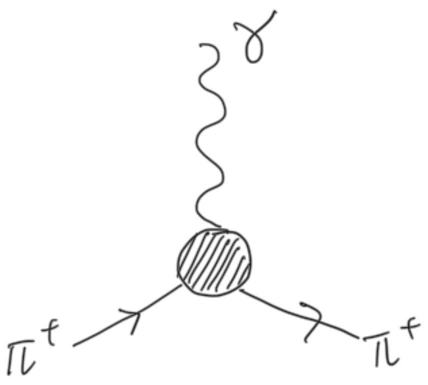

access through a three-point correlation function

$$\langle 0 \,|\, \underbrace{\bar{\psi}\gamma_5\psi(\Delta t)}_{\text{annihilate pion q.n.}} \; \underbrace{\bar{\psi}\gamma^\mu\psi(t)}_{\text{vector current}} \; \underbrace{\bar{\psi}\gamma_5\psi(0)}_{\text{create pion q.n.}} \,|\, 0 \rangle$$

annihilate pion q.n. — vector current — create pion q.n.

three-point correlation functions and matrix elements

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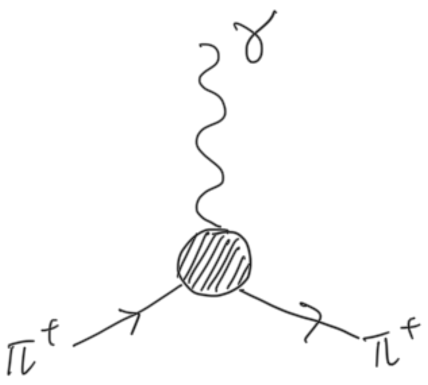
$$\langle \pi^+(\vec{p}\,') \,|\, \overline{\psi}\gamma^\mu\psi(0) \,|\, \pi^+(\vec{p}) \rangle = (p+p')^\mu \, F_\pi(Q^2)$$



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$$= \langle 0 \,|\, \overline{\psi}\gamma_5\psi \,|\, \pi(\vec{p}\,') \rangle \, e^{-E_\pi(\vec{p}\,')(\Delta t - t)} \, \underbrace{\langle \pi(\vec{p}\,') \,|\, \overline{\psi}\gamma^\mu\psi \,|\, \pi(\vec{p}) \rangle}_{\text{desired matrix element}} \, e^{-E_\pi(\vec{p})t} \, \langle \pi(\vec{p}) \,|\, \overline{\psi}\gamma_5\psi \,|\, 0 \rangle \; + \ldots$$

three-point correlation functions and matrix elements

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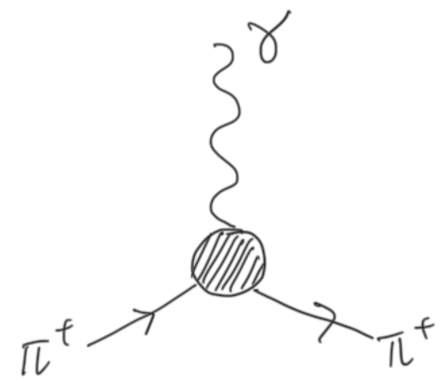

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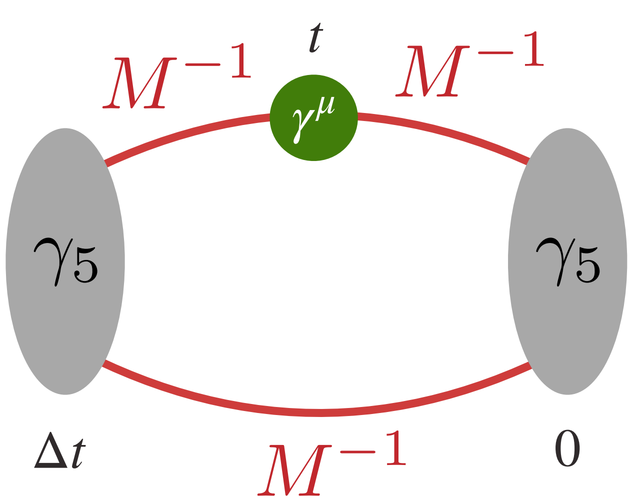

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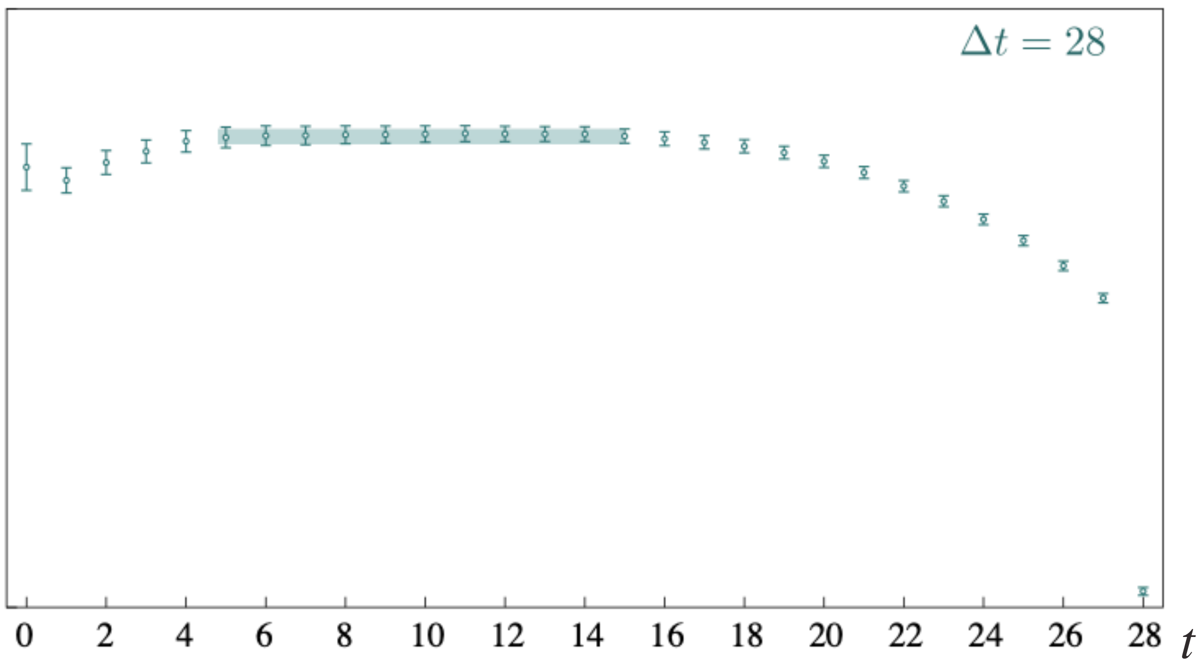

pion form-factor

$$\langle 0 \,|\, \overline{\psi}\gamma_5\psi(\Delta t)\, \overline{\psi}\gamma^\mu\psi(t)\, \overline{\psi}\gamma_5\psi(0) \,|\, 0 \rangle$$

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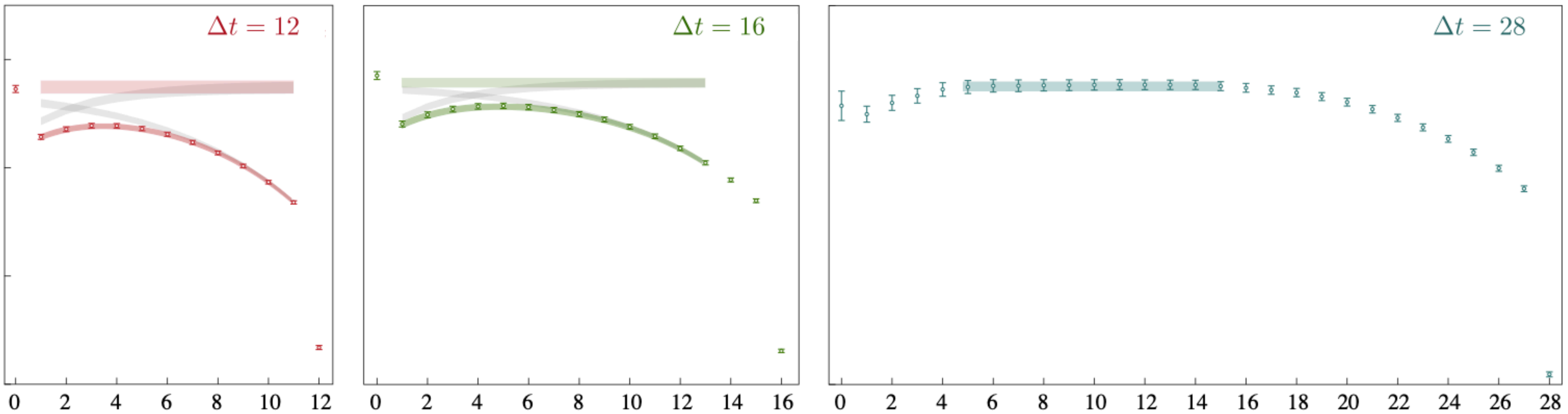

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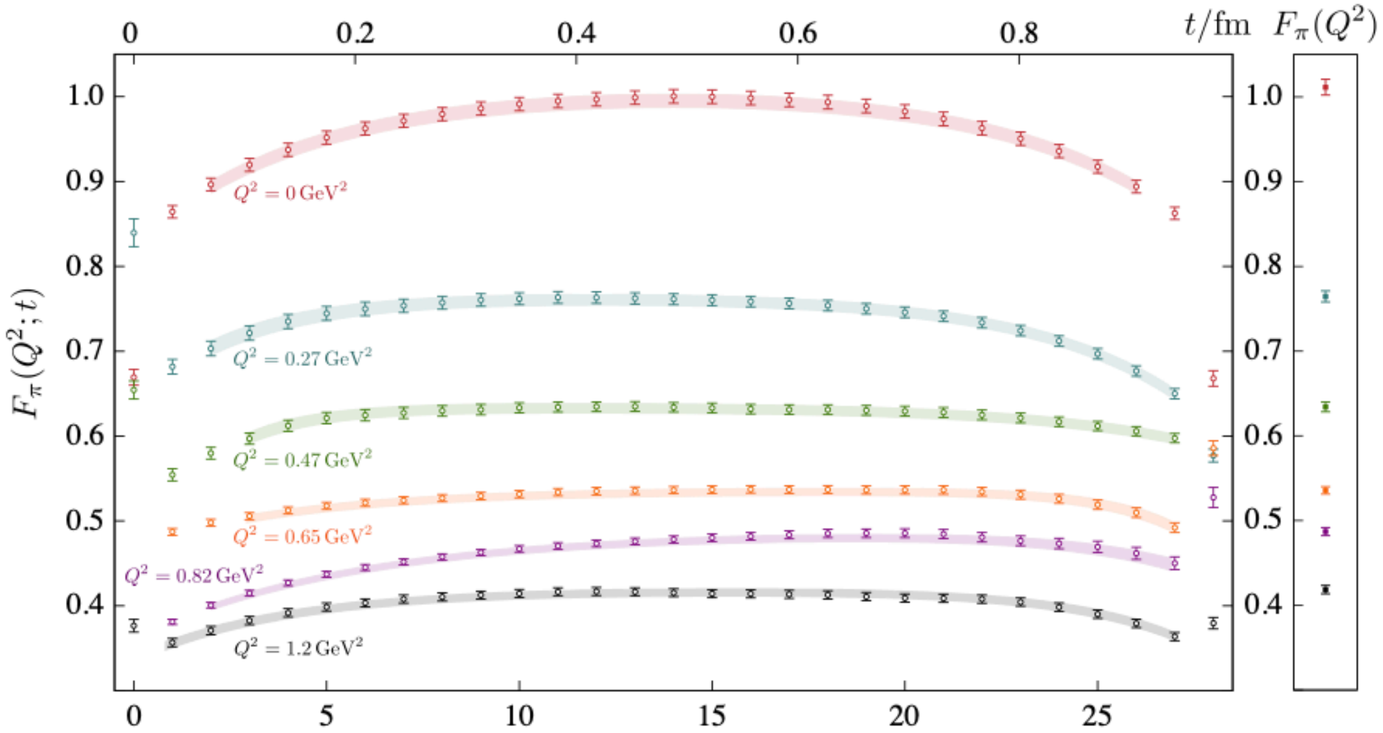

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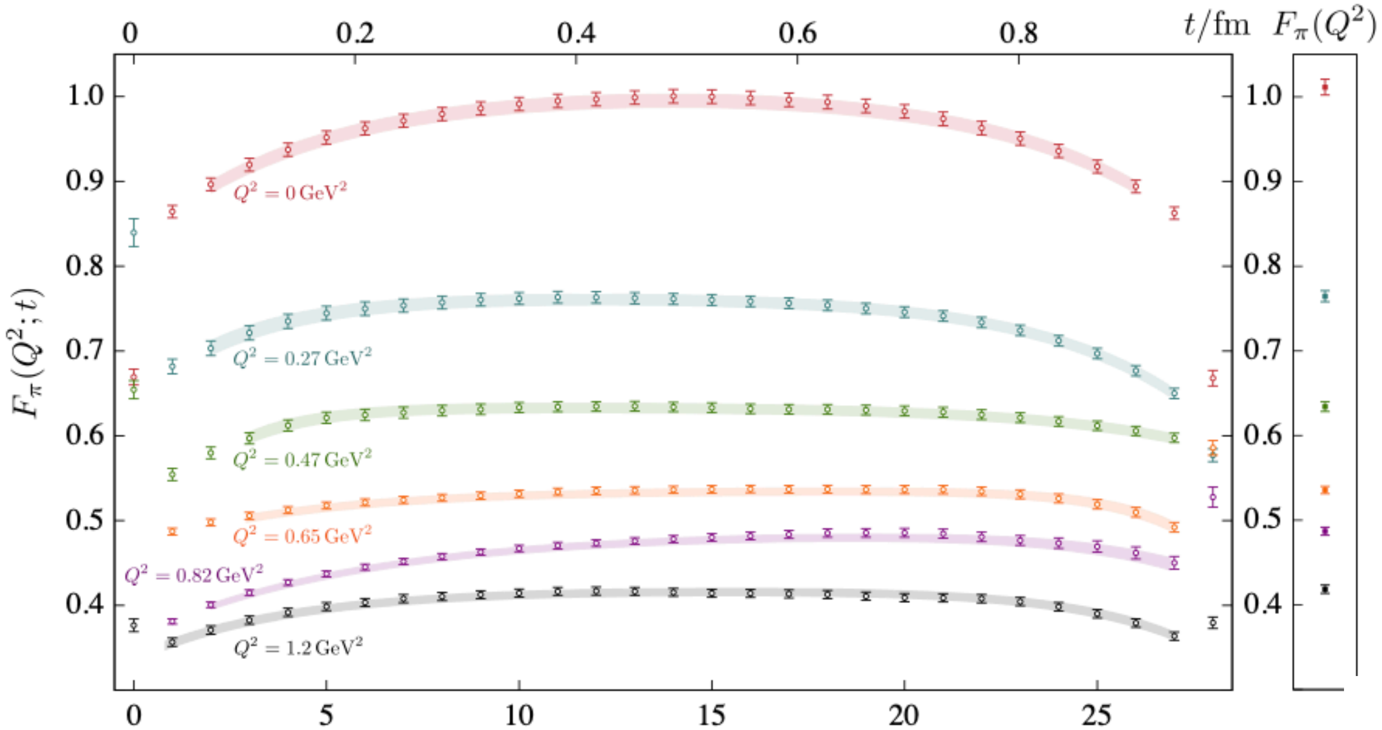
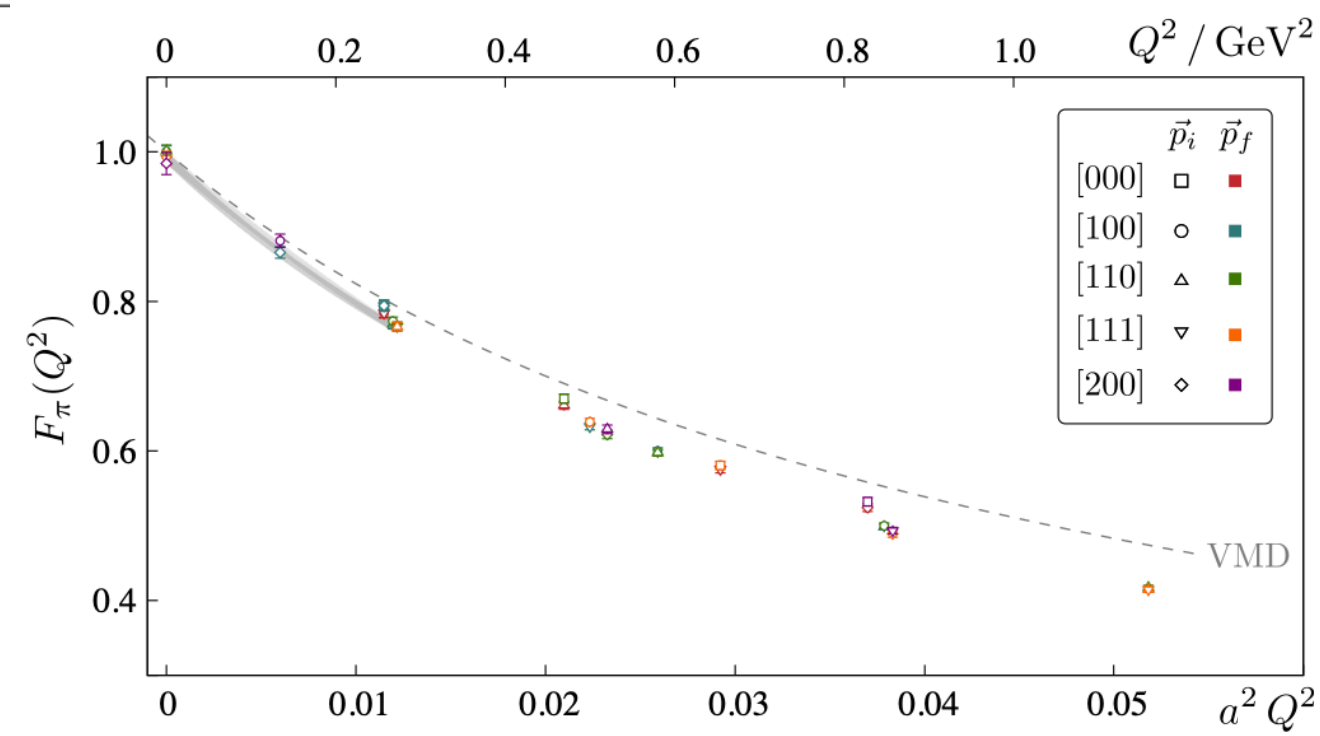


$$\overrightarrow{p} = \frac{2\pi}{L}[n_x, n_y, n_z]$$



this calculation done for a quark mass very far away from the physical value

and in fact using ‘pion’ operators much more intelligently built than $\overline{\psi}\gamma_5\psi$

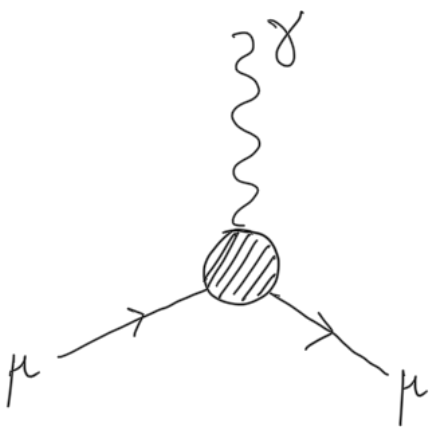
hadron spectroscopy — masses of ‘stable’ hadrons

hadron structure — operator matrix-elements between hadron states

thermodynamics of QCD — put theory at finite temperature by reducing the periodic time extent

remove unwanted QCD effects — e.g. heavy-flavor decays for CP-violation, muon g-2 …

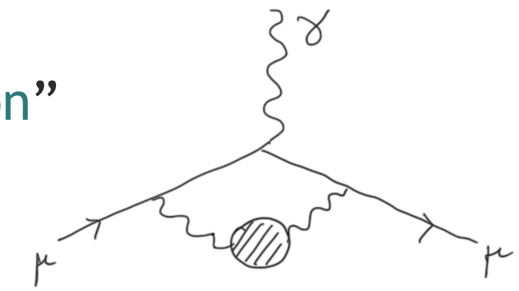
muon $g-2$

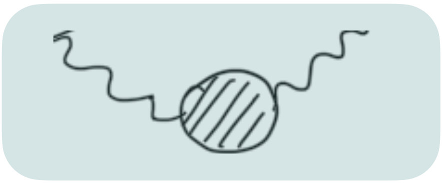


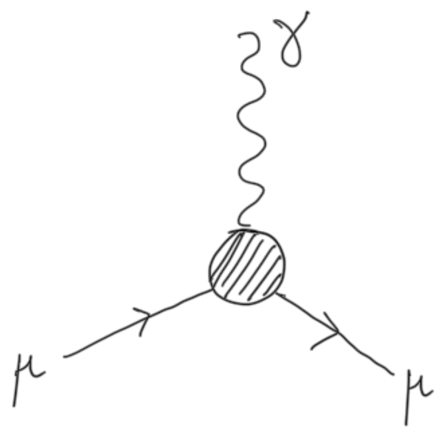
are there beyond the standard model particles in  ?

need to precisely determine the standard model contribution & this includes QCD

e.g. the “vacuum polarization”







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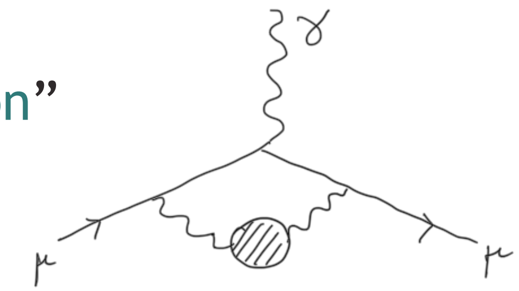
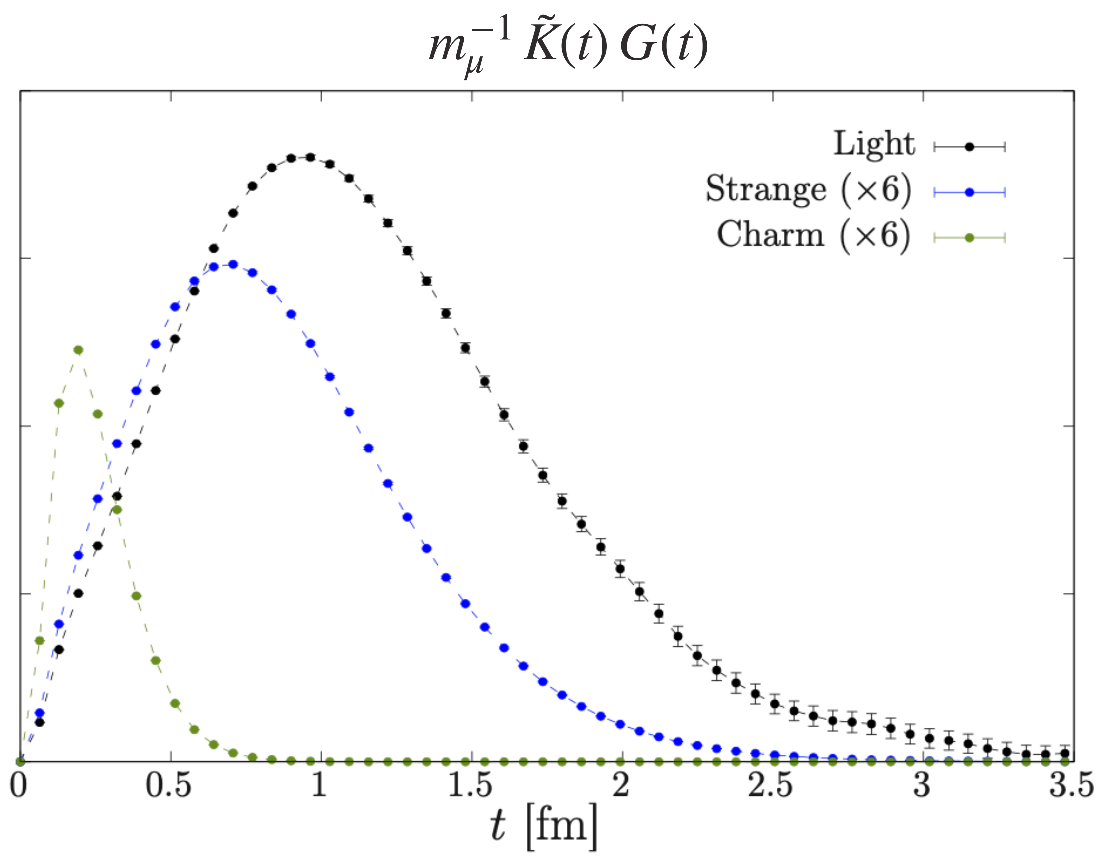
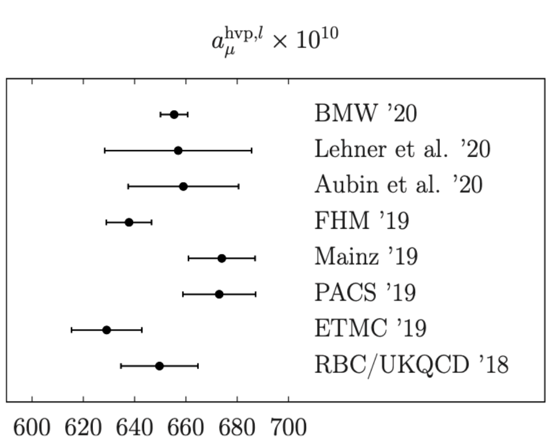


hadronic contribution:

$$a_\mu = \left(\frac{\alpha}{\pi}\right)^2 \int_0^\infty dt\, \tilde{K}(t)\, G(t)$$

$$G(t) = \frac{1}{3}\sum_{k=1}^{3} \int d^3x\, \langle 0 | J_k(x,t)\, J_k(0,0) | 0 \rangle$$

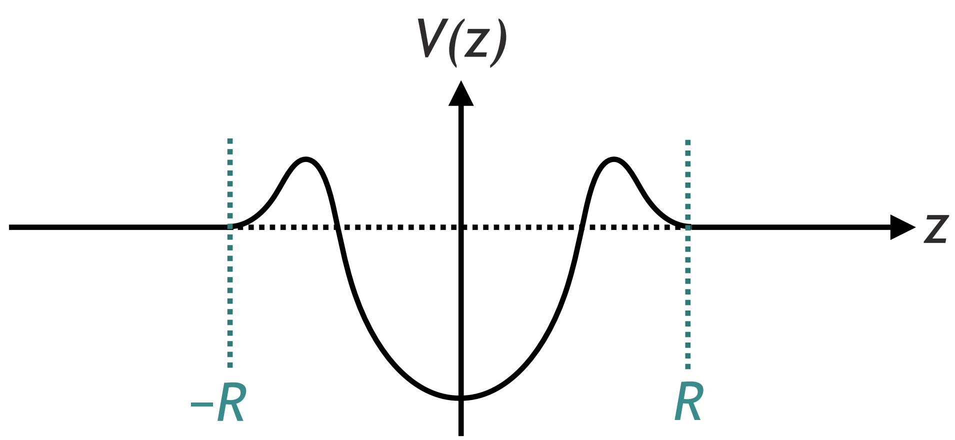




lattice QCD — what can't you do with it ?

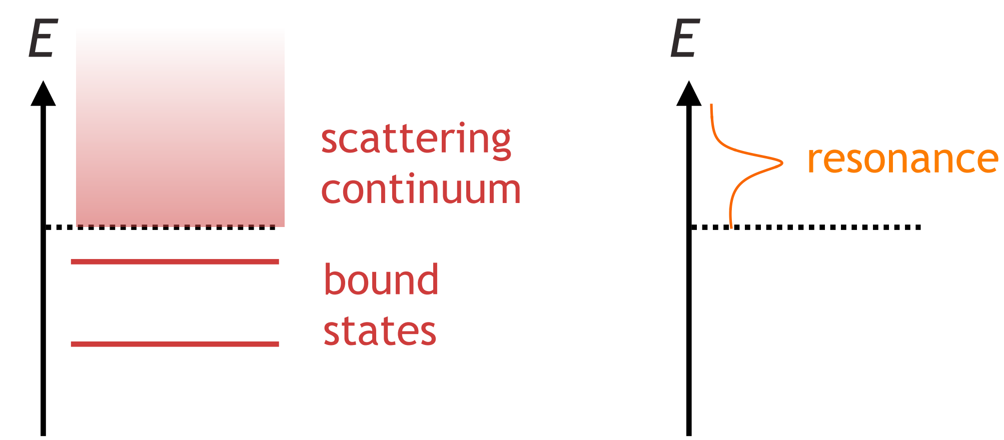
at first glance, looks like you can't study **hadron-hadron scattering**

scattering states have a continuous energy spectrum,
but in a finite-volume there are only discrete energy states



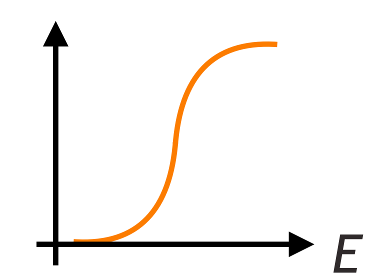
solve the Schrödinger equation

$$-\frac{1}{m}\frac{d^2\psi}{dz^2} + V(z)\psi(z) = E\psi(z)$$



$$\psi(|z| > R) \sim \cos\big(p\,|z| + \boxed{\delta(p)}\big)$$

phase-shift



'scattering' in a finite-volume

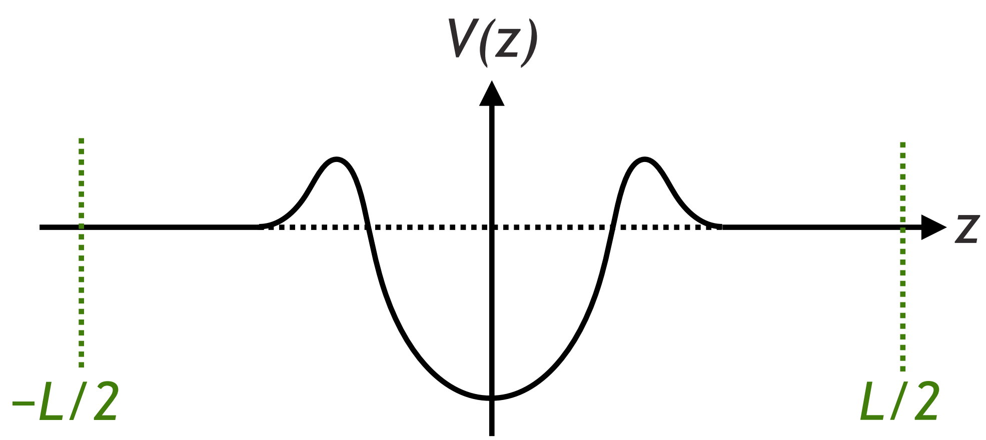
now put the system in a 'box' — periodic boundary condition at $z = \pm L/2$

$$\psi(|z| > R) \sim \cos\big(p\,|z| + \delta(p)\big)$$

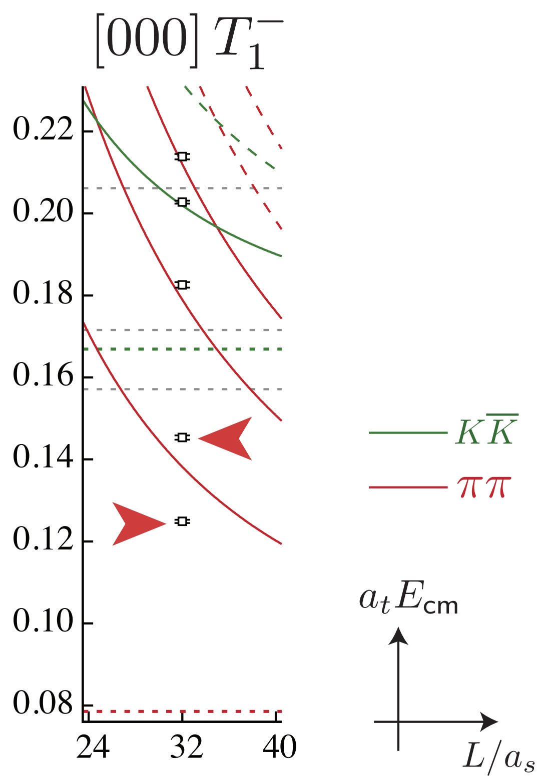
$$\psi(L/2) = \psi(-L/2)$$
$$\frac{d\psi}{dz}(L/2) = \frac{d\psi}{dz}(-L/2)$$

momentum quantization condition

$$p = \frac{2\pi}{L}n - \frac{2}{L}\delta(p)$$

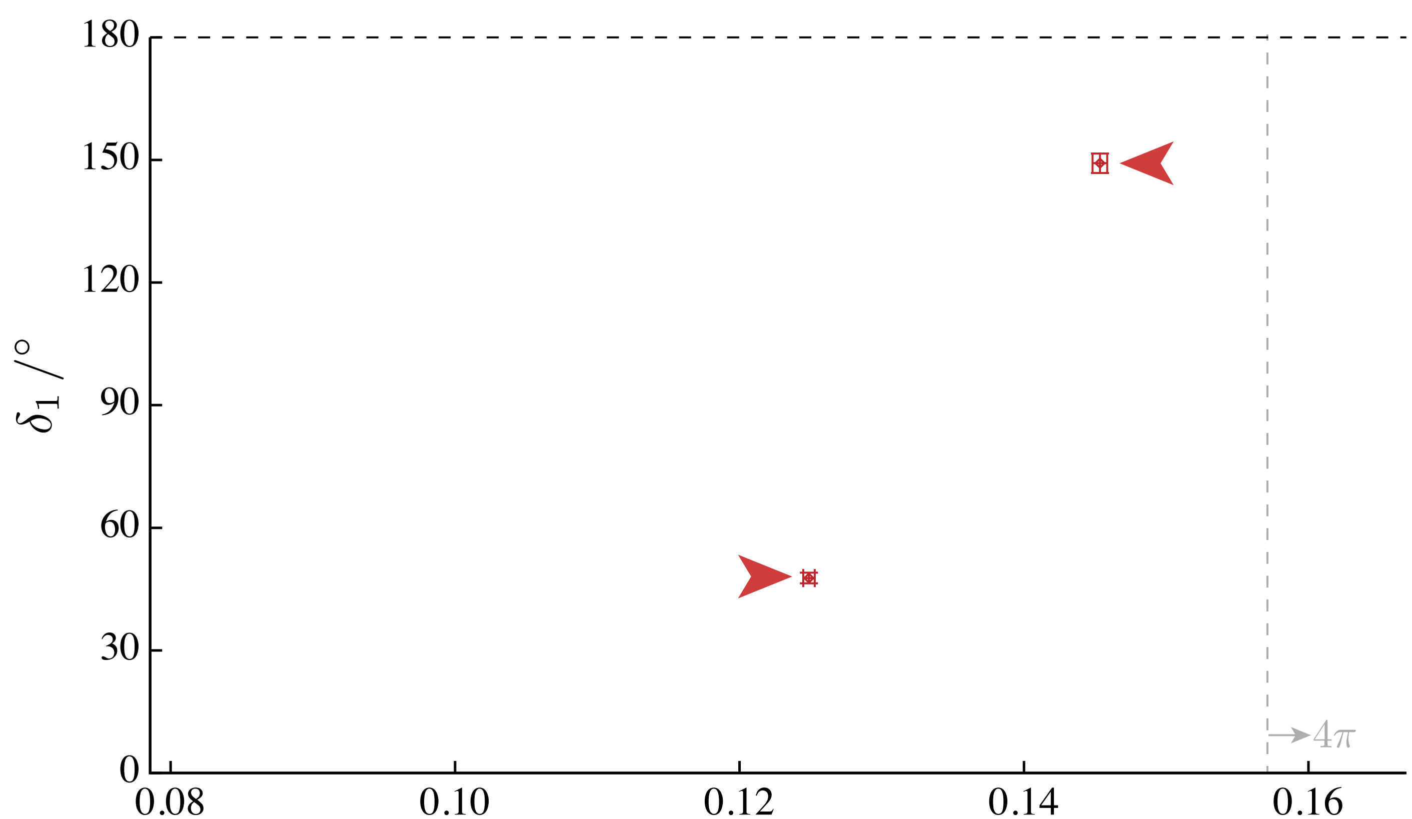


you can access scattering, but indirectly, from the discrete spectrum



$$t(E) = \frac{1}{\rho(E)} e^{i\delta(E)} \sin\delta(E)$$

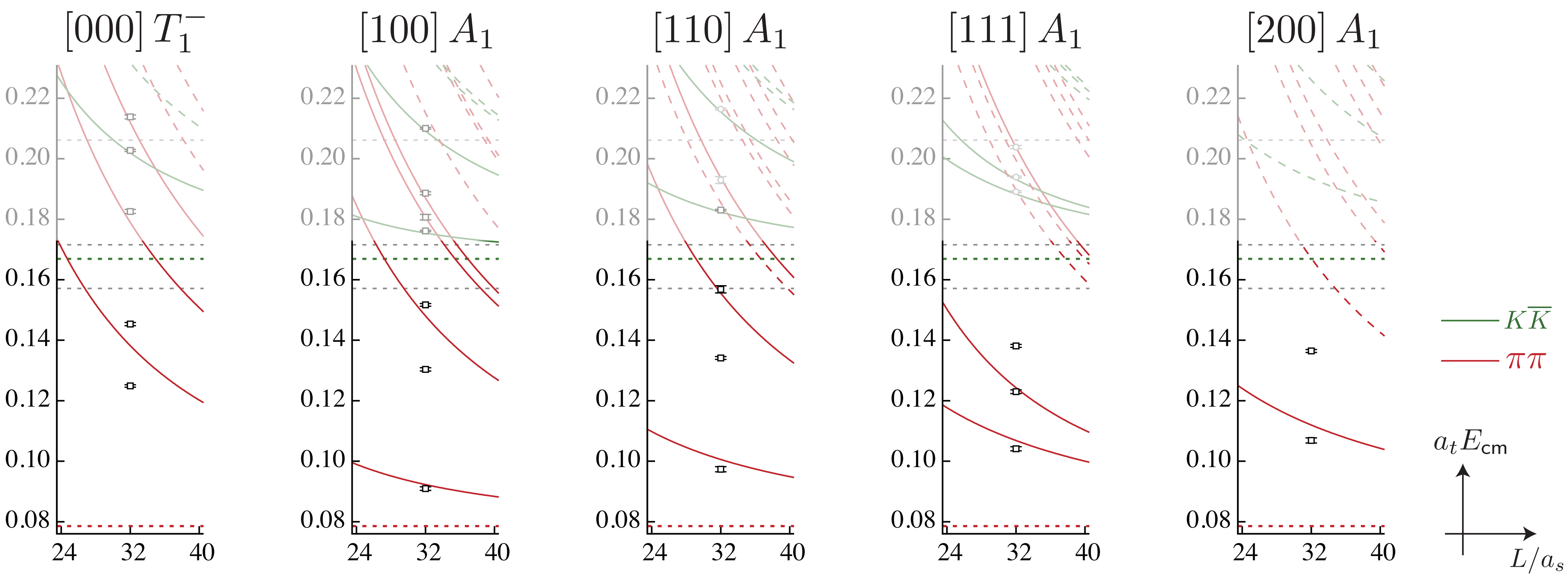
$$\rho(E) = \frac{2k}{E}$$



m_π = 0.039
m_K = 0.083
L ~ 3.8 fm

… and in moving frames …

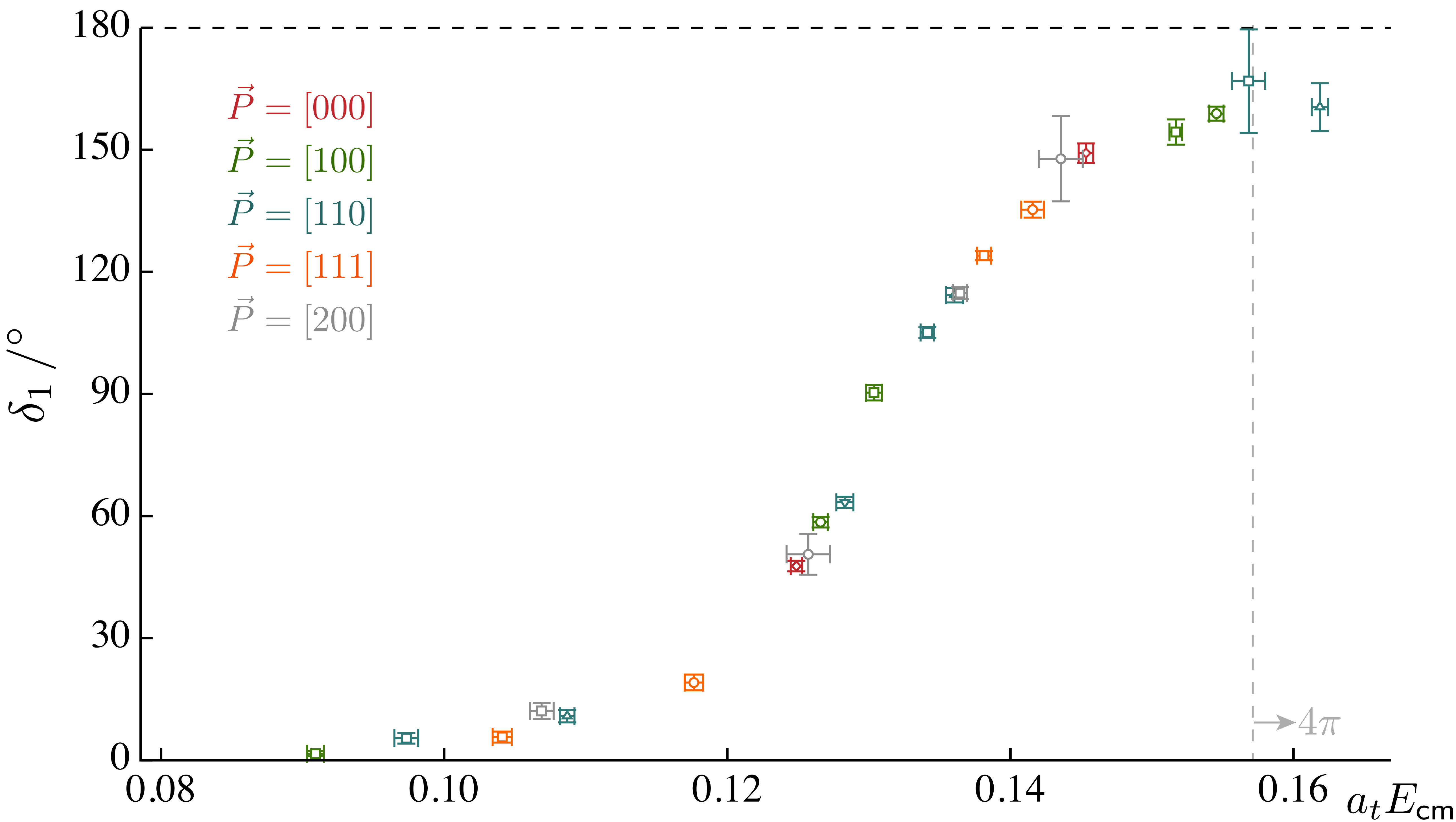
PRD92 094502 (2015)



$m_\pi = 0.039$
$m_K = 0.083$

L ~ 3.8 fm

… giving a phase-shift

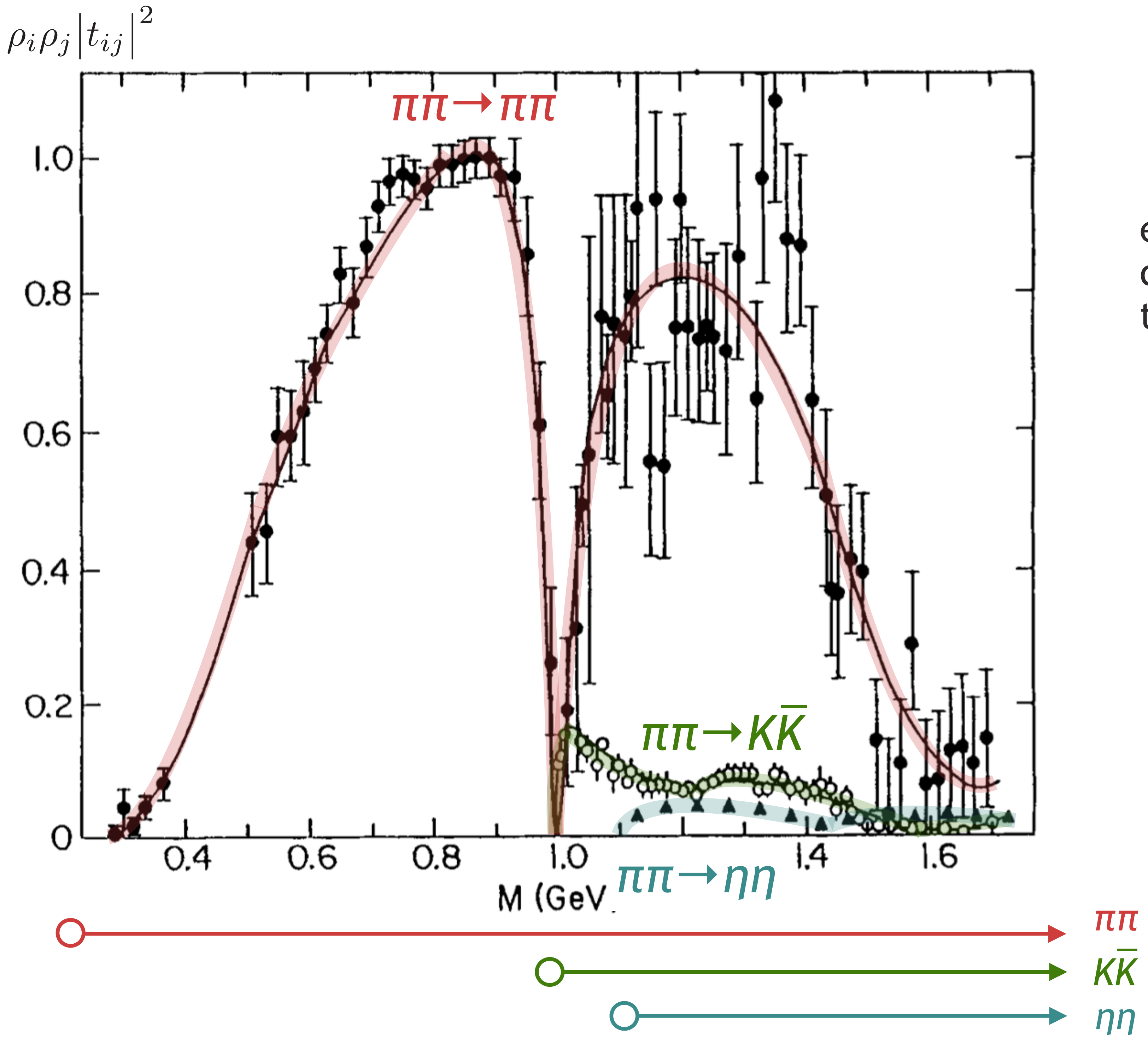


$m_\pi = 0.039$
$m_K = 0.083$
L ~ 3.8 fm

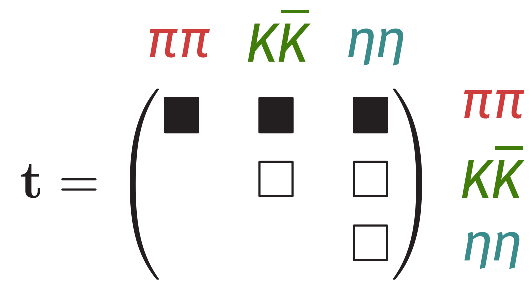
… looks like a classic resonance signal …

hadron-hadron scattering can be non-trivial

e.g. $\pi\pi$, KK, $\eta\eta$ S-wave scattering



experimentally quite difficult to fill out the whole matrix



isolating kaon exchange hard & η beams don't exist

$\pi\pi$, $K\bar{K}$, $\eta\eta$ scattering with m_π~391 MeV

PRD 97 054513 (2018)

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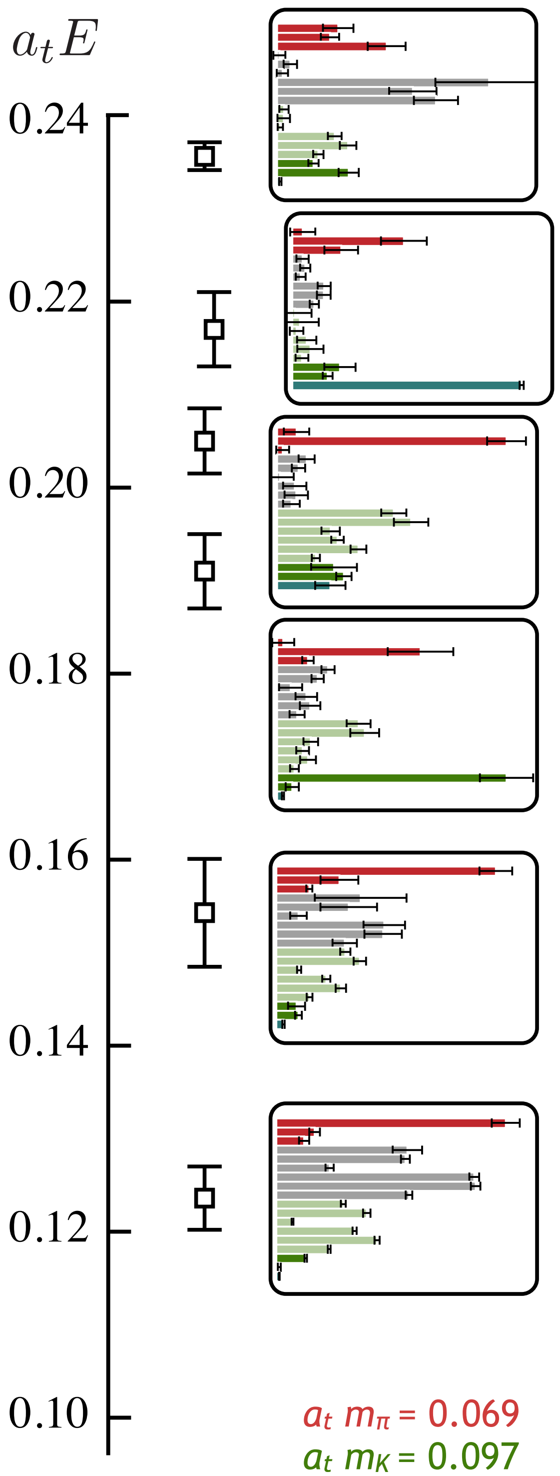
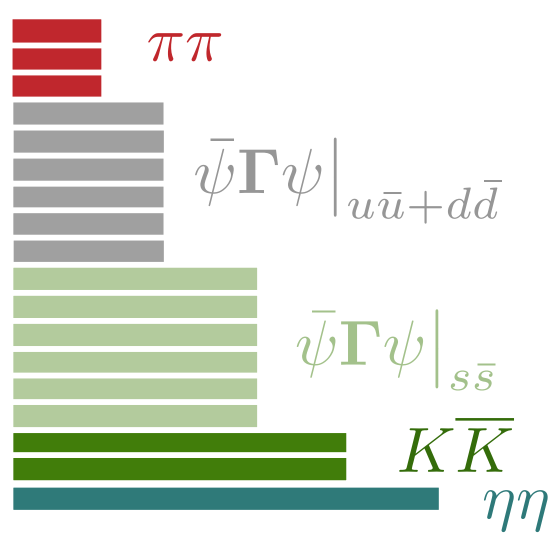
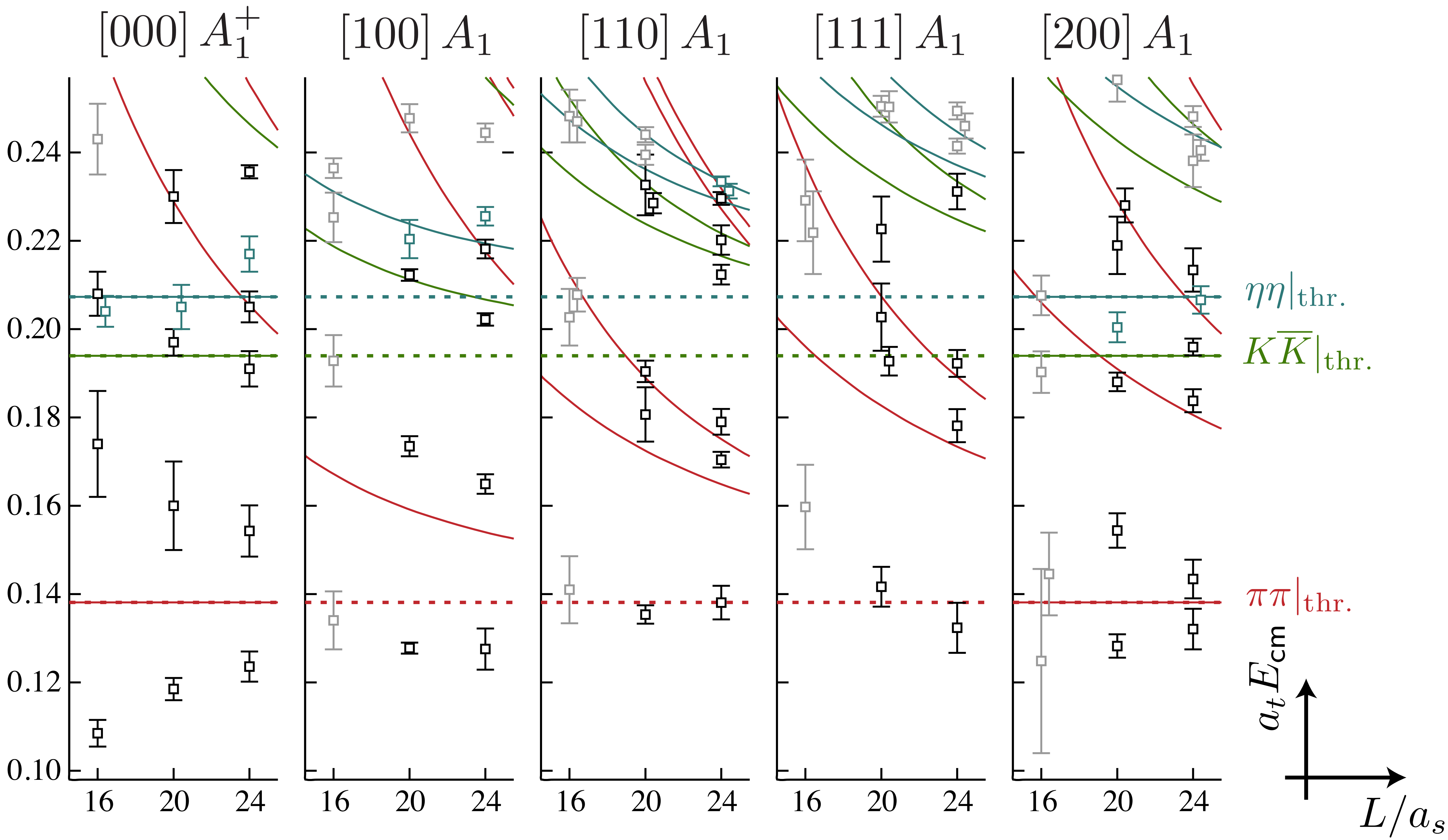


$a_t\, m_\pi = 0.069$
$a_t\, m_K = 0.097$
$a_t\, m_\eta = 0.104$

operator basis



$\pi\pi$, $K\bar{K}$, $\eta\eta$ scattering with m_π~391 MeV



what ***t***-matrix gives these spectra ?

$\pi\pi$, $K\bar{K}$, $\eta\eta$ scattering with m_π~391 MeV

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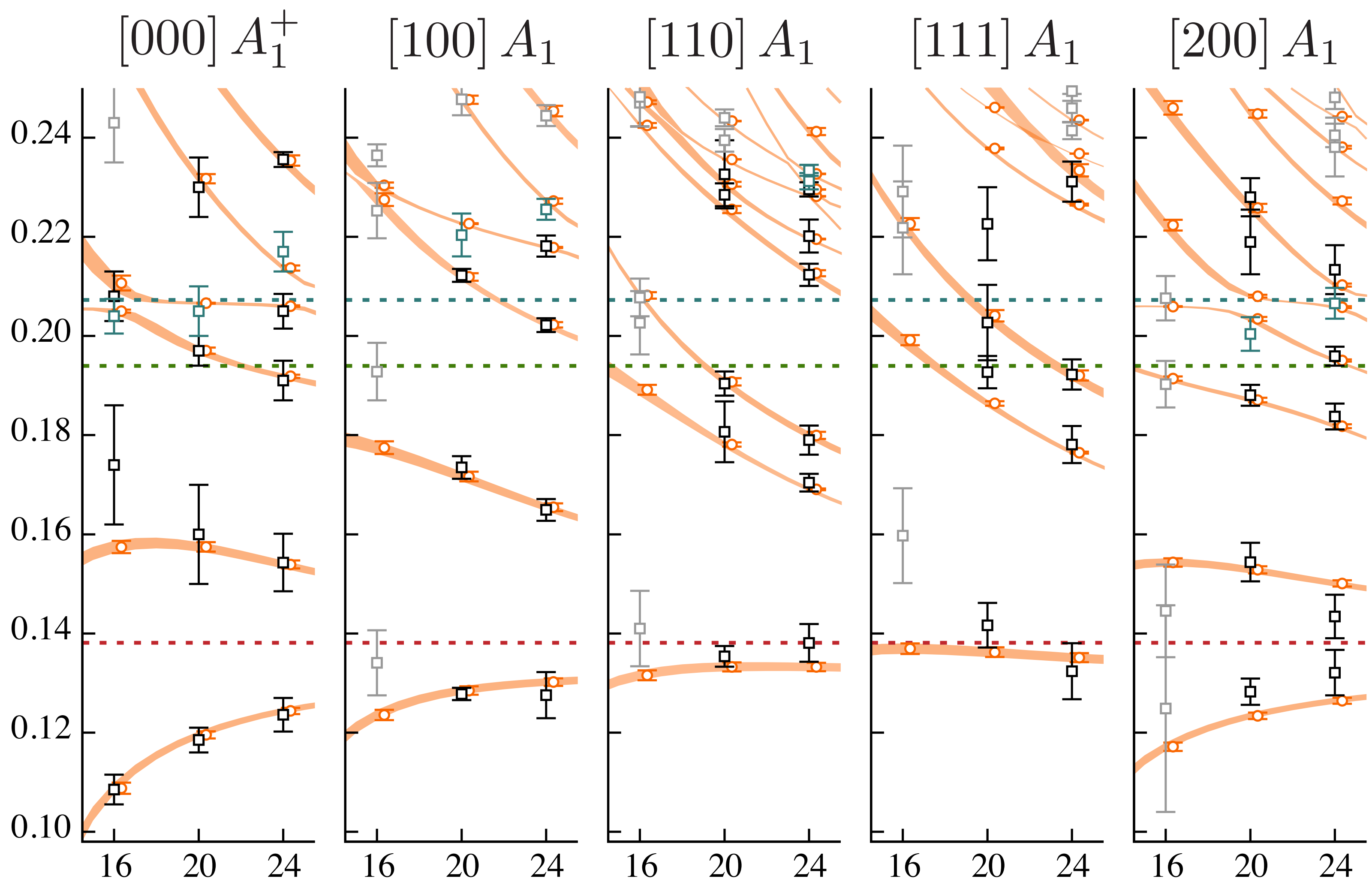
best fit to lattice spectra



$$\frac{\chi^2}{N_{\rm dof}} = \frac{44.0}{57-8} = 0.90$$

$\pi\pi$, $K\bar{K}$, $\eta\eta$ scattering with m_π~391 MeV

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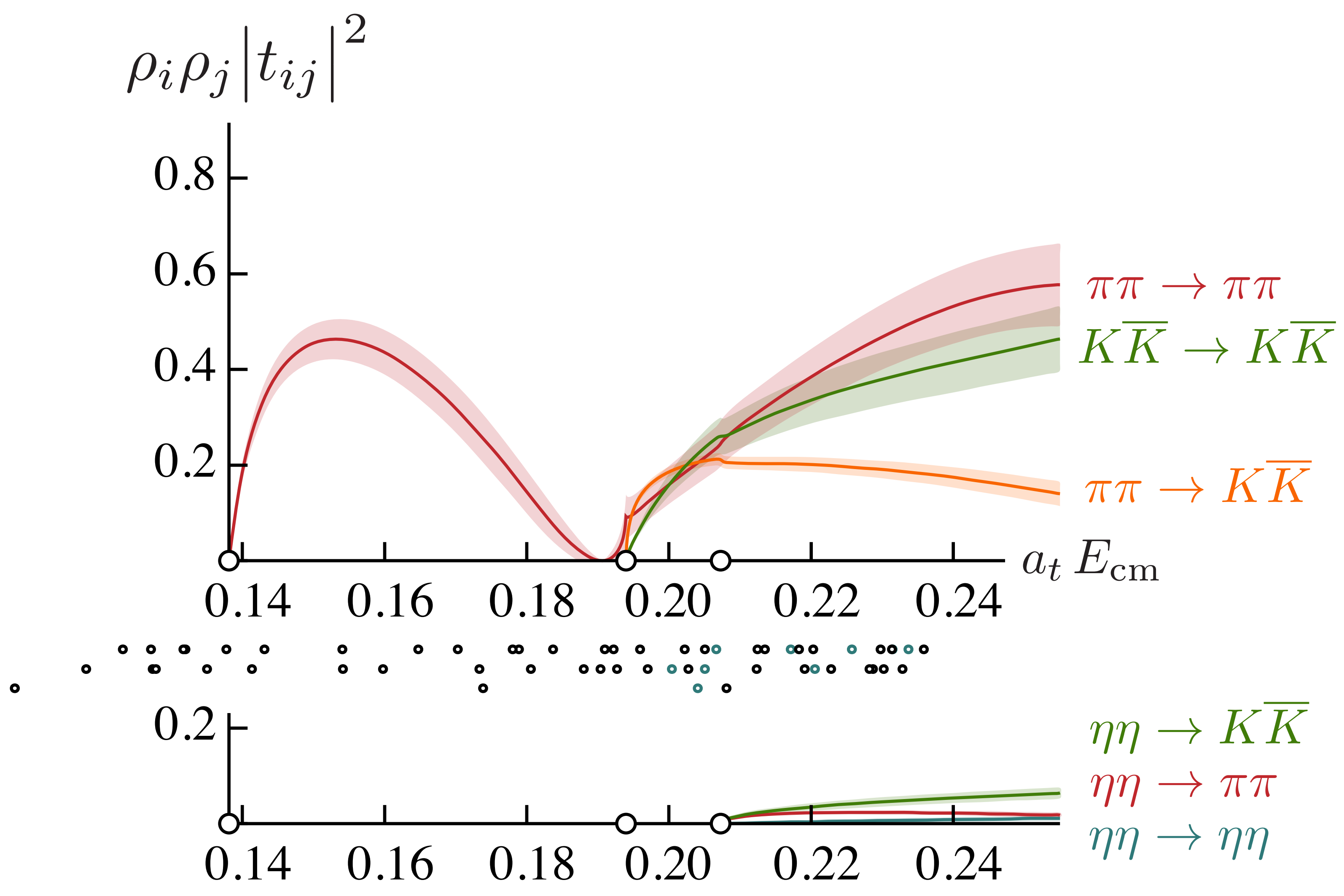
S-wave amplitudes



$\pi\pi$, $K\bar{K}$, $\eta\eta$ scattering with m_π~391 MeV

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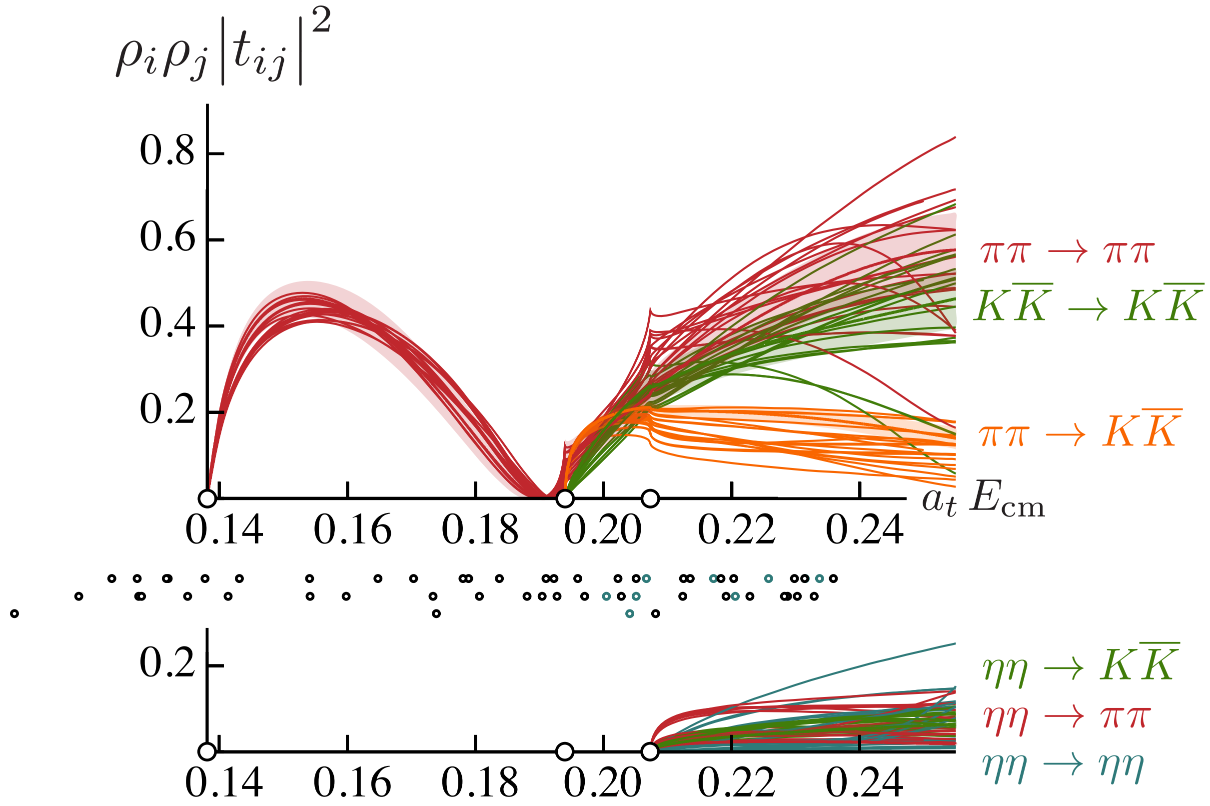
scattering amplitude 'prediction'



'analogous' experimental data