Lattice QCD: Finite-volume spectrum

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EXOHAD
EXOTIC HADRONS TOPICAL COLLABORATION

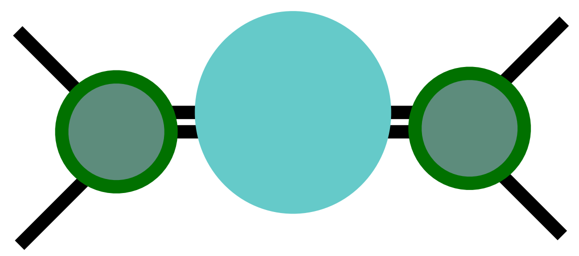
Spectroscopy in lattice QCD

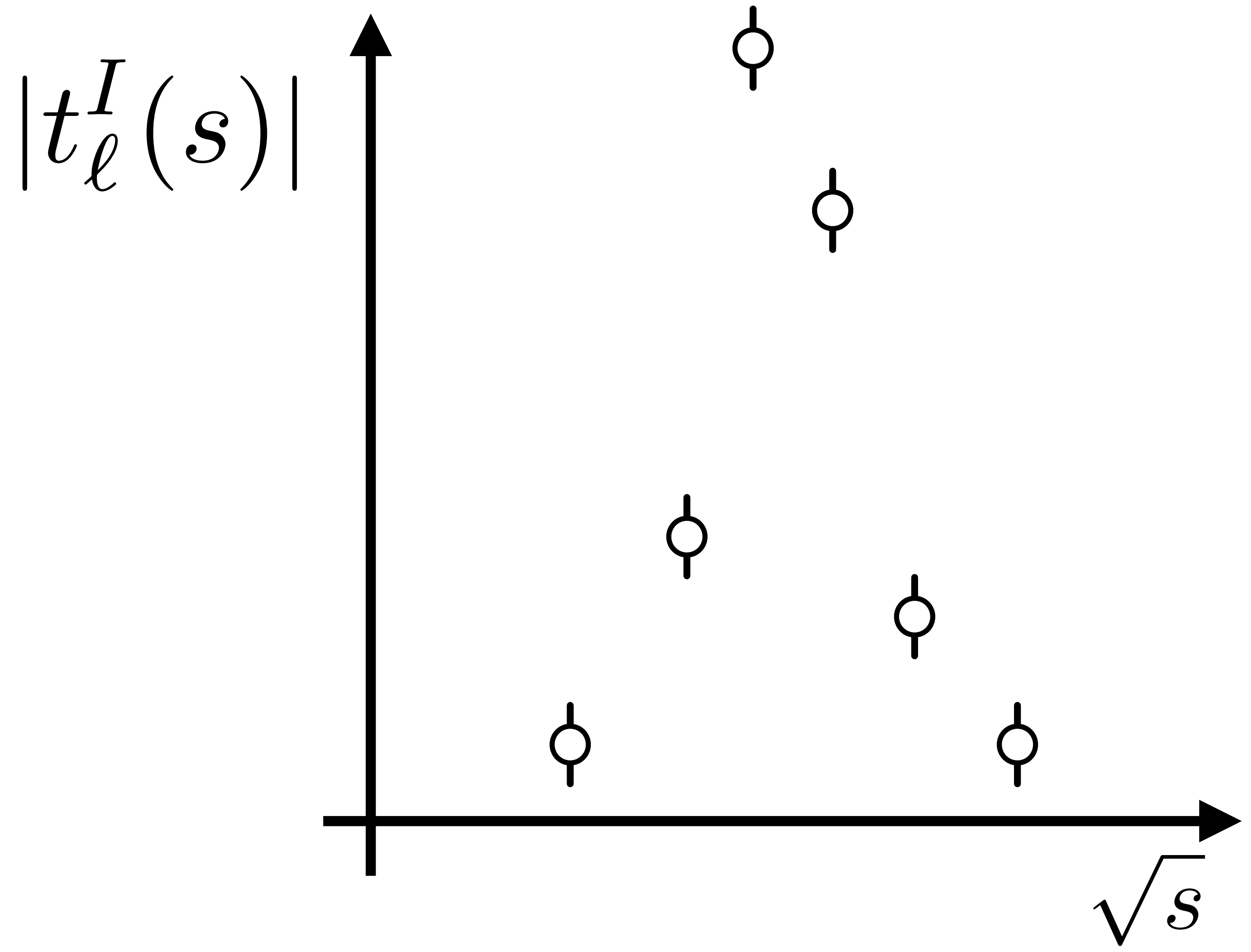
Extracting resonances from 2-body data 101

Assume we have scattering data for well-defined angular momentum

Assume the resonance is narrow and isolated

$$t_\ell^I(s) = \frac{1}{\rho(s)} \frac{\sqrt{s}\Gamma}{m_{\rm BW}^2 - s - i\sqrt{s}\Gamma}$$





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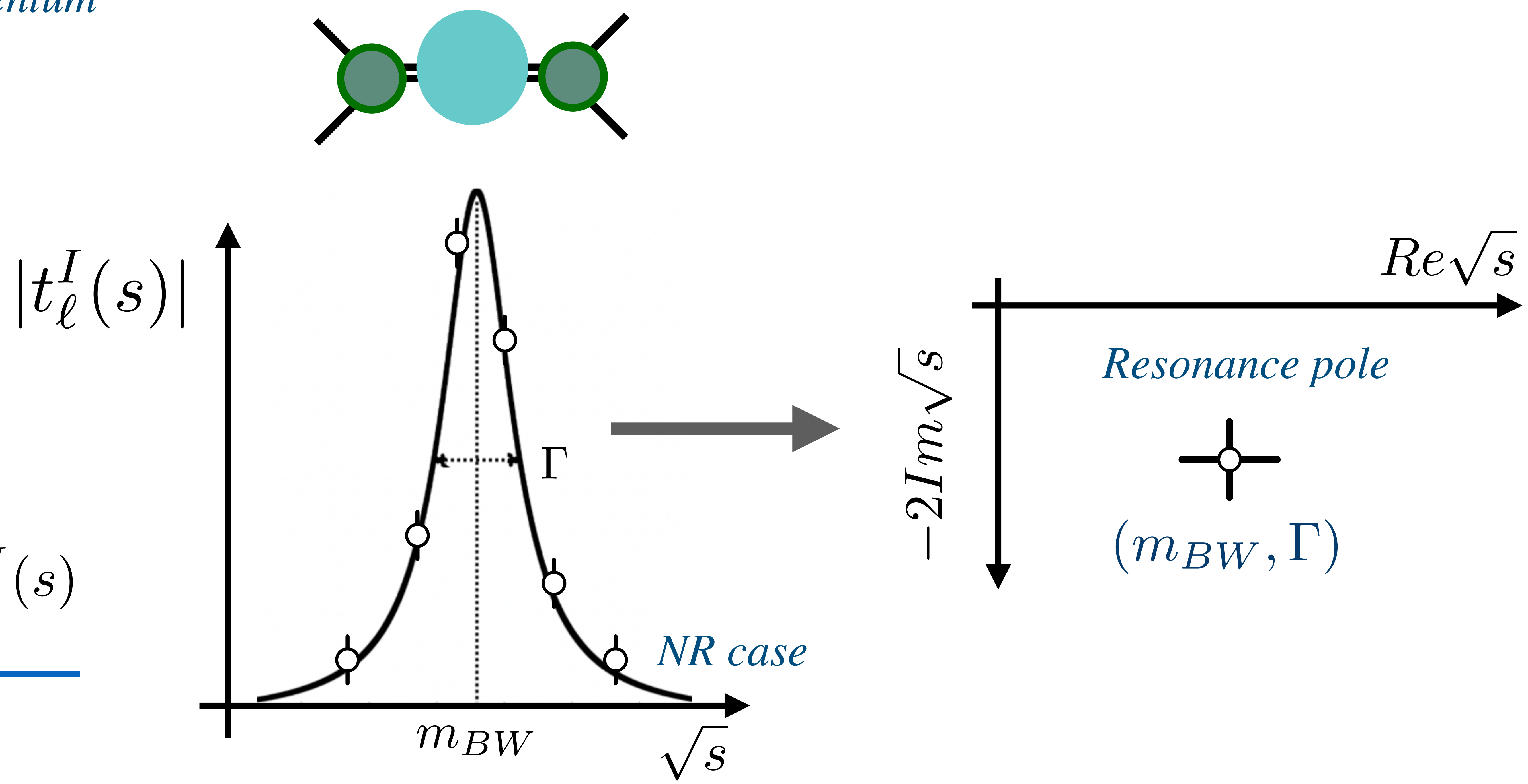

More general form for the amplitude

$$t_\ell^I(s) = \frac{1}{\rho(s)} \frac{K(s)}{1 - i\rho(s)K(s)} = \frac{1}{\rho(s)} e^{i\delta_\ell^I(s)} \sin\delta_\ell^I(s)$$

Elastic case

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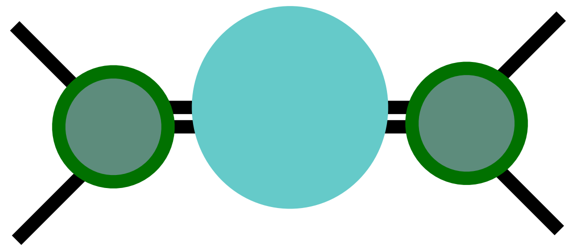

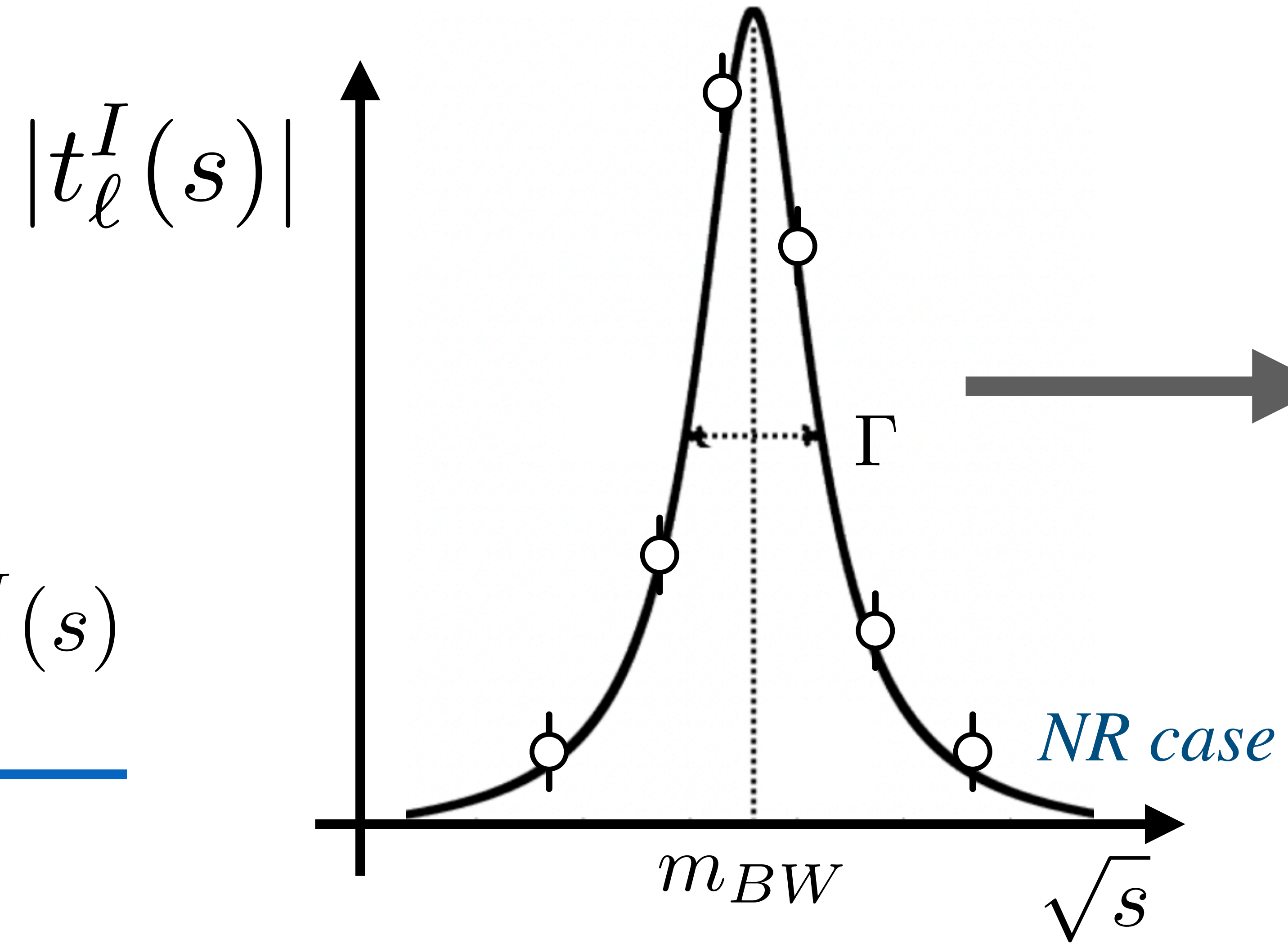

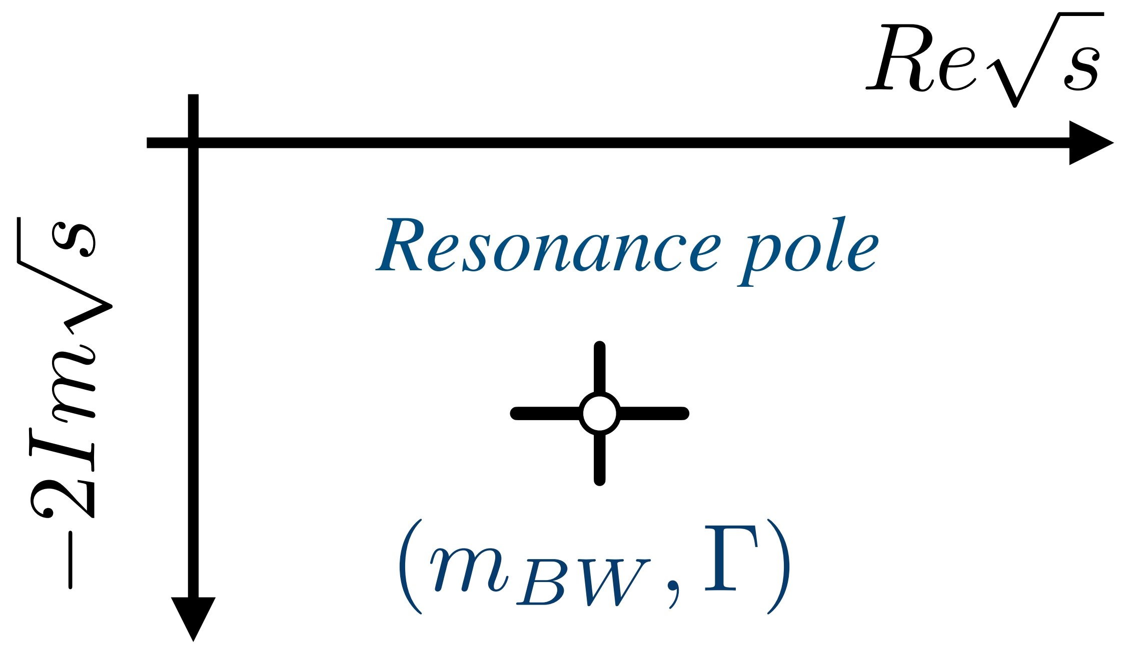

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Elastic case

In lattice QCD, our basic equation is the Lagrangian

$$\mathcal{L}_{\mathrm{QCD}} = \sum_f \bar{\psi}_f \left(i\not{D} - m_f\right)\psi_f - \frac{1}{2g_s^2}\,\mathrm{Tr}\,G_{\mu\nu}G^{\mu\nu}$$

Quark masses are a parameter for us → m_π is a "choice"

Our basic observables are correlation functions

$$\langle O_f(t) O_i^\dagger(0)\rangle = \frac{1}{Z_T}\int \mathcal{D}[\Phi] \mathrm{e}^{-S_E[\Phi]} O_f[\Phi] O_i^\dagger[\Phi]$$

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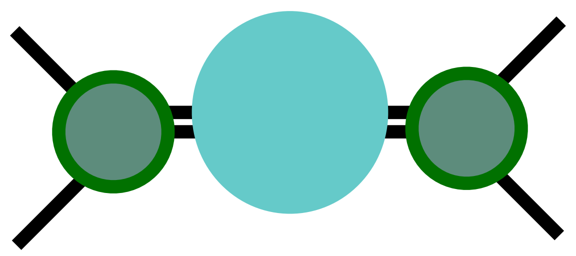

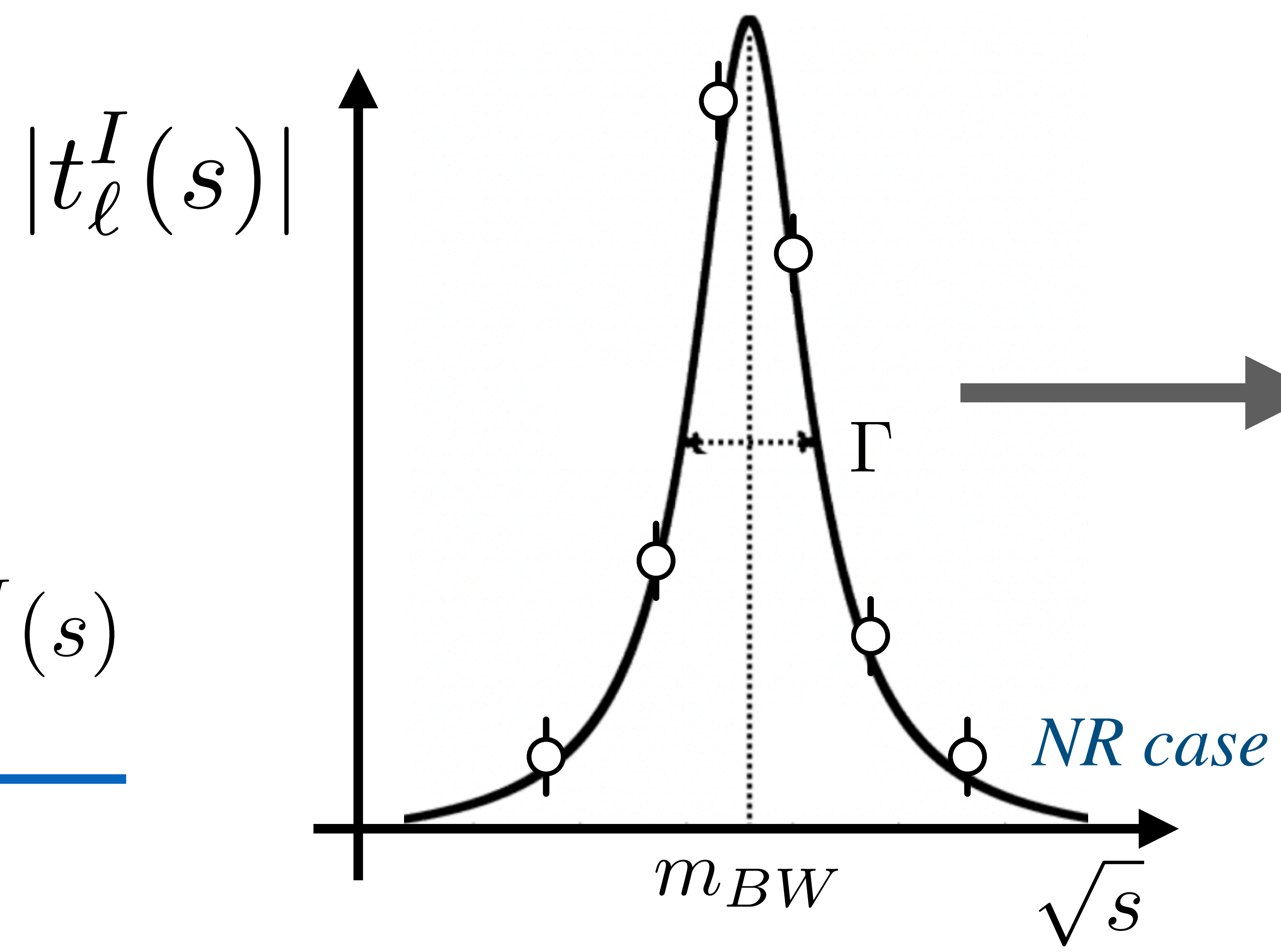

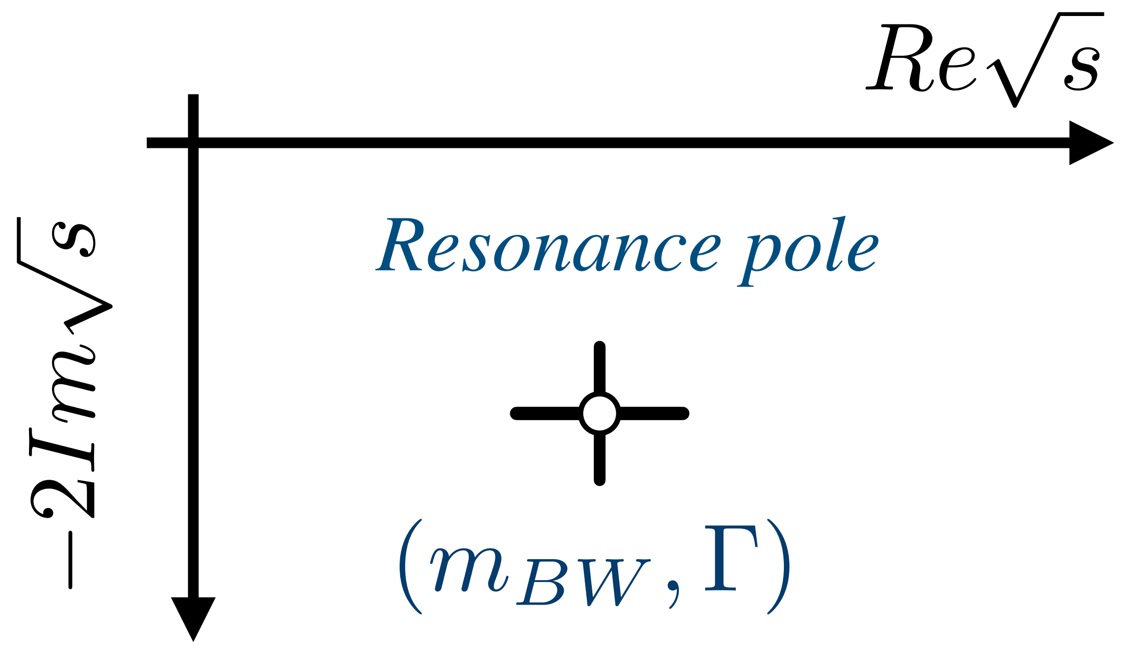

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How do we go from here to there??

Lattice QCD: Continuation

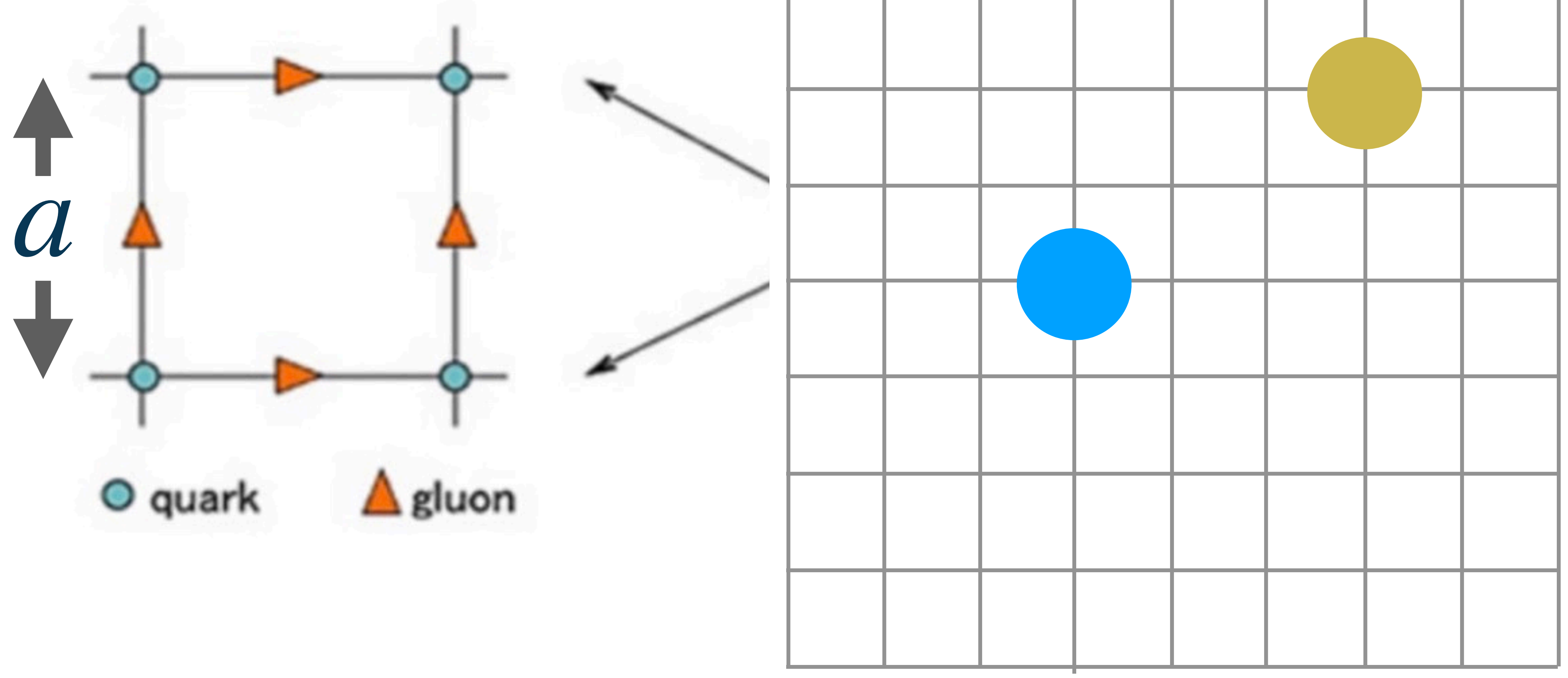
- [x] **Discretized lagrangian/hamiltonian formulations**
- [x] **Importance sampling and algorithms**
- [x] **Correlators**

- [ ] **Intro to 2-pt correlation building and fitting**
- [ ] **Finite-volume symmetry**
- [ ] **Generalized eigenvalue problem**

Lattice QCD: Continuation

$$\left\langle \varphi_{\mathrm{f}} \left| e^{-i\hat{H}(t_{\mathrm{f}}-t_{\mathrm{i}})} \right| \varphi_{\mathrm{i}} \right\rangle = \int \mathcal{D}\varphi(x) e^{-iS[\varphi(x)]}$$

Regulator



Discretization

Sum over all paths

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

Advantages

1. **Systematic approach**
2. **Quark mass is a parameter**

Major obstacles

1. **Highly dimensional integral** $10^6 - 10^8$
2. **Highly oscillatory** $e^{-iS[\varphi(x)]}$

Lattice QCD: Continuation

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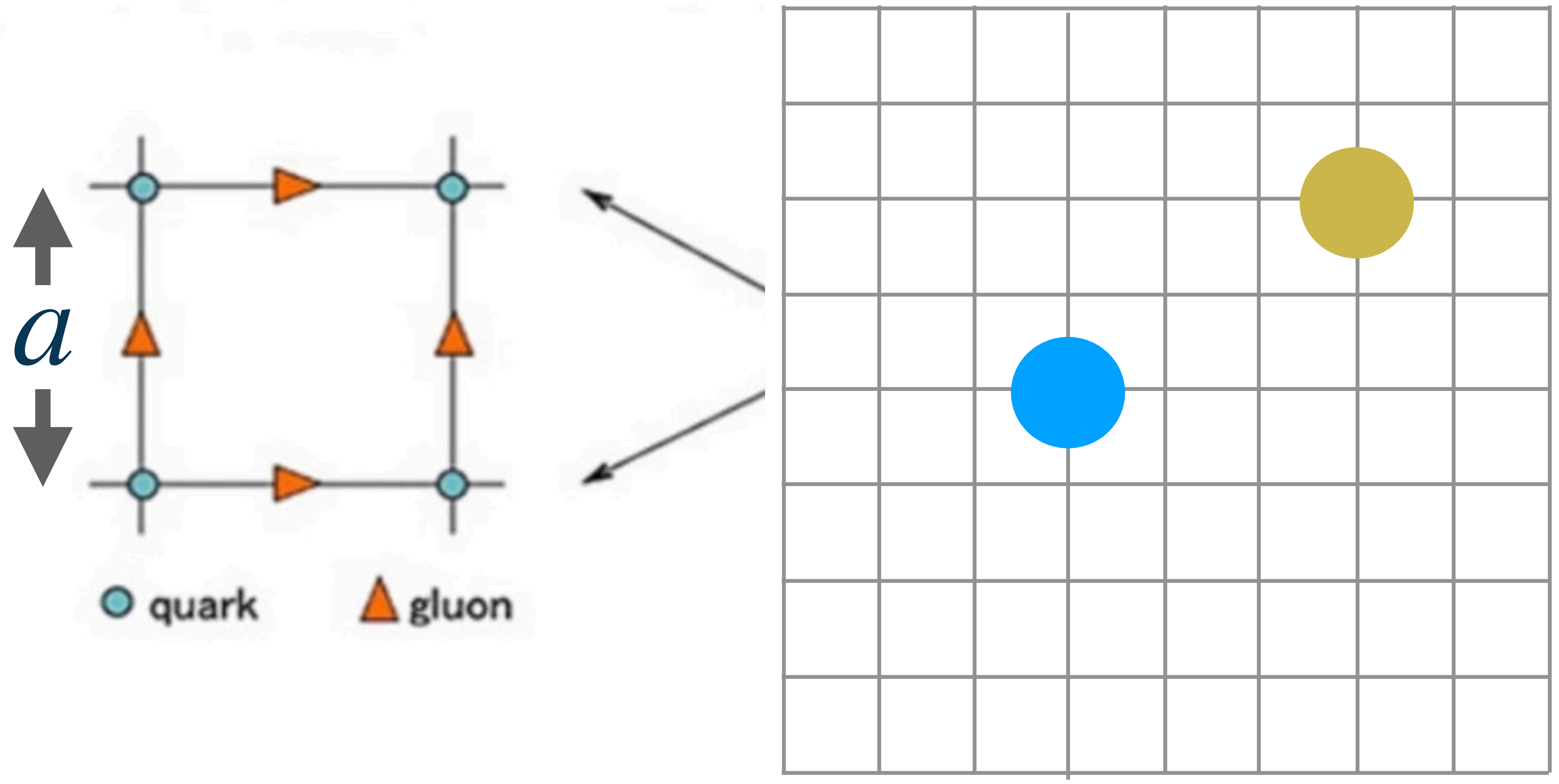

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Euclidean action $t \to -it$

$$-iS = -i \int d^3x dt \mathcal{L} \to -\int d^3x dt \mathcal{L}_{\mathrm{E}} = -S_{\mathrm{E}}$$

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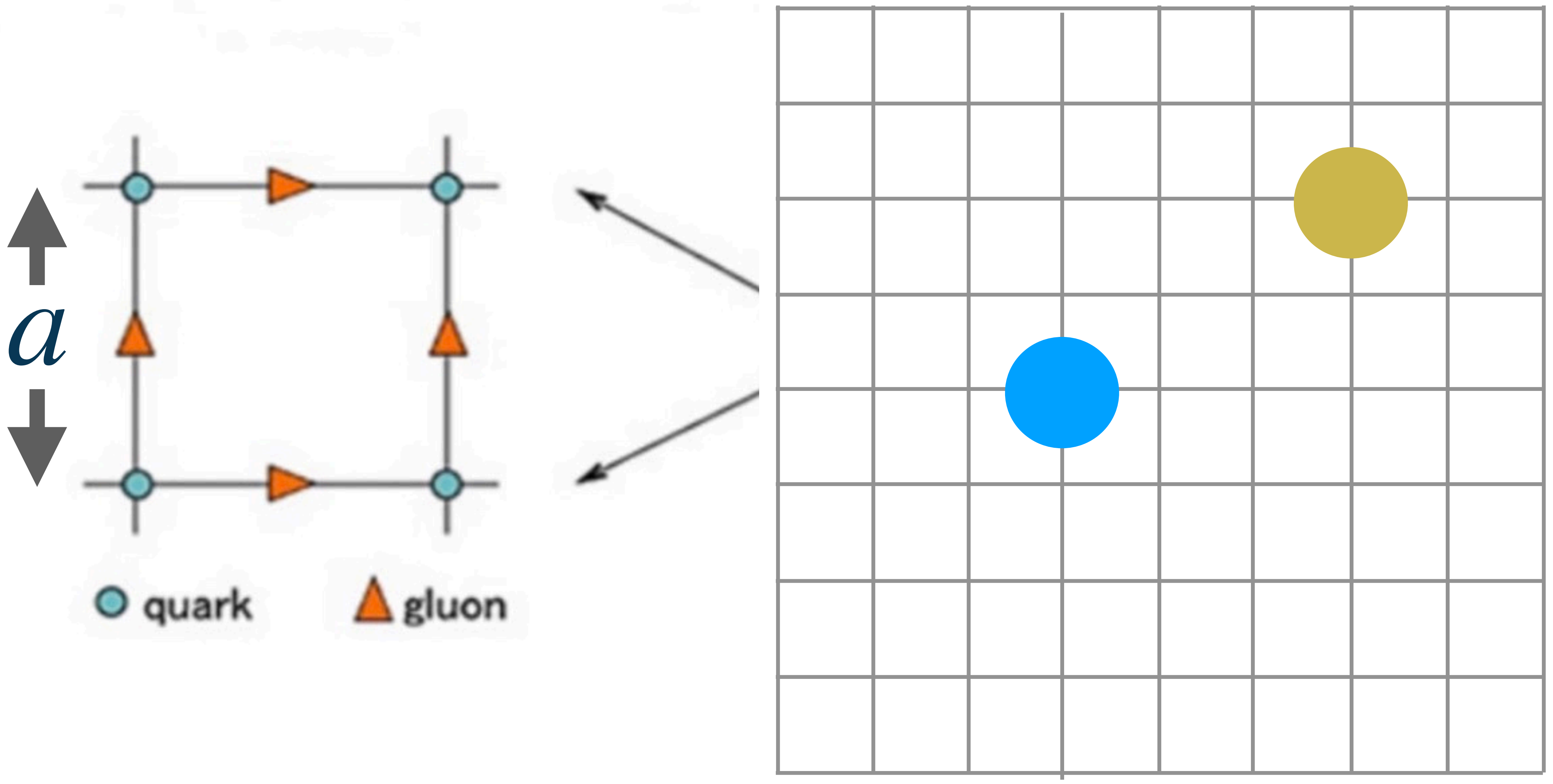


Discretization

Sum over all paths

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

$$\mathcal{L}_{\rm E} = \bar{\psi}\left(\gamma_\mu D_\mu + m\right)\psi + \frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu}$$

Euclidean action $t \to -it$

$$-iS = -i \int d^3x dt \mathcal{L} \to - \int d^3x dt \mathcal{L}_{\rm E} = -S_{\rm E}$$

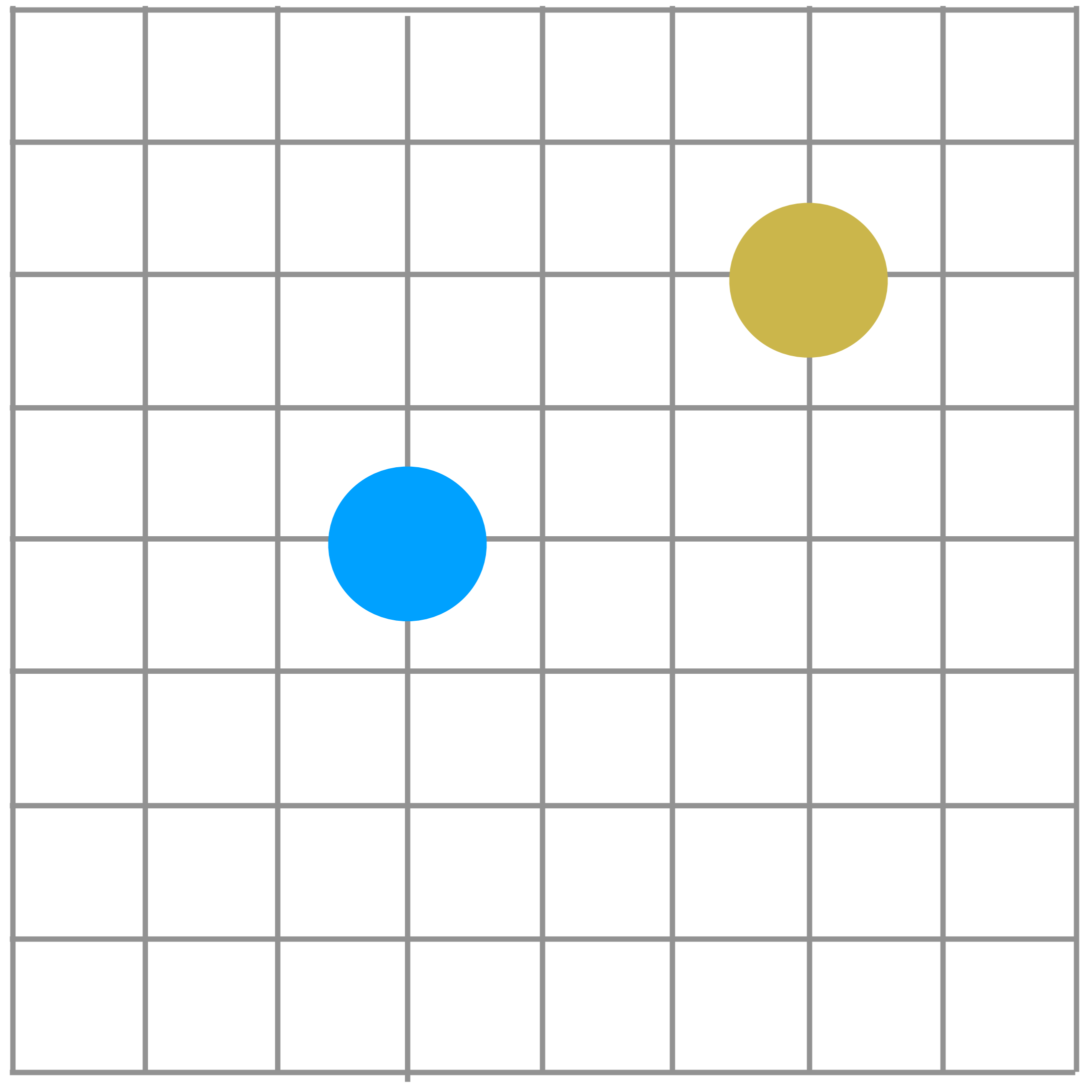
$$0 < \qquad < 1$$

$$\left\langle \varphi_{\rm f} \left| e^{-i\hat{H}(t_{\rm f}-t_{\rm i})} \right| \varphi_{\rm i} \right\rangle = \int \mathcal{D}\varphi(x) e^{-iS[\varphi(x)]} = \int \mathcal{D}\varphi(x) e^{-S_{\rm E}[\varphi(x)]}$$

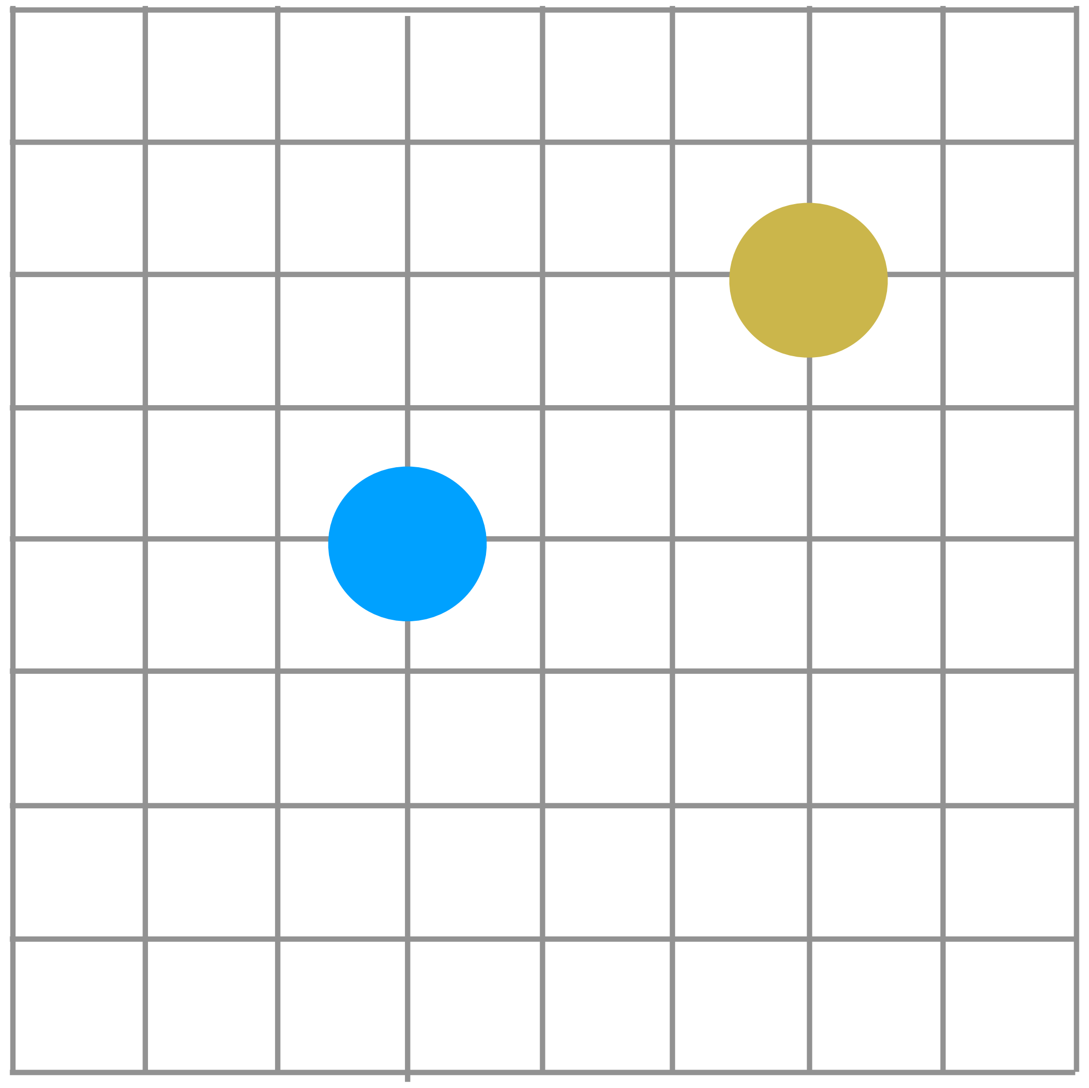
Probability like

Quark propagator

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



Quark propagator



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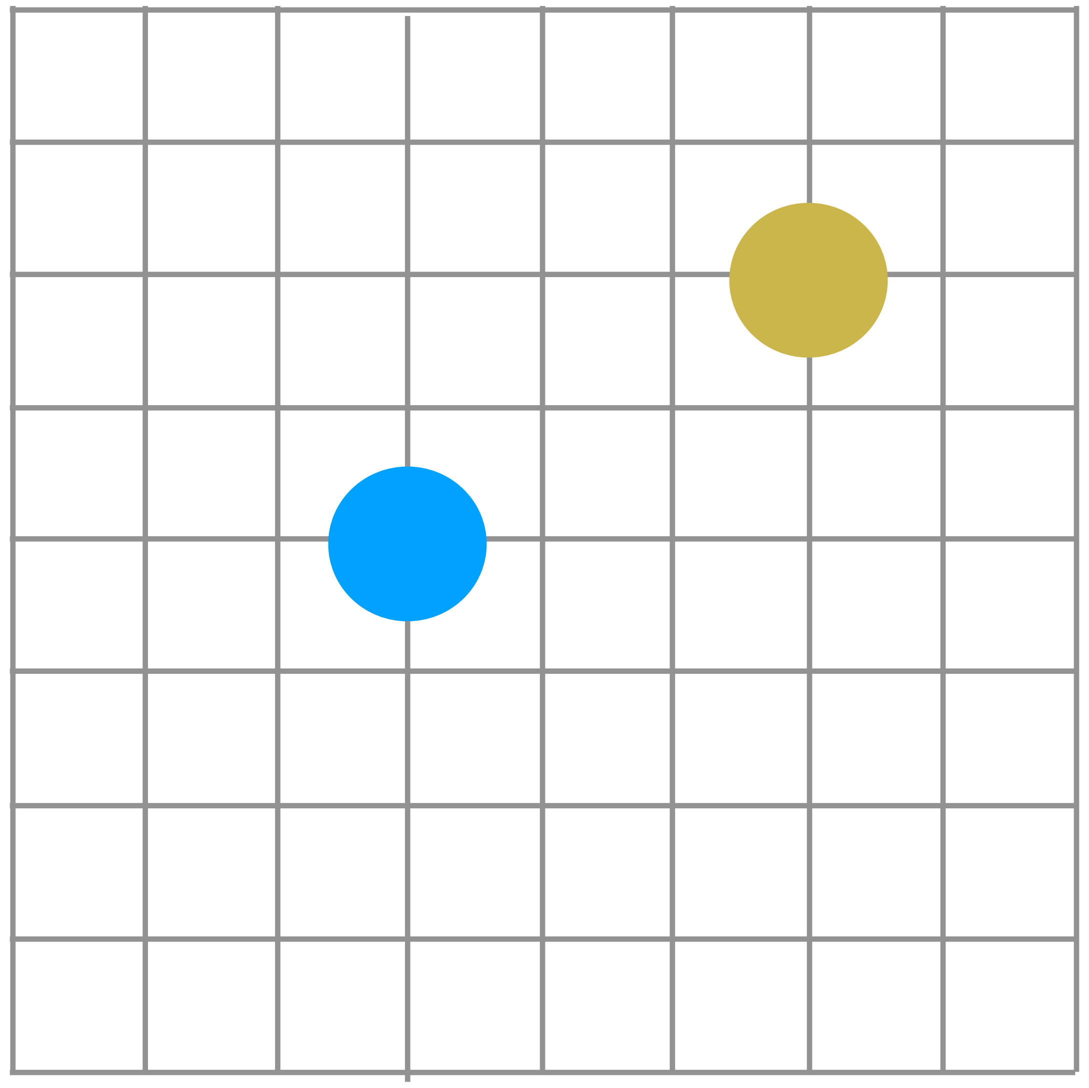
Splitting the fermions

$$= \int \mathcal{D}U e^{-S_{\rm E}^{\rm g}[U]} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \psi_x^{i\alpha} \bar{\psi}_y^{j\beta} e^{-\bar{\psi} D[U] \psi}$$

Quark Propagator



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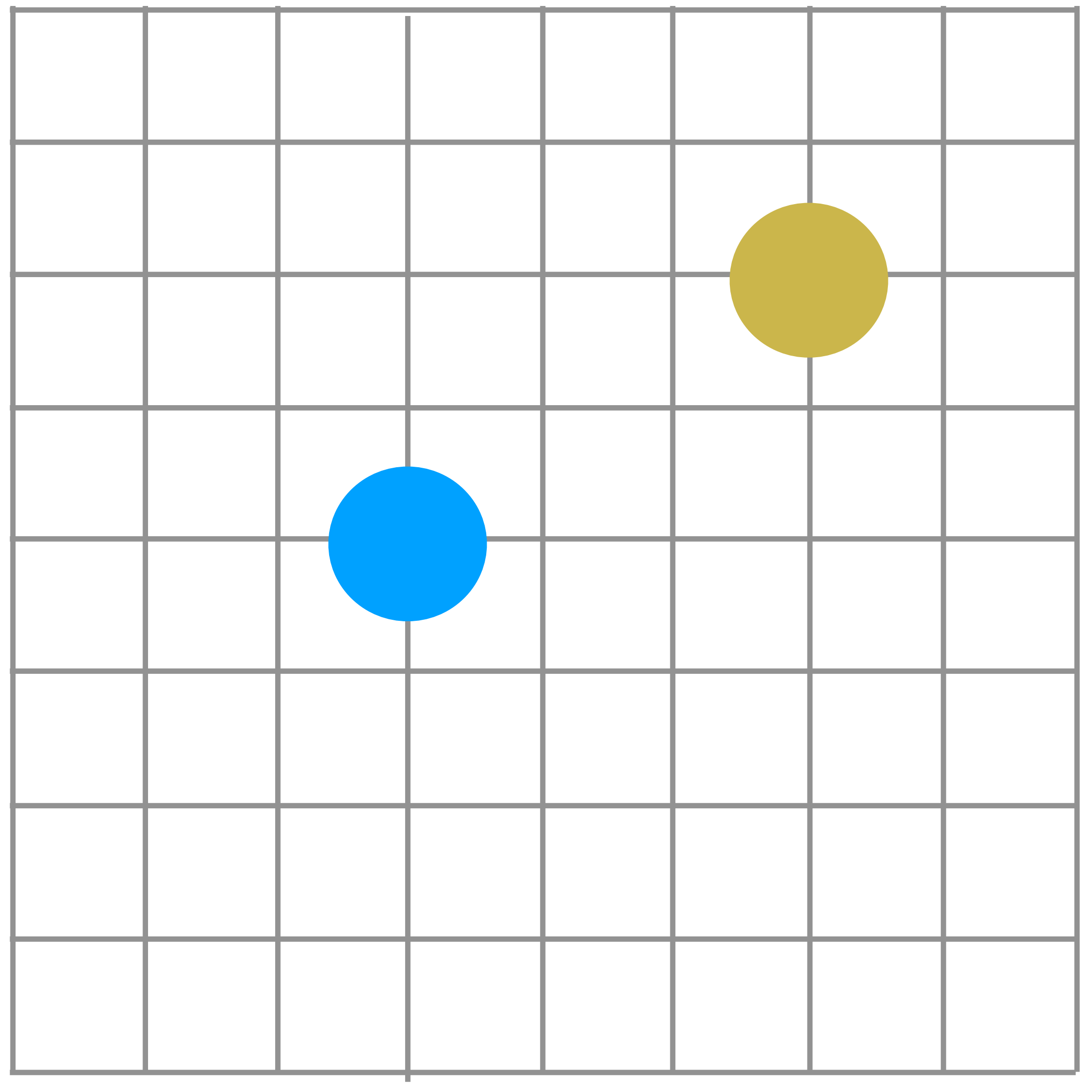
Algebra

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

Probability

Quark Propagator



Quark propagator

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Algebra

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

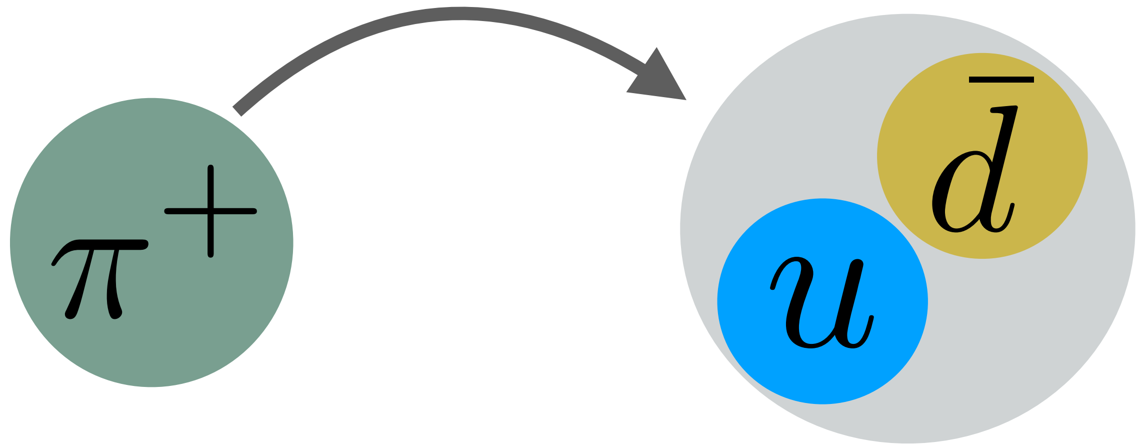
Sampling according to this

$$= \sum_n^N \left[D^{-1}[U_n]\right]_{x,y}^{i\alpha,j\beta}$$

Our quark propagator, one per configuration

Wick contractions

Lets study the temporal evolution of a pion at at fixed position in the lattice



$$|\pi^+\rangle = |\bar{d}\gamma_5 u\rangle$$

$$C(t) \equiv \langle 0 | \mathcal{O}(t)\, \mathcal{O}^\dagger(0) | 0 \rangle$$

Where

$$\mathcal{O}_{\pi^+}(\vec{x},t) = \bar{d}(\vec{x},t)\gamma_5 u(\vec{x},t) \quad \mathcal{O}_{\pi^-}(\vec{x},t) = \bar{u}(\vec{x},t)\gamma_5 d(\vec{x},t)$$

$$O_{\pi^0}(\vec{x},t) = \frac{1}{\sqrt{2}}\left(\bar{u}(\vec{x},t)\gamma_5 u(\vec{x},t) - \bar{d}(\vec{x},t)\gamma_5 d(\vec{x},t)\right)$$

Are P and C correct?

Afternoon…

Wick contractions

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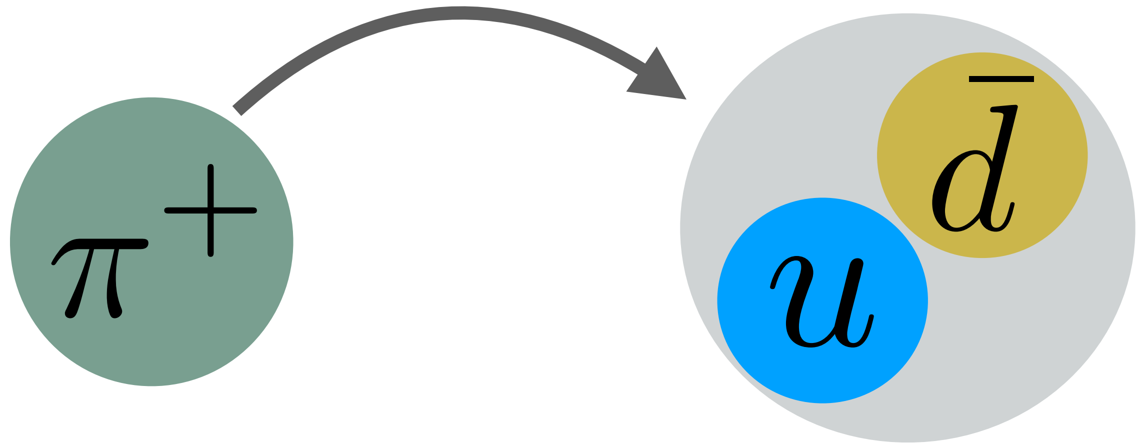

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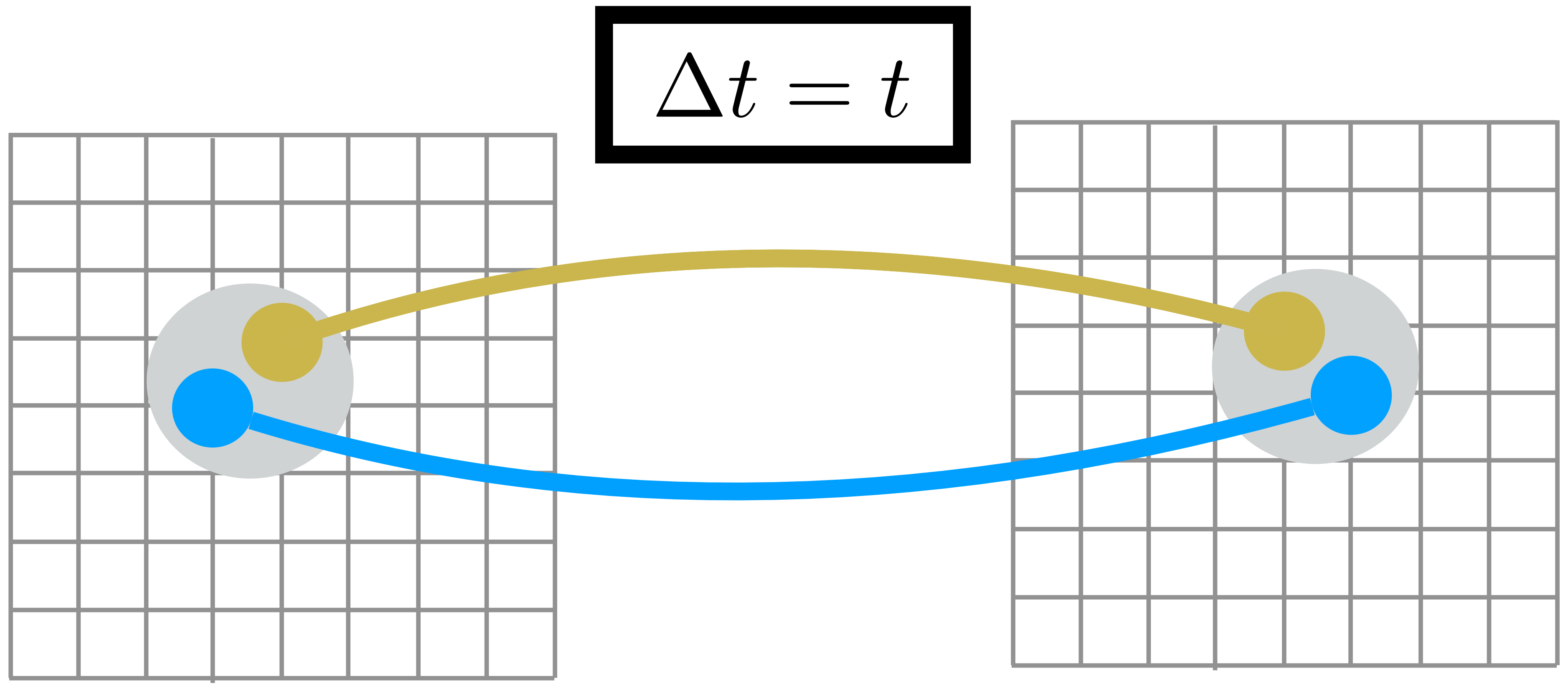
$$\langle \mathcal{O}_{\pi^+}(x)\mathcal{O}^\dagger_{\pi^+}(0)\rangle = \langle \bar{d}(x)\gamma_5 u(x)\bar{u}(0)\gamma_5 d(0)\rangle = \gamma_5^{\alpha_1\beta_1}\gamma_5^{\alpha_2\beta_2}\langle \bar{d}(x)_{\substack{\alpha_1\\c_1}} u(x)_{\substack{\beta_1\\c_1}} \bar{u}(0)_{\substack{\alpha_2\\c_2}} d(0)_{\substack{\beta_2\\c_2}}\rangle$$

$$= -\gamma_5^{\alpha_1\beta_1}\gamma_5^{\alpha_2\beta_2}\langle u(x)_{\substack{\beta_1\\c_1}} \bar{u}(0)_{\substack{\alpha_2\\c_2}}\rangle_u \langle d(0)_{\substack{\beta_2\\c_2}} \bar{d}(x)_{\substack{\alpha_1\\c_1}}\rangle_d = -\sum_n^N \gamma_5^{\alpha_1\beta_1}\gamma_5^{\alpha_2\beta_2} D_u^{-1}(x\mid 0)_{\substack{\beta_1\alpha_2\\c_1c_2}} D_d^{-1}(0\mid x)_{\substack{\beta_2\alpha_1\\c_2c_1}}$$

$$= -\sum_n^N \mathrm{tr}[\gamma_5 (D_u[U_n]^{-1})_{x,0}\gamma_5 (D_d[U_n]^{-1})_{0,x}]$$



Wick contractions

More general constructions are possible

$$O_M(x) = \bar{\psi}^{(f_1)}(x)\Gamma\psi^{(f_2)}(x)$$

State	J^{PC}	Γ	Particles
Pseudoscalar	0^{-+}	$\gamma_5, \gamma_4\gamma_5$	$\pi^\pm, \pi^0, \eta, K^\pm, K^0, \ldots$
Scalar	0^{++}	$\mathbf{1}, \gamma_4$	$f_0, a_0, K_0^*, \ldots$
Vector	1^{--}	$\gamma_i, \gamma_4\gamma_i$	$\rho^\pm, \rho^0, \omega, K^*, \phi, \ldots$
Axial vector	1^{++}	$\gamma_i\gamma_5$	$a_1, f_1, \ldots$
Tensor	1^{+-}	$\gamma_i\gamma_j$	$h_1, b_1, \ldots$

Γ **can take many different forms to produce desired quantum numbers**

One way of creating more general operators is to also include covariant derivatives

$$O_M(x) = \bar{\psi}^{(f_1)}(x)\Gamma(D_{i1}^{n1}, D_{i2}^{n2}, ..., D_{iN}^{nN})\psi^{(f_2)}(x)$$

n is the order, and i the direction

$$D_i\psi(x) \to \frac{1}{2a}\left(U_i(x)\psi(x+i) - U_i^\dagger(x-i)\psi(x-i)\right)$$

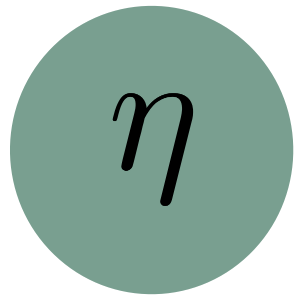
On a discrete lattice they are finite displacements of quark fields, connected by links

In our last step, we sum over position space to create operator of well-defined momenta

$$\widetilde{O}(\vec{p},t) = \frac{1}{\sqrt{|\Lambda_3|}}\sum_{\vec{x}\in\Lambda_3} O(\vec{x},t)\mathrm{e}^{-\mathrm{i}\vec{x}\vec{p}} \xrightarrow[p=0,\ \Lambda_3=O]{} \sum_{\vec{x}} O(\vec{x},t)$$

Wick contractions

Lets study the temporal evolution of an eta at at fixed position in the lattice

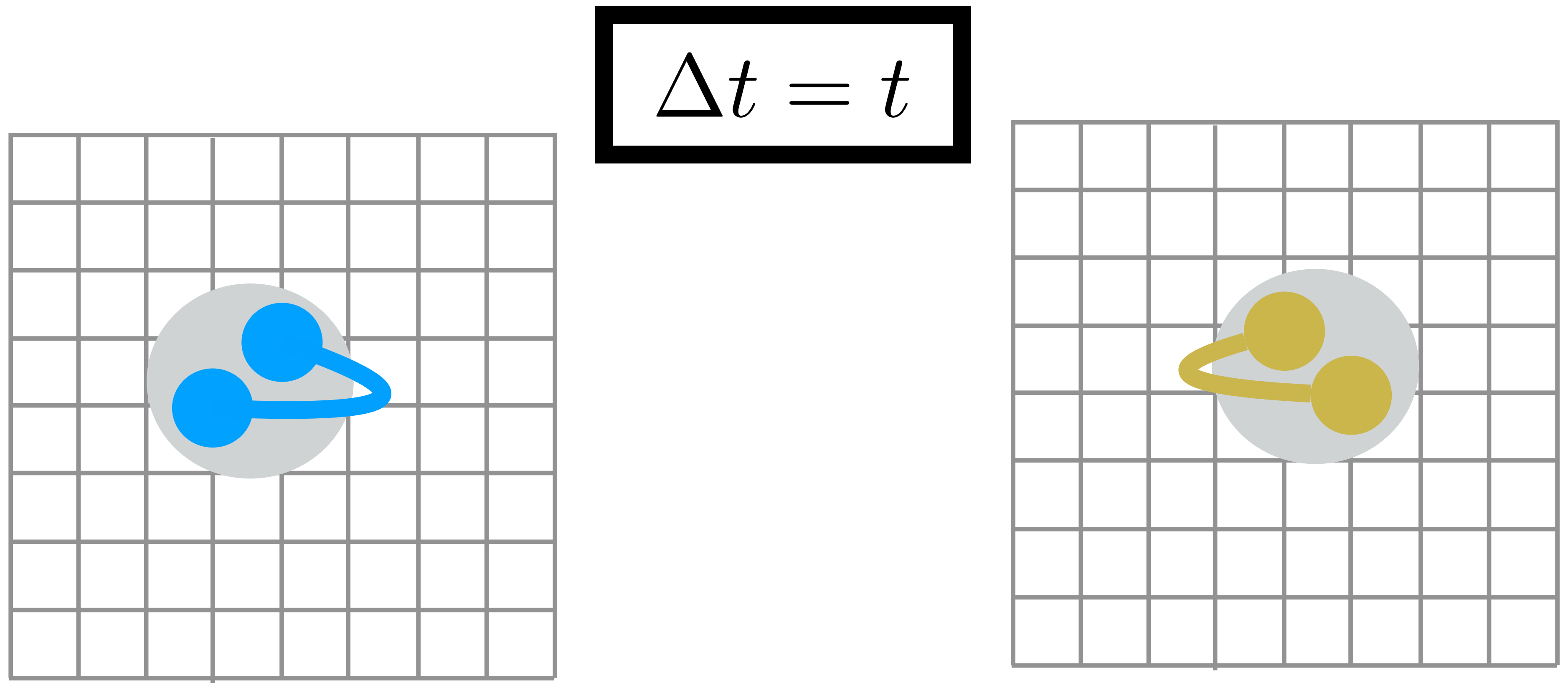


$$|\eta\rangle = \frac{|\bar{u}\gamma_5 u\rangle + |\bar{d}\gamma_5 d\rangle}{\sqrt{2}}$$

$$C(t) \equiv \left\langle 0 \middle| \mathcal{O}(t)\, \mathcal{O}^\dagger(0) \middle| 0 \right\rangle$$

$$\left\langle \mathcal{O}_\eta(x)\mathcal{O}_\eta^\dagger(0)\right\rangle = -\sum_n \left(\frac{1}{2}\,\mathrm{tr}\left[\gamma_5 D_u^{-1}(x \mid 0)\gamma_5 D_u^{-1}(0 \mid x)\right] + \frac{1}{2}\,\mathrm{tr}\left[\gamma_5 D_u^{-1}(x \mid x)\right]\mathrm{tr}\left[\gamma_5 D_u^{-1}(0 \mid 0)\right] + \frac{1}{2}\,\mathrm{tr}\left[\gamma_5 D_u^{-1}(x \mid x)\right]\mathrm{tr}\left[\gamma_5 D_d^{-1}(0 \mid 0)\right]\right) + u \leftrightarrow d$$

Disconnected pieces



Disconnected pieces are typically noisier

They share the same initial and final time

One trick is to compute them on all time-slices and average (translational invariance)

Point-to-all vs all-to-all

This is a common result when dealing with iso-singlet operators

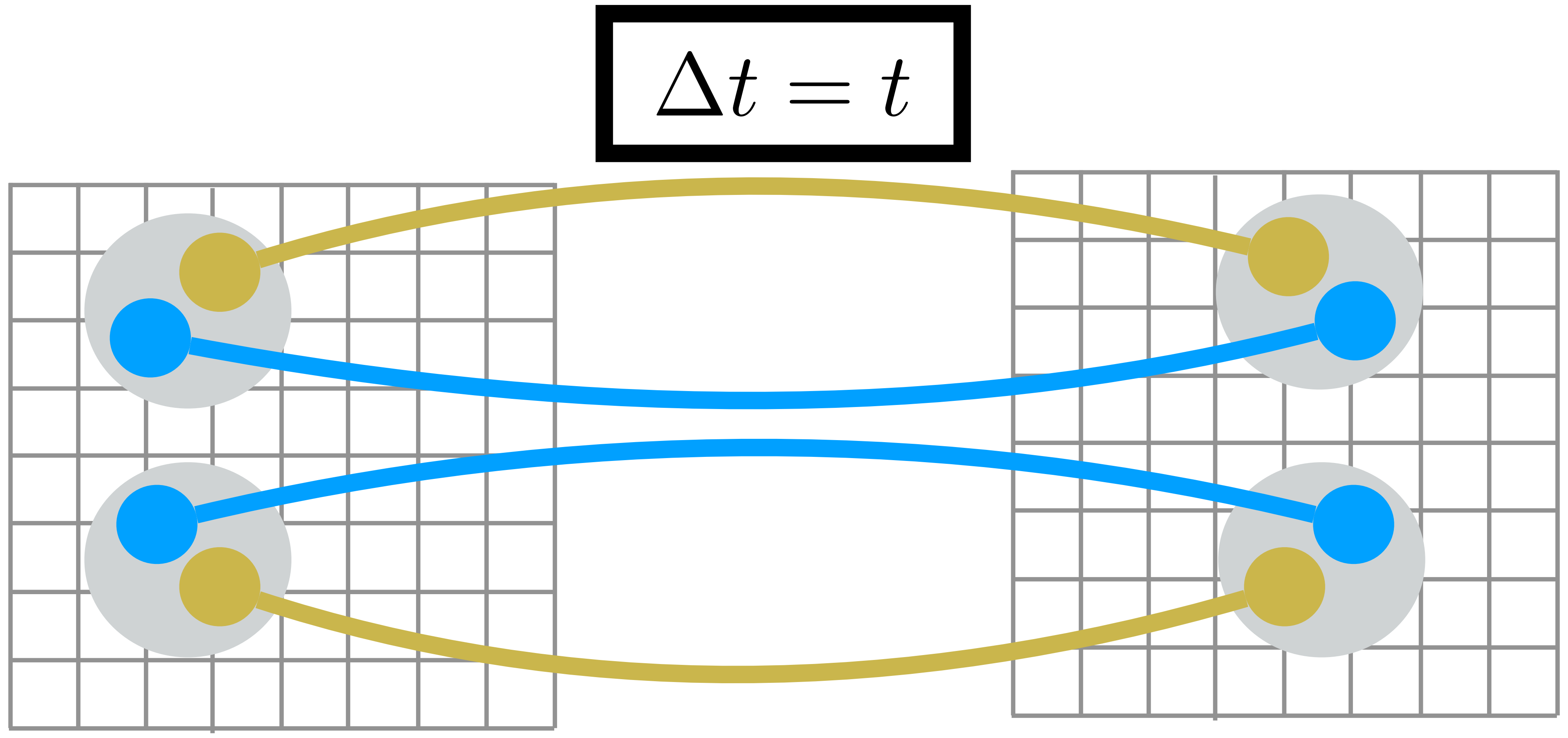
The situation is similar when studying two-pion states

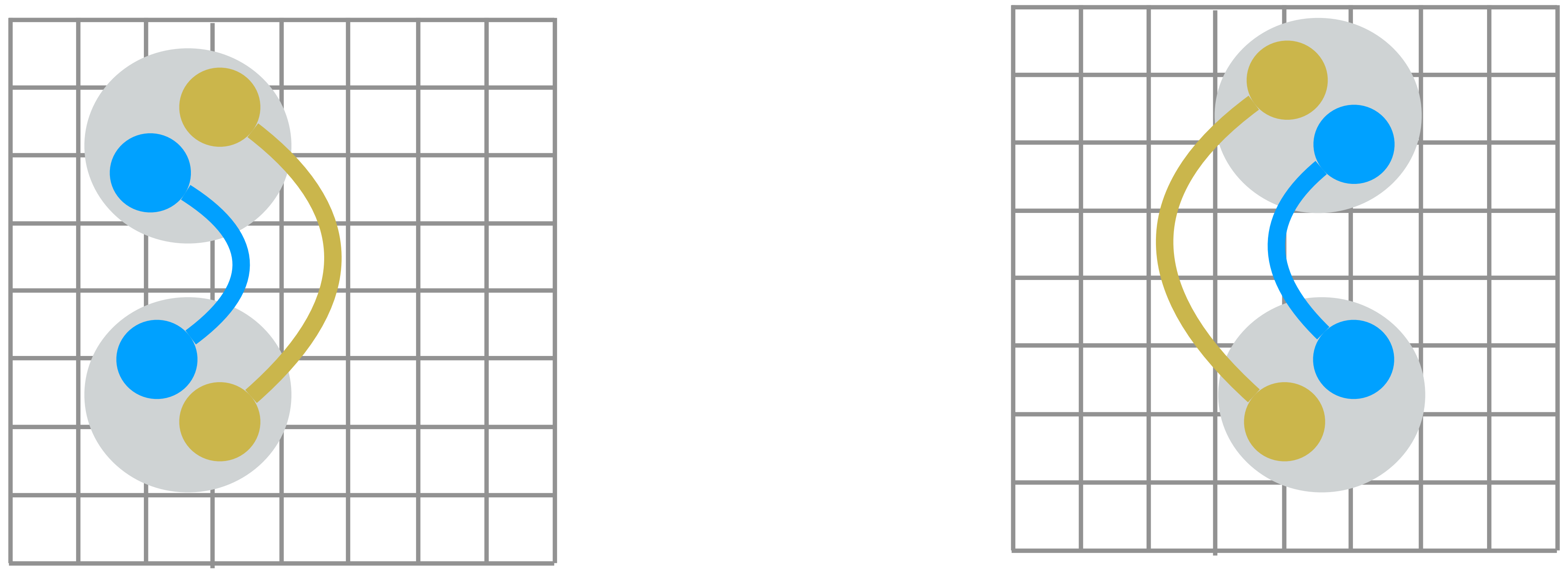
For I=2 scattering, only connected pieces contribute to the contractions

$$\mathcal{O}_{\pi\pi}^{I=2} = \bar{d}\gamma_5 u \bar{d}\gamma_5 u$$

However, I=0 also contains extra disconnected pieces

$$\mathcal{O}_{\pi\pi}^{I=0} = \frac{1}{2}(\bar{u}\Gamma u - \bar{d}\Gamma d)(\bar{u}\Gamma u - \bar{d}\Gamma d)$$





Smearing

We are studying low-energy objects → relatively large distances

Our hadrons are of the order of $\mathcal{O}(1)$ fm

But our operators are based on a local-type construction??

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But our operators are based on a local-type construction??

We will optimize the coupling of our operators to the physics of interest by smearing our constructions

$$\psi(\vec{x},t) = \sum_{\vec{x'}} F(\vec{x},\vec{x'},U(t))\psi(\vec{x'},t)$$

Respect Gauge invariance

We will focus here on Gaussian smearing types

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Smearing

On top of Gauge invariance, we want our operation to have translational, rotational, parity and charge conjugation invariance

$$\psi(\vec{x},t) = \sum_{\vec{x'}} F(\vec{x},\vec{x'},U(t))\psi(\vec{x'},t)$$

Turns out the Laplacian operator fulfills these requirements

$$\nabla^2(\vec{x},\vec{y};t) = -6\delta_{\vec{x},\vec{y}} + \sum_{k=1}^{3}\left(U_k(\vec{x},t)\delta_{\vec{x}+\hat{k},\vec{y}} + U_k^\dagger(\vec{x},t)\delta_{\vec{x}-\hat{k},\vec{y}}\right)$$

A prototypical smearing operator is the "exponentiated", discretized version of the laplacian on the lattice

$$J_{\sigma,n_\sigma}(t) = \left(1 + \frac{\sigma\nabla^2(t)}{n_\sigma}\right)^{n_\sigma}$$

Where

$$\square(t) = \lim_{n_\sigma\to\infty} J_{\sigma,n_\sigma}(t) = \exp\left(\sigma\nabla^2(t)\right)$$

Can we ask for anything else??

Smearing

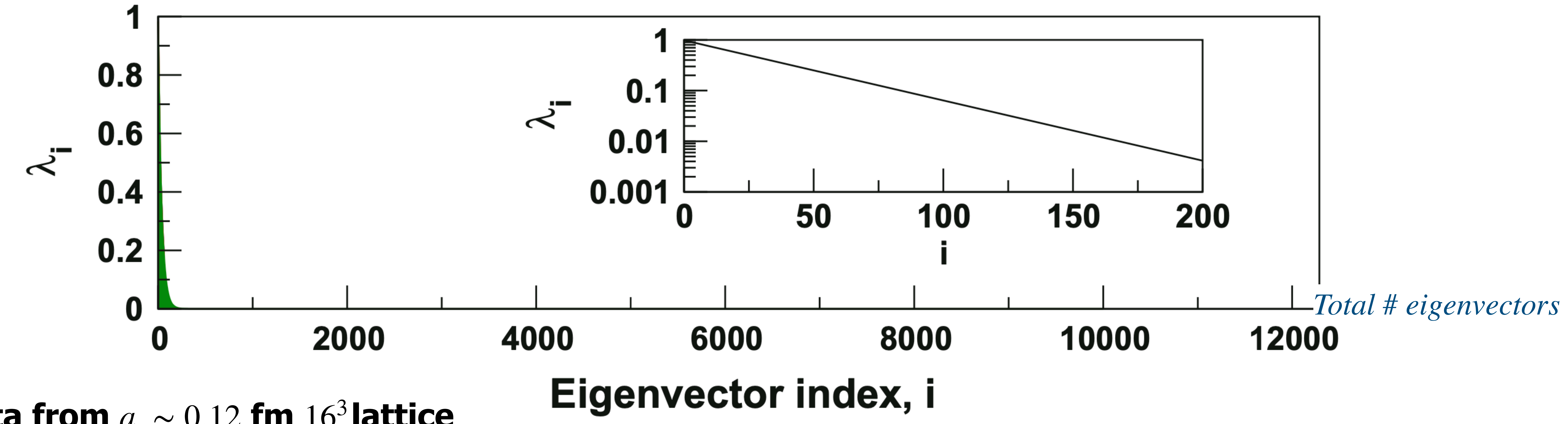
The exponential takes care of the shape of our smeared operator, approximating a gaussian-type line shape of the wave function, centered around $\vec{x}$, the profile also depends on the σ parameter

$$\Box(t) = \lim_{n_\sigma \to \infty} J_{\sigma,n_\sigma}(t) = \exp\left(\sigma \nabla^2(t)\right)$$

Remember that we can represent the operator by its eigenstate decomposition

$$\Box(t) = \sum_i |i\rangle \lambda_i \langle i|$$

Decomposition in space of coloured scalar fields on a time-slice $N_s \times N_c$



Data from $a_s \sim 0.12$ fm 16^3 lattice

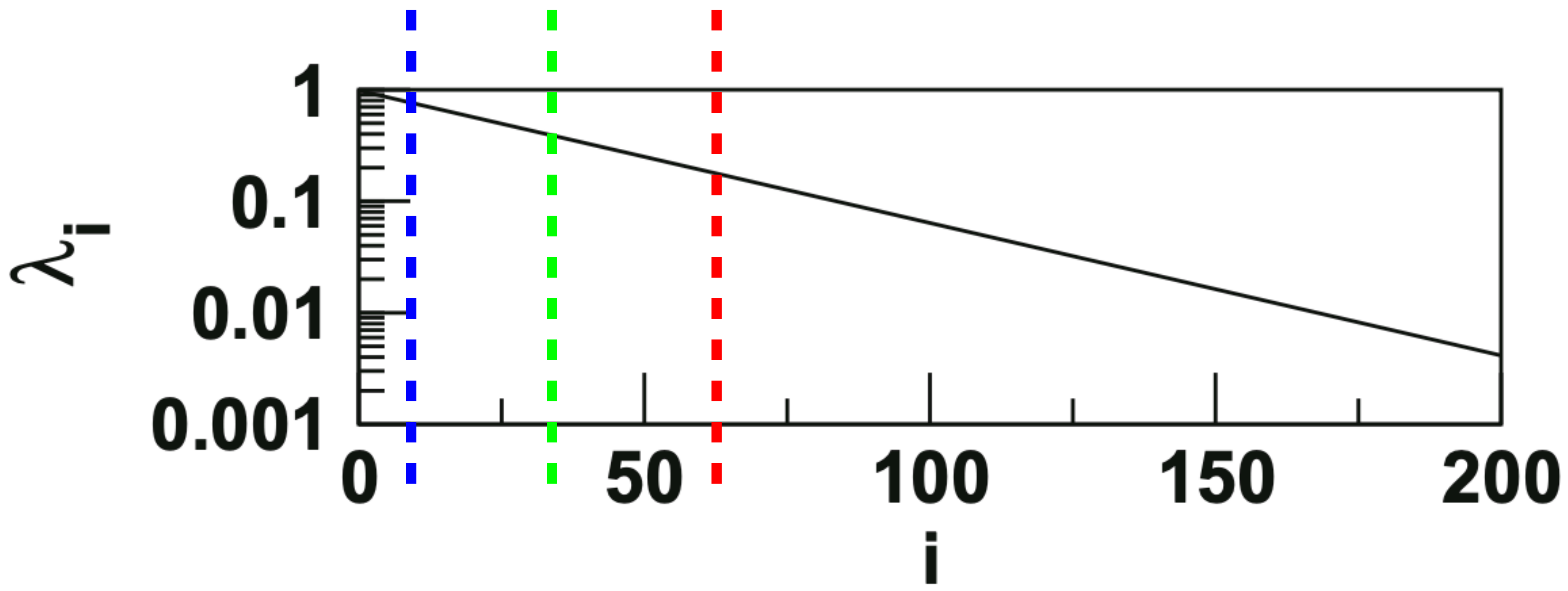
Smearing: Distillation

Phys.Rev.D 80 (2009)

We truncate the eigenvector decomposition to a VERY low number

$$\Box(t) = \sum_{i}^{N_D} |i\rangle \lambda_i \langle i|$$

Where $N_D << N_s \times N_c$



It approximates to a good extent the previous smearing algorithm

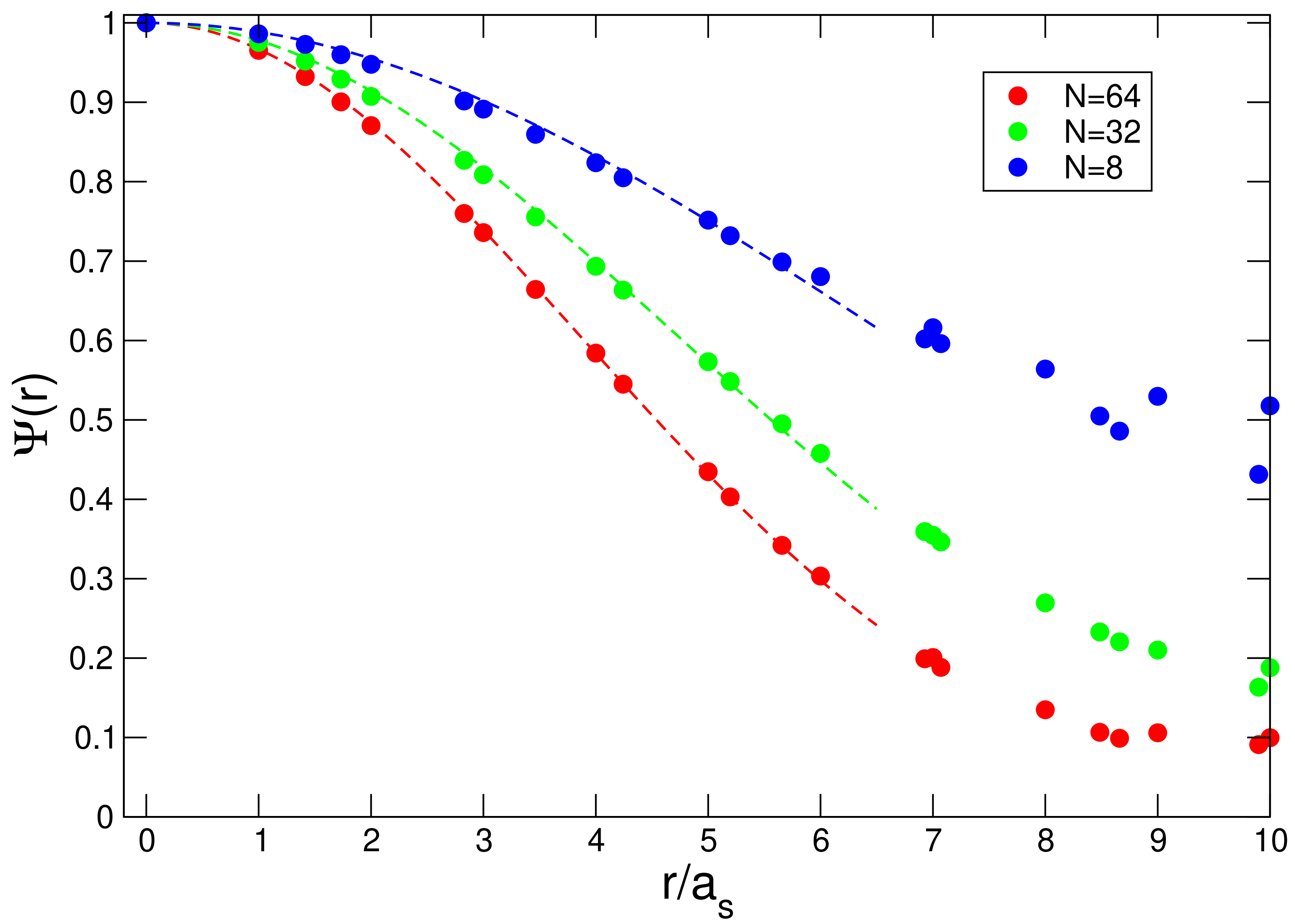
$$\Box(t) = \underline{V(t)}V^\dagger(t)$$

$(N_s \times N_c) \times N_D$

N_D **is now a free parameter we use to produce a sensible linehsape for thewave function**

As N_D **approaches the total number of eigenvectors, the profile approaches a delta**

Why??



Smearing: Distillation

Phys.Rev.D 80 (2009)

Now, we define our operators in the following way

$$O_M(t) = \bar{\tilde{\psi}}^{(f_1)}(t)\Gamma\tilde{\psi}^{(f_2)}(t) \qquad \tilde{\psi}(t) = \Box[t]\psi(t) \qquad \Box(t) = V(t)V^\dagger(t)$$

Our correlation functions are defined accordingly

$$\langle O(t)O^\dagger(0)\rangle = -\sum_n^N \mathrm{tr}\left[\phi(t)\tau_u(t,0)\phi(0)\tau_u(0,t)\right](U_n)$$

Where

$$\phi(t) = V^\dagger(t)\Gamma V(t)$$

Elemental

$$\tau_i(t,t') = V^\dagger(t)D_i^{-1}(t,t')V(t')$$

Perambulator

Now, our correlation functions are much cheaper

$$4 \times \underbrace{3 \times L^3}_{98304} \times T \to 4 \times \underbrace{N_D}_{\sim 100-300} \times T$$

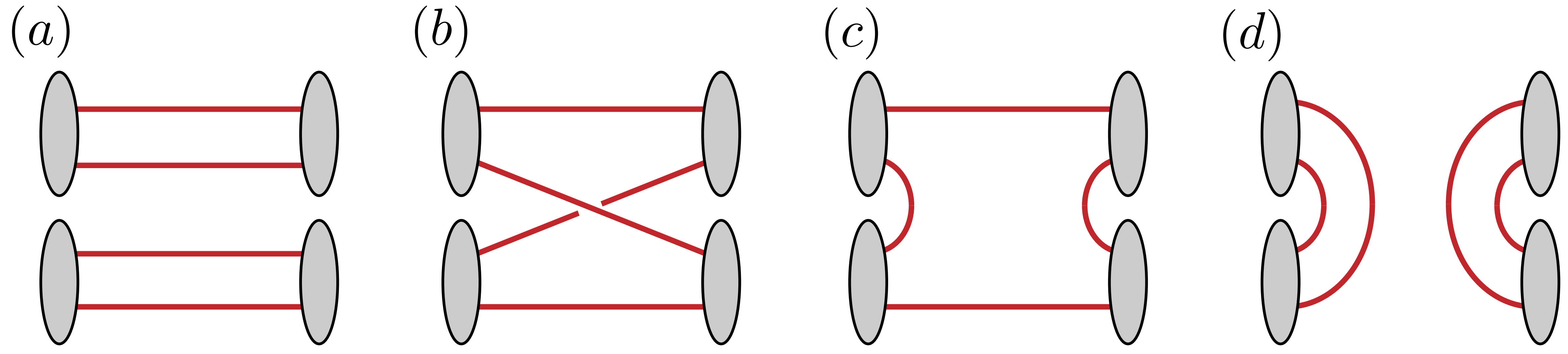
Smearing: Distillation

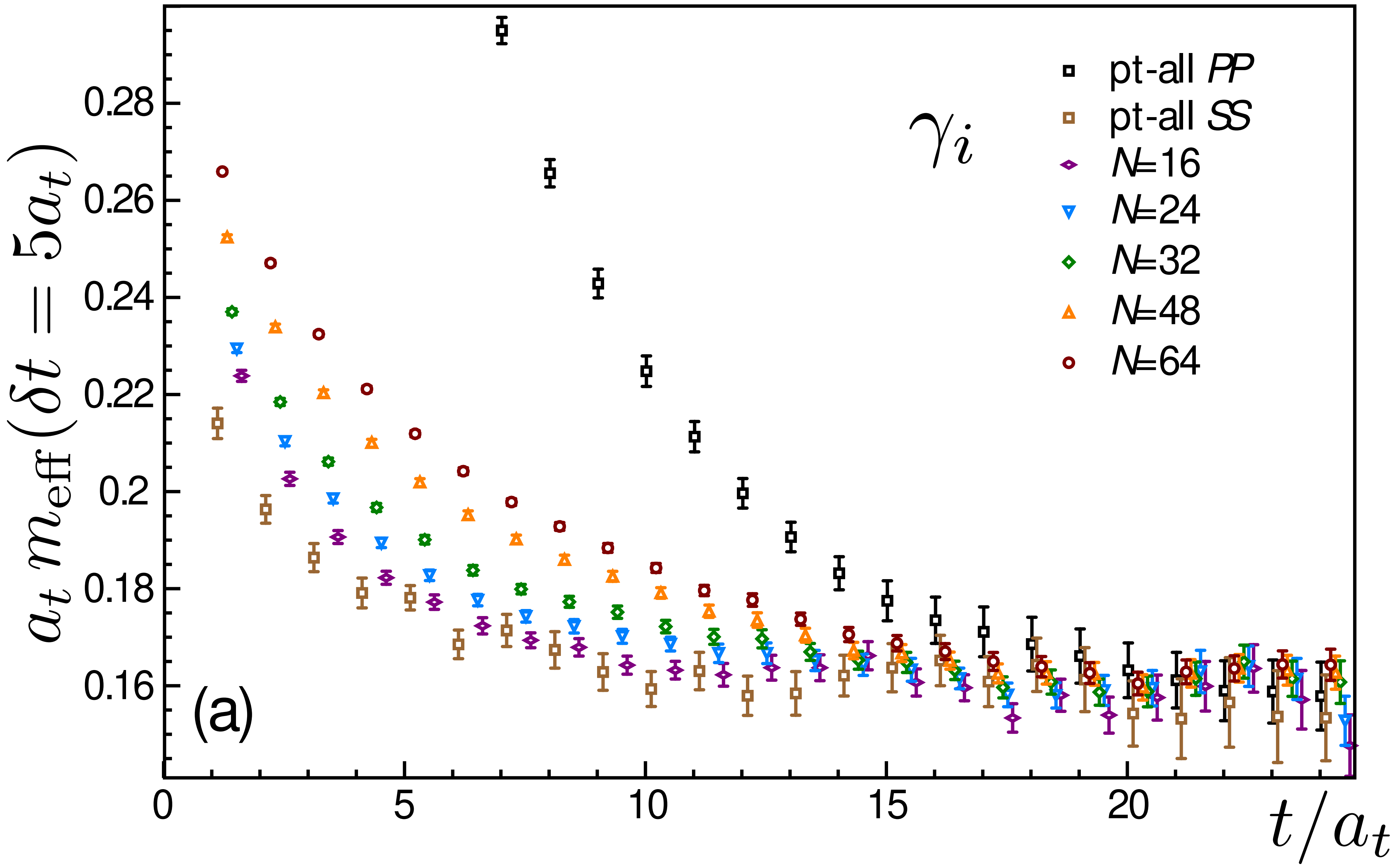
Compare PP (non-smeared) with all the other smearing procedures

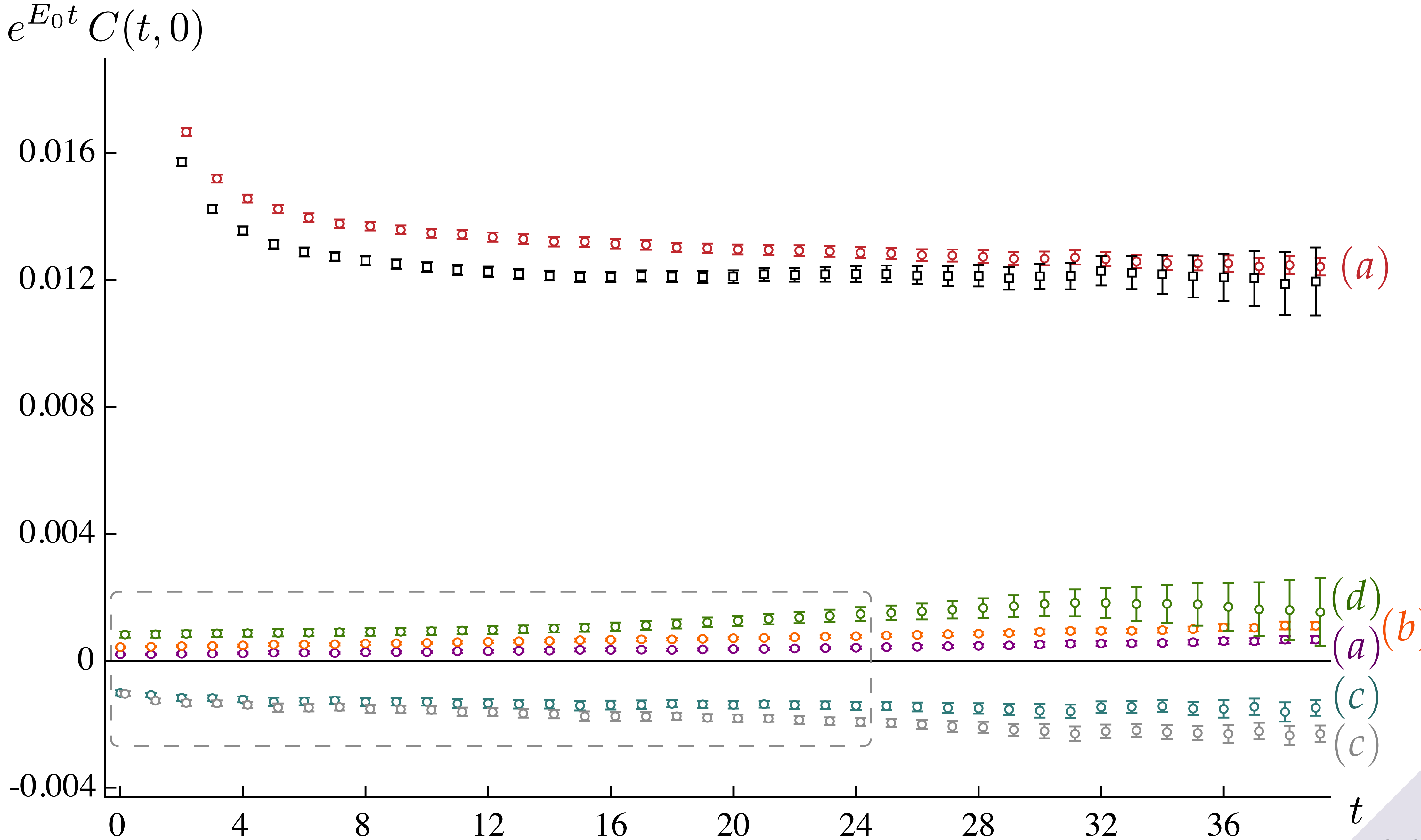
Increasing N_D introduces more ultraviolet effects, but increases the precision around the plateau

Setting N_D is a balancing game

As discussed, Wick contractions for I=0 $\pi\pi$ scattering include disconnected pieces, which we compute in full using distillation

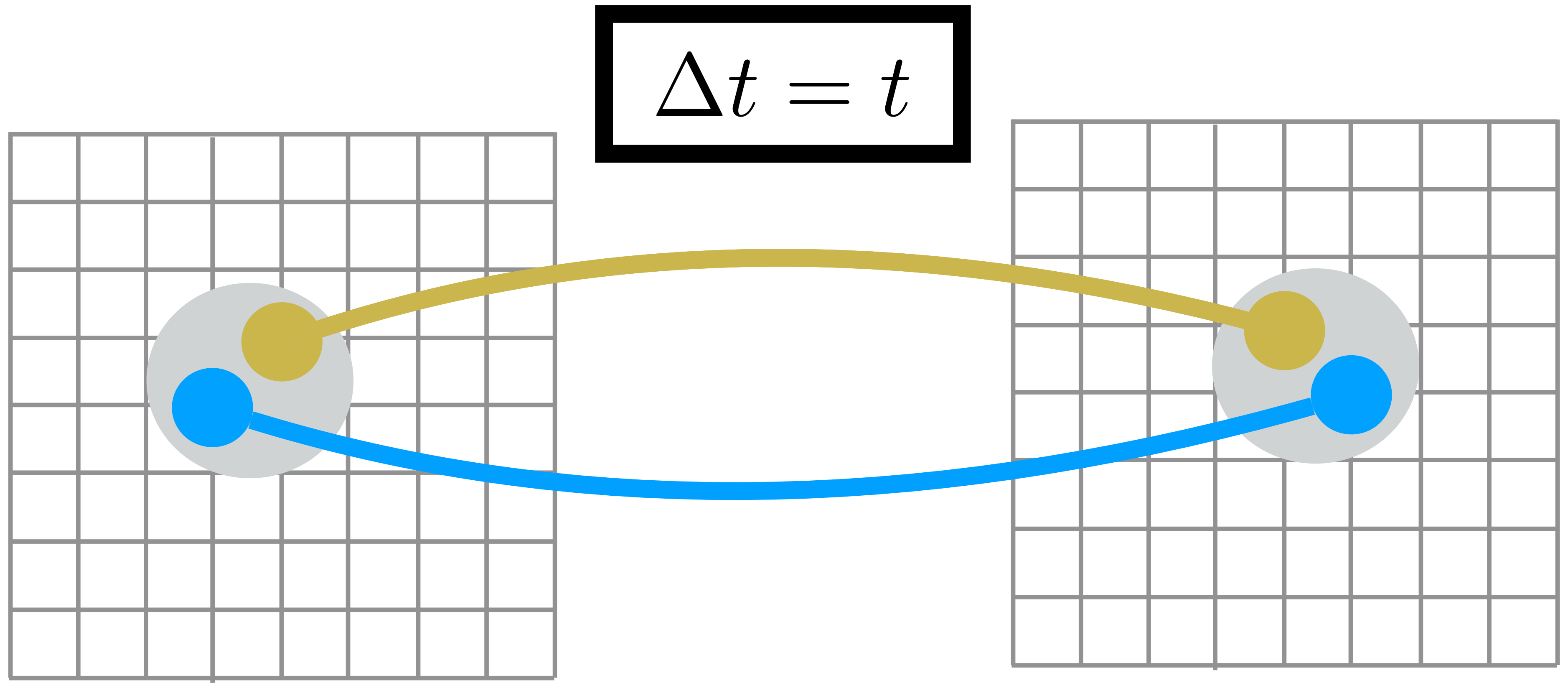






Questions?

Pions on the lattice



Lets study the temporal evolution of a single particle

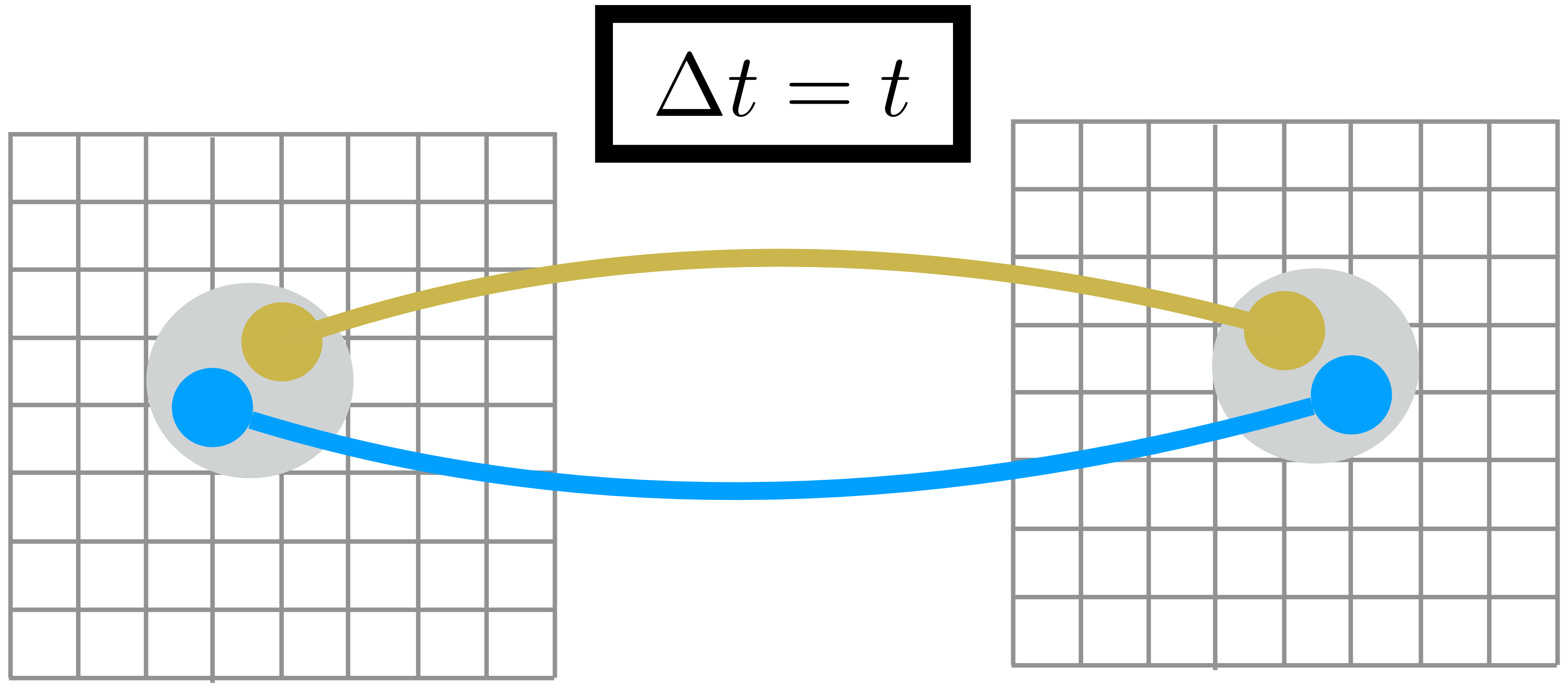
$$C(t) \equiv \langle 0 | \mathcal{O}(t) \mathcal{O}^\dagger(0) | 0 \rangle$$

Basis

$$= \sum_n \langle 0 | \mathcal{O}(t) | n \rangle \langle n | \mathcal{O}^\dagger(0) | 0 \rangle$$

$$\rightarrow e^{-iHt_M/\hbar}$$

Pions on the lattice



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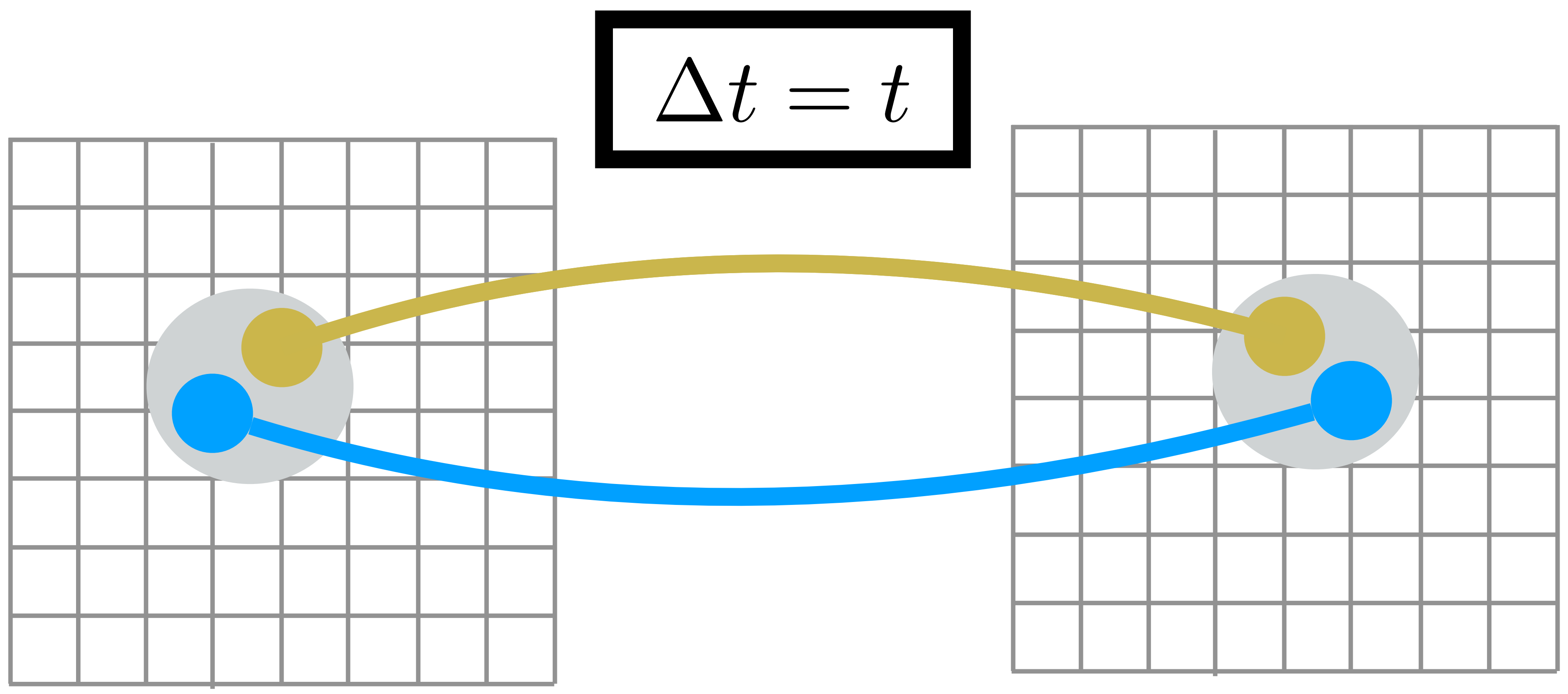
Euclidean time

$$= \sum_n A_n e^{-E_n t}$$

Pions on the lattice



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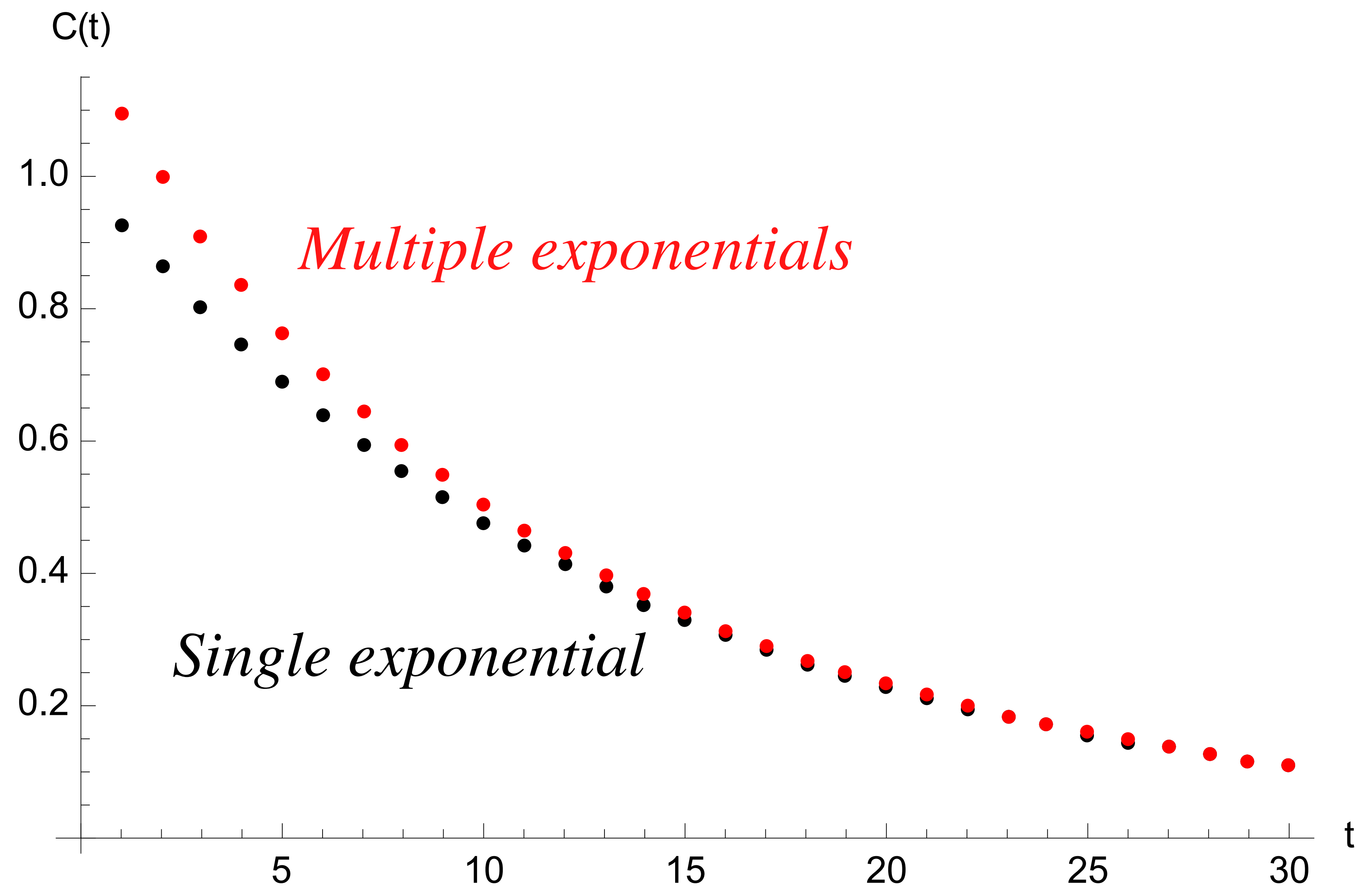
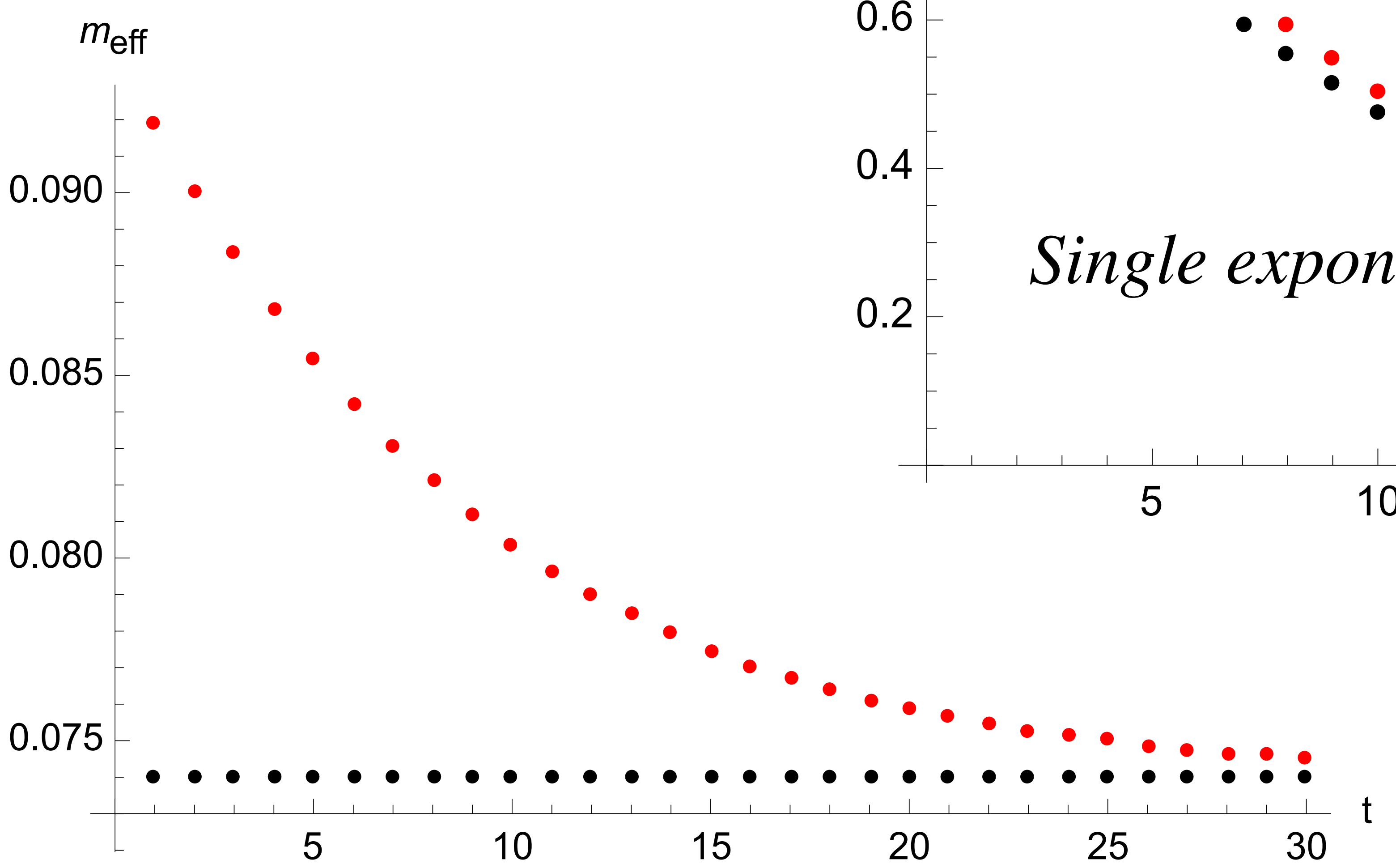
Afternoon…



We determine these energies from fitting the temporal evolution of the system

$$m_{\text{eff}} = log\left[\frac{C(t)}{C(t+1)}\right]$$

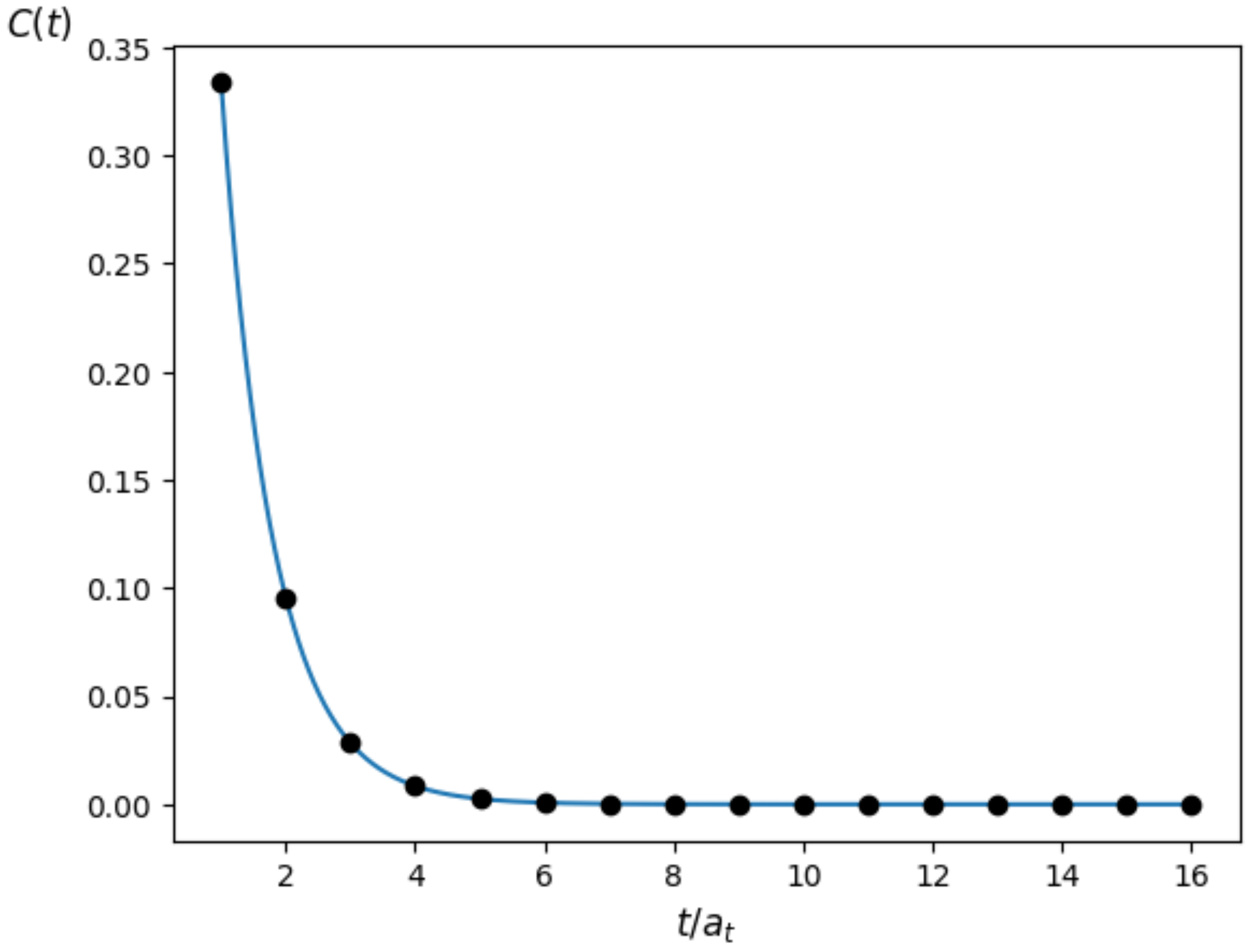


Tomorrow…

Signal-to-noise ratio

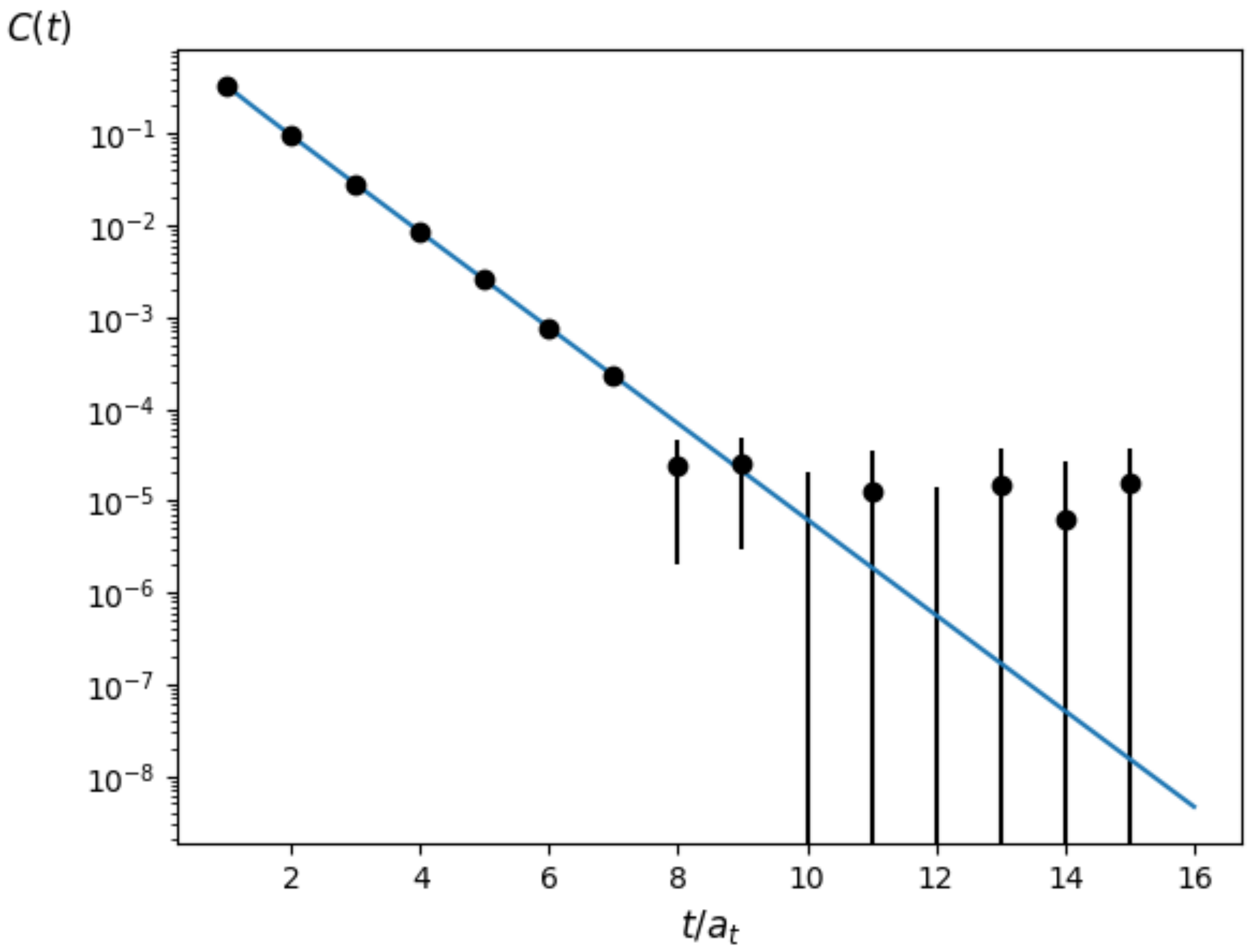
For a correlator, the signal decreases exponentially

This one looks incredibly precise



The error decreases at best (only for π), at same speed

In any practical calculation, the data becomes noisy, pretty early



We define the signal-to-noise value by using simple averages and variances

$$\mathrm{StN}(\mathcal{O}) = \frac{\langle \mathcal{O} \rangle}{\sqrt{\mathrm{Var}(\mathcal{O})}}$$

If StN is lower than 1, then the error is greater than the value, we lost all signal

Signal-to-noise ratio

Remember that for us, the observables are correlation functions

$$\langle \mathcal{O} \rangle \equiv \langle \mathcal{O}(t)\mathcal{O}^\dagger(0)\rangle \qquad Var(\mathcal{O}) = \langle |\mathcal{O}|^2\rangle - \langle \mathcal{O}\rangle^2$$

By definition

$$|\mathcal{O}|^2 = \mathcal{O}\mathcal{O}^*$$

For mesons, the signal decreases with the ground state mass

$$\langle \mathcal{O} \rangle \sim e^{-m_M t}$$

The variance, $|\mathcal{O}|^2 = \mathcal{O}\mathcal{O}^*$ **can contain operators that couple to two pions**

Why??

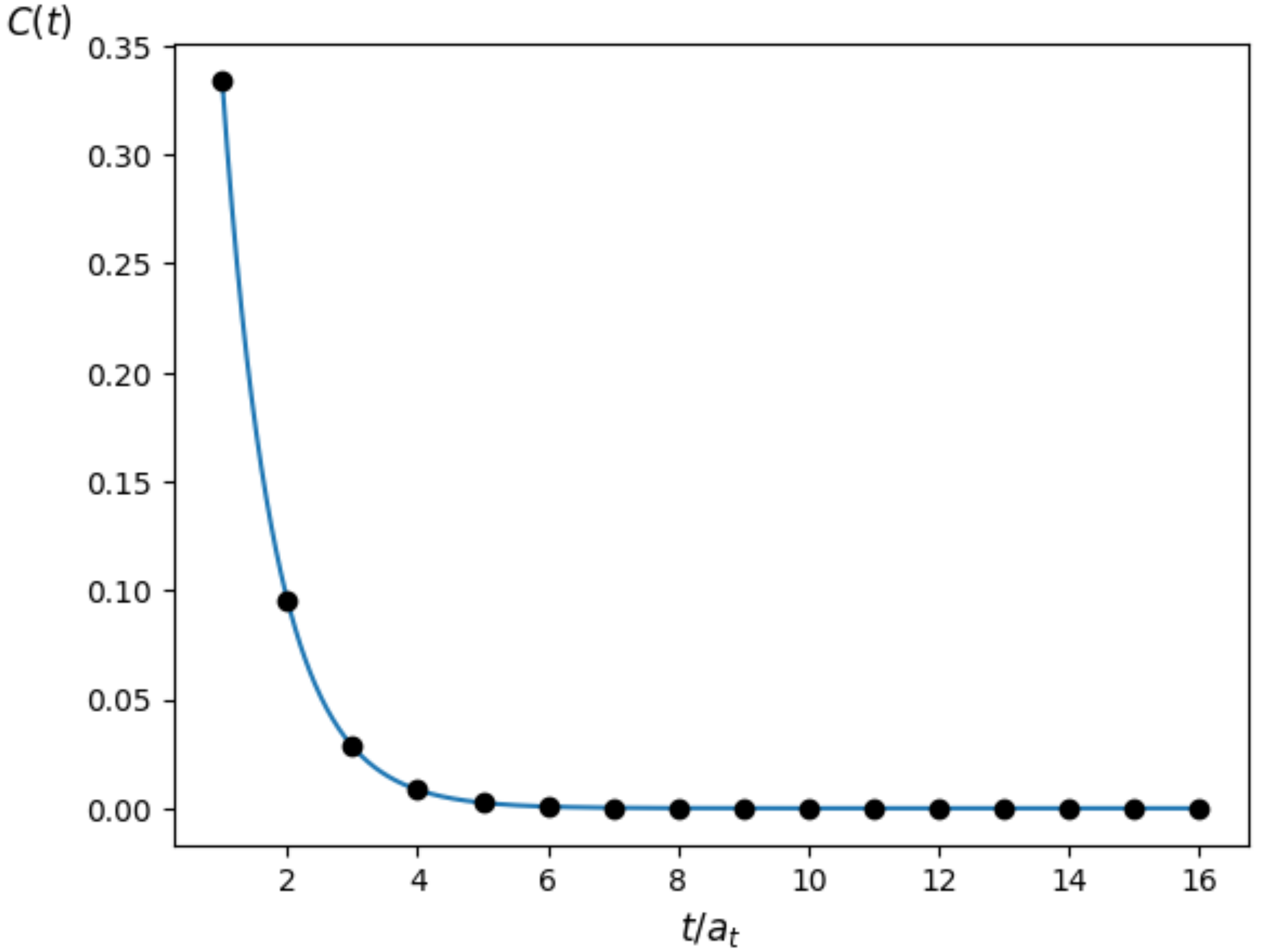
$$\langle |\mathcal{O}|^2 \rangle \sim e^{-2m_\pi t}$$

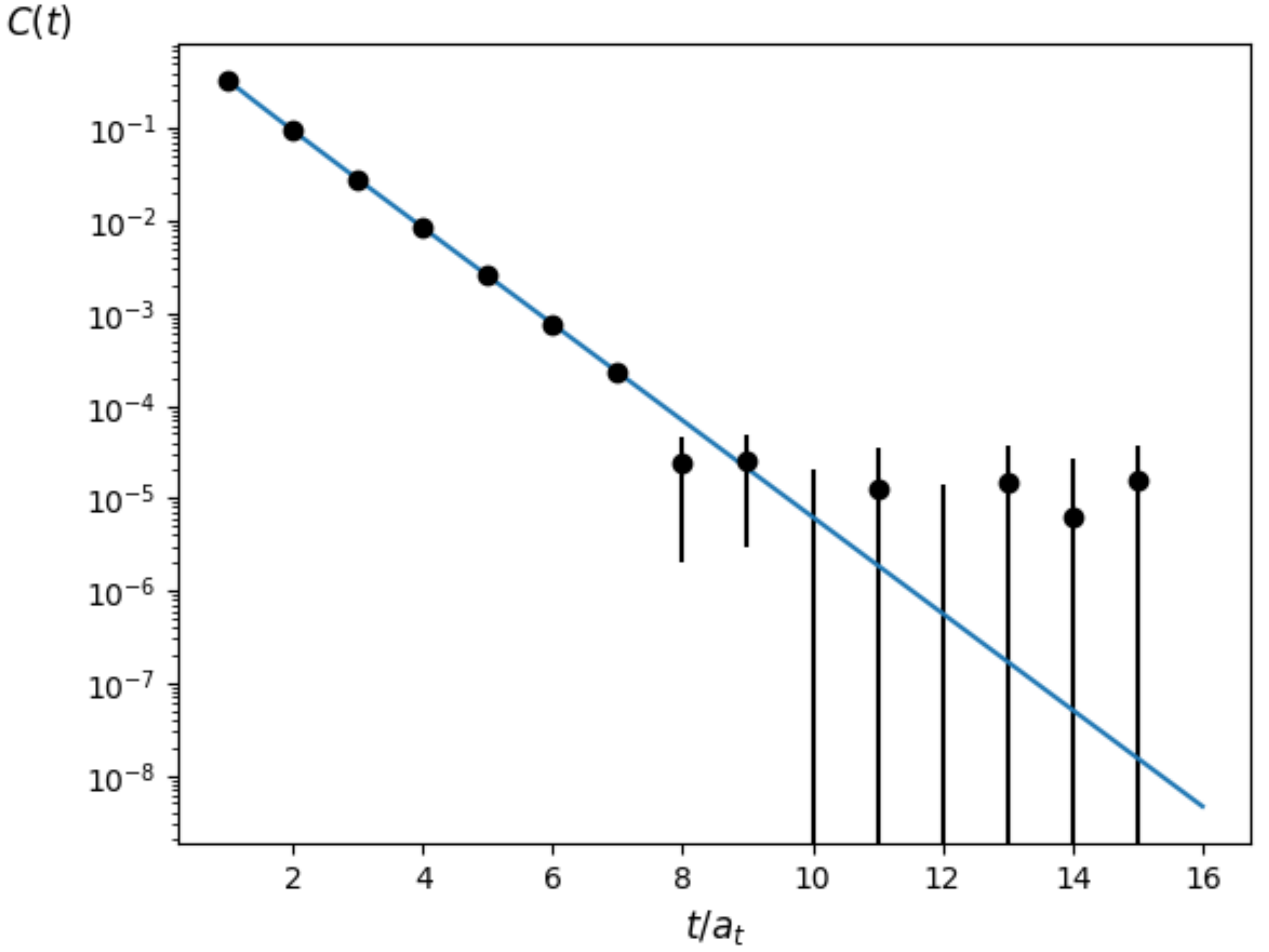
All in all, for mesons the ratio decreases like

$$\mathrm{StN}(\mathcal{O}) \sim \exp\left[-\left(m_M - m_\pi\right) t\right]$$

For baryons, the situation is only slightly different

$$\mathrm{StN}(\mathcal{O}) \sim \exp\left[-\left(m_B - (3/2)m_\pi\right) t\right]$$





2-pt correlation fitting

How would we naively fit the correlation function?

$$\chi^2 = \sum_i \left(\frac{C(t_i) - f(\mathbf{a}^\star, t_i)}{\Delta C(t_i)} \right)^2 \qquad f(\mathbf{a}^\star, t) = \sum_n A_n \exp(-E_n t)$$

However, in this case, all our values at different times come from the same Montecarlo samples

Think about samples U_n as the main variable now

If our the distance between two times is small (small spacing a) then the value of the correlation function must be similar

$$C(t_1)(U_n) \sim C(t_2)(U_n)$$

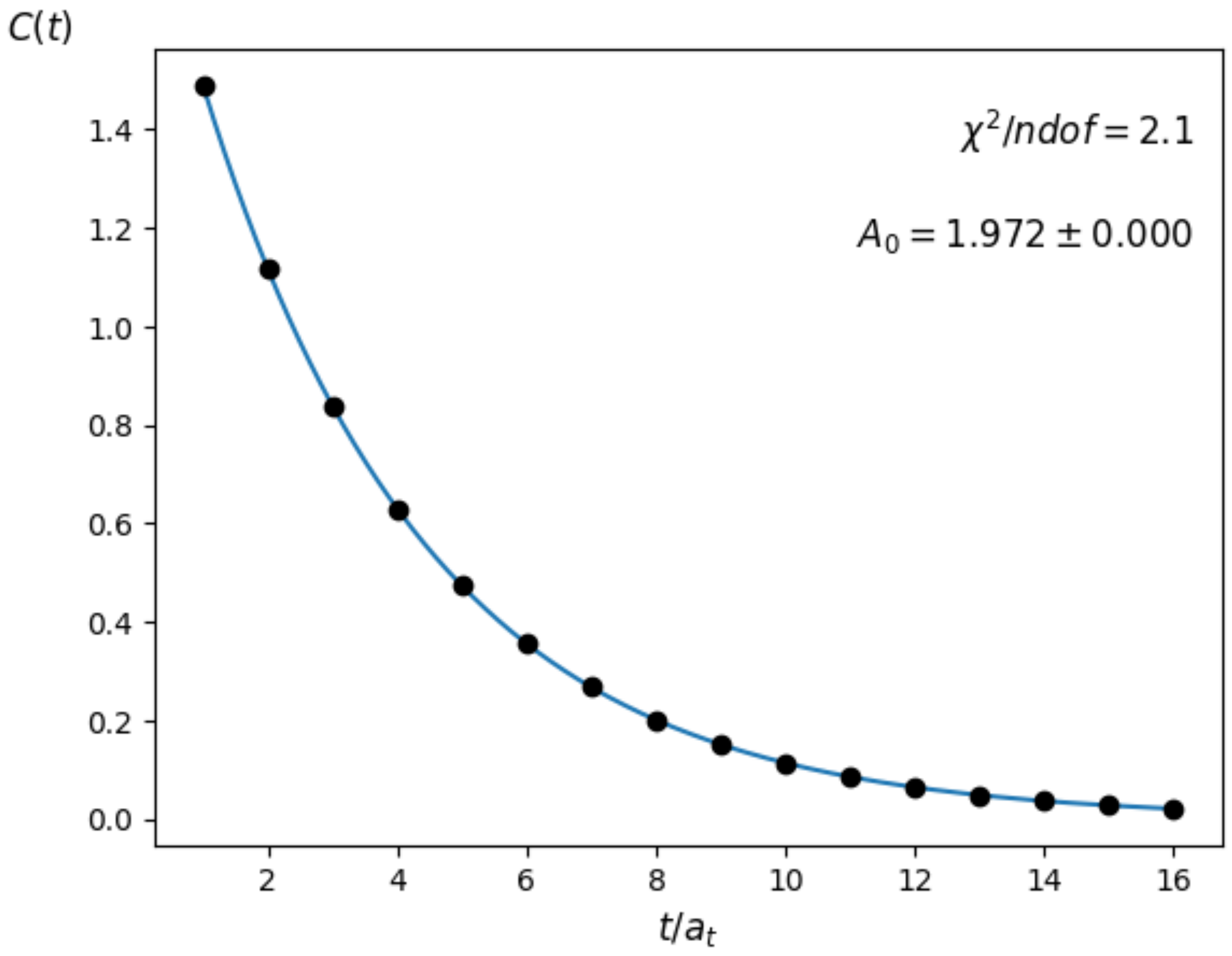
Data IS correlated

$$\Sigma_{ij} = Cov(t_i, t_j) \neq 0$$

We therefore modify our penalty function to account for this

$$\chi^2 = \sum_{i,j} (C(t_i) - f(\mathbf{a}^\star, t_i)) \Sigma_{ij}^{-1} (C(t_j) - f(\mathbf{a}^\star, t_j))$$

2-pt correlation fitting



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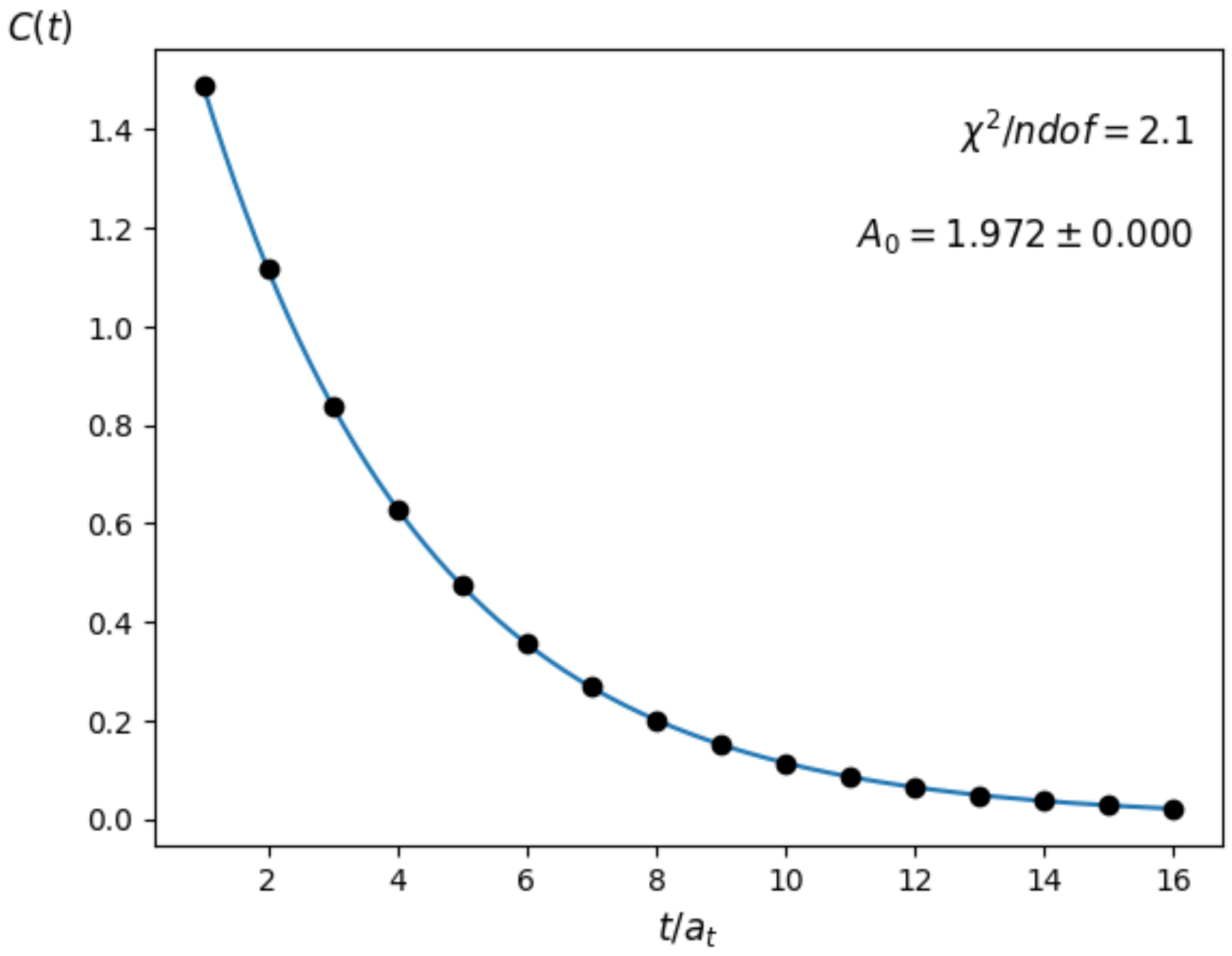
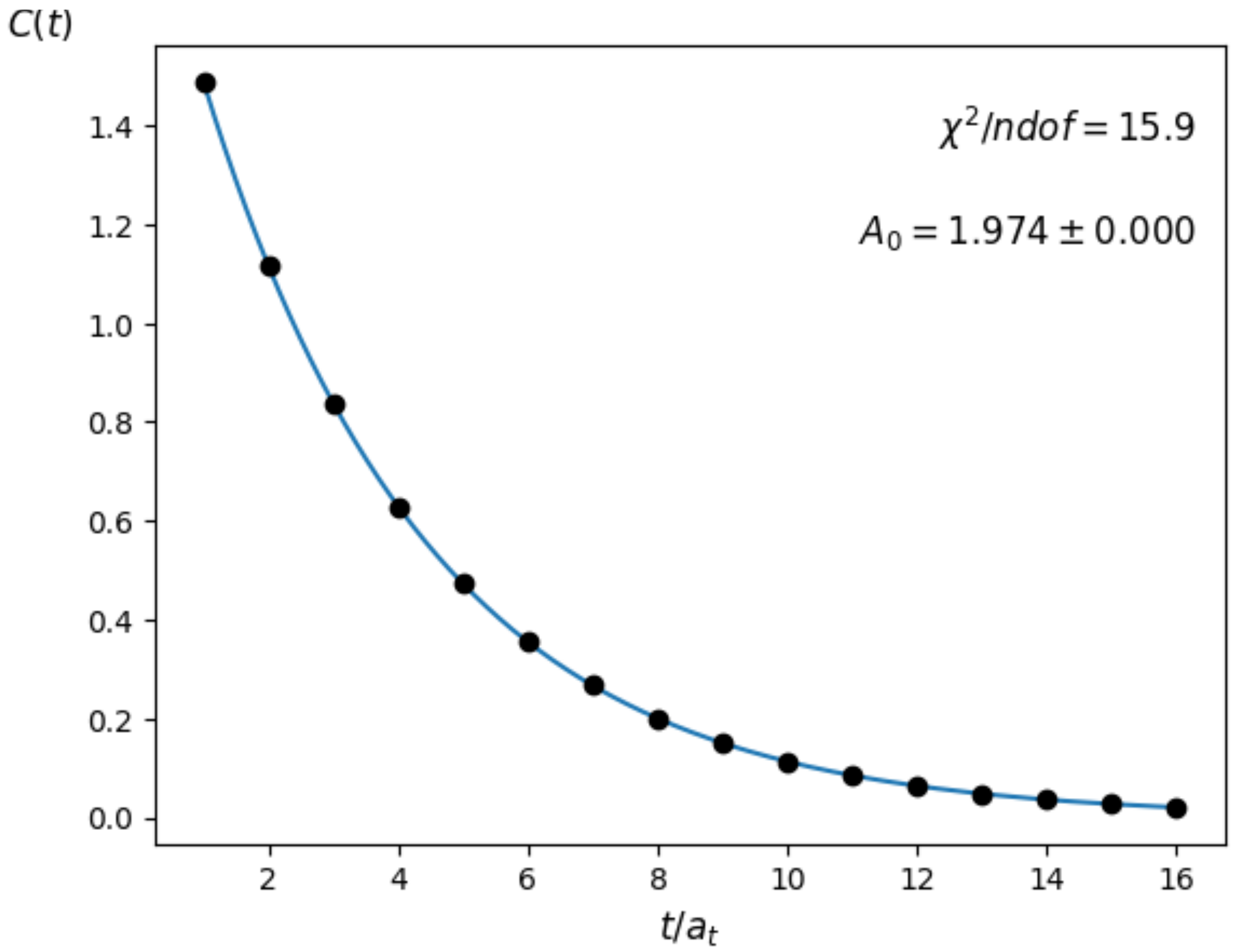




2-pt correlation fitting: Statistics

How do we estimate errors and correlations of observables

Remember our inputs are discretized sampled numbers (they come without errors)

Average $$\langle C(t)\rangle = \frac{1}{N}\sum_{i=1}^{N} C(t)_i$$

Error of the average $$\Delta\langle C(t)\rangle = \frac{\left\langle C(t)^2\right\rangle - \langle C(t)\rangle^2}{N-1}$$

Covariance $$Cov(t_i, t_j) = \frac{1}{N(N-1)}\sum_{n=1}^{N}\left(C(t_i)_n - \langle C(t_i)\rangle\right)\left(C(t_j)_n - \langle C(t_j)\rangle\right)$$

How do we estimate unbiased error propagation?

Function f *Parameters* $\mathbf{a}^\star \quad \Delta\mathbf{a}^\star$

Central value $f(\mathbf{a}^\star)$

Errors (correlated) $$\Delta f(\mathbf{a}^\star)^2 = \sum_{ij}\frac{\partial f(\mathbf{a}^\star)}{\partial a_i}\underline{Cov_{ij}}\frac{\partial f(\mathbf{a}^\star)}{\partial a_j}$$

Parameter fit covariance

2-pt correlation fitting: Jackknife

How do we estimate unbiased error propagation?

Central value $f(\mathbf{a}^\star)$

Errors (correlated) $$\Delta f(\mathbf{a}^\star)^2 = \sum_{ij} \frac{\partial f(\mathbf{a}^\star)}{\partial a_i} Cov_{ij} \frac{\partial f(\mathbf{a}^\star)}{\partial a_j}$$

How to do this based on our samples? → Jackknife

Jackknife samples from raw samples $$\widehat{C(t)}_n = \frac{1}{N-1}\sum_{i\neq n}^{N} C(t)_i = \langle C(t)\rangle - \frac{\langle C(t)\rangle - C(t)_n}{N-1}$$

Average is preserved $$\langle C(t)\rangle = \frac{1}{N}\sum_{i=1}^{N}\widehat{C(t)}_i = \langle C(t)\rangle = \frac{1}{N}\sum_{i=1}^{N} C(t)_i$$

Covariance of averages from Jackknife $$Cov(t_i, t_j) \equiv \Sigma_{ij} = \frac{N-1}{N}\sum_{n=1}^{N}\left(\widehat{C(t_i)}_n - \langle C(t_i)\rangle\right)\left(\widehat{C(t_j)}_n - \langle C(t_j)\rangle\right)$$

2-pt correlation fitting: Jackknife

How to do this based on our samples? → Jackknife

Returning to raw samples

$$C(t)_n = \widehat{C(t)}_n + N(\langle C(t)\rangle - \widehat{C(t)}_n)$$

How does it work?

Start with a collection of raw parameters and produce the Jackknife samples $(\mathbf{a}^\star)_i \to \widehat{\mathbf{a}^\star}_n$

Obtain the Jackknife sample for the function $\widehat{f\left(\mathbf{a}^\star\right)}_n = f\left(\widehat{\mathbf{a}^\star}_n\right)$

Best fit $f\left(\mathbf{a}^\star\right) = \left\langle \widehat{f\left(\mathbf{a}^\star\right)}_n \right\rangle$

Errors $\Delta f(\mathbf{a}^\star)^2 = \dfrac{N-1}{N}\sum_n (\widehat{f(\mathbf{a}^\star)}_n - f(\mathbf{a}^\star))^2$

Do not confuse this sampling procedure with experimental data resampling

The procedures are not the same

Experimental data resampling propagates bias

2-pt correlation fitting: Jackknife

Why does it work so well?

Note that (single parameter) $\hat{\mathbf{a}}_n \sim \mathbf{a} + \Delta\mathbf{a}/\sqrt{N}$

$$\widehat{f(\mathbf{a})}_n^2 - f(\mathbf{a})^2 \sim f'(\mathbf{a})\Delta\mathbf{a}/\sqrt{N}$$

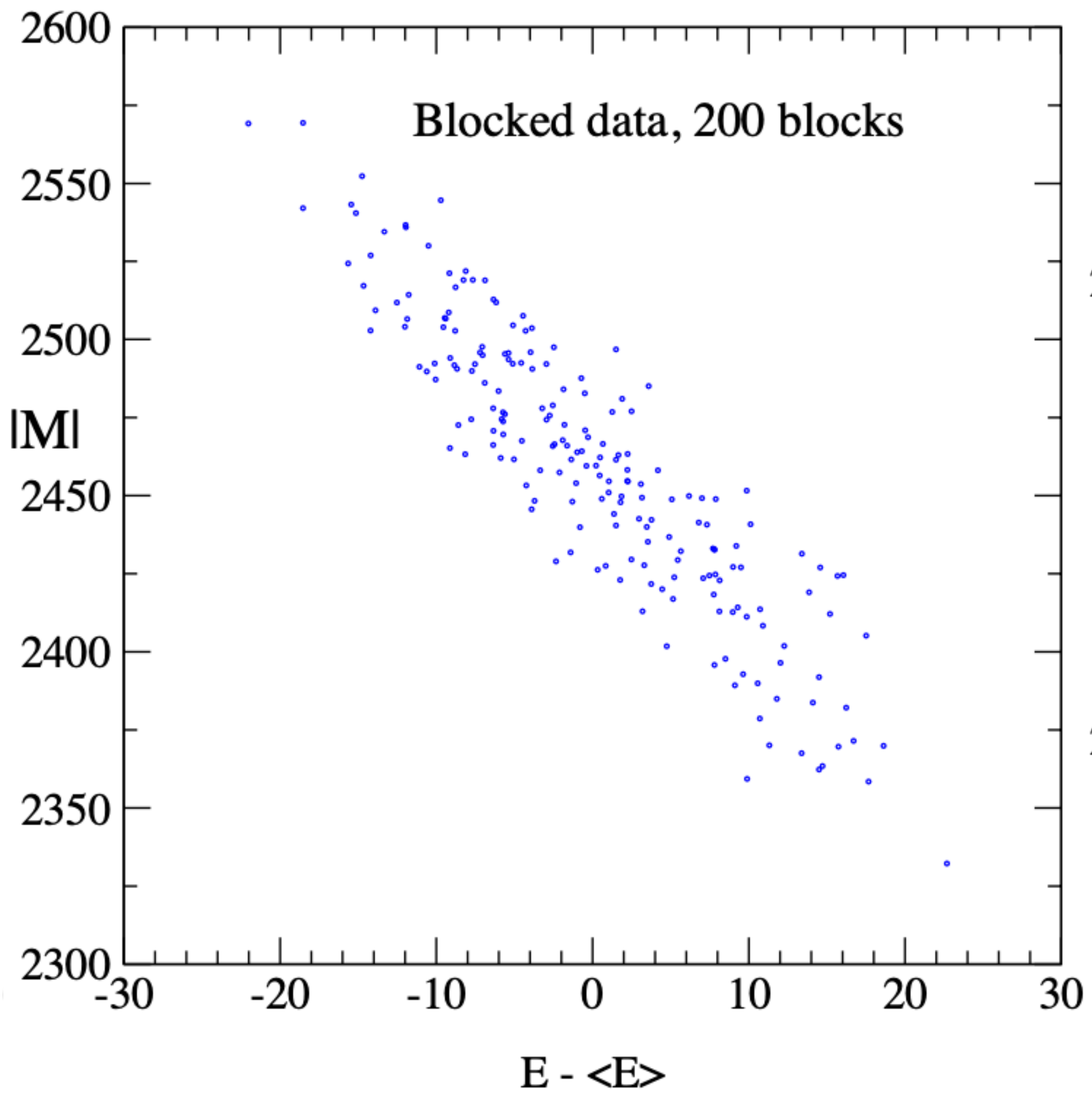
In which case

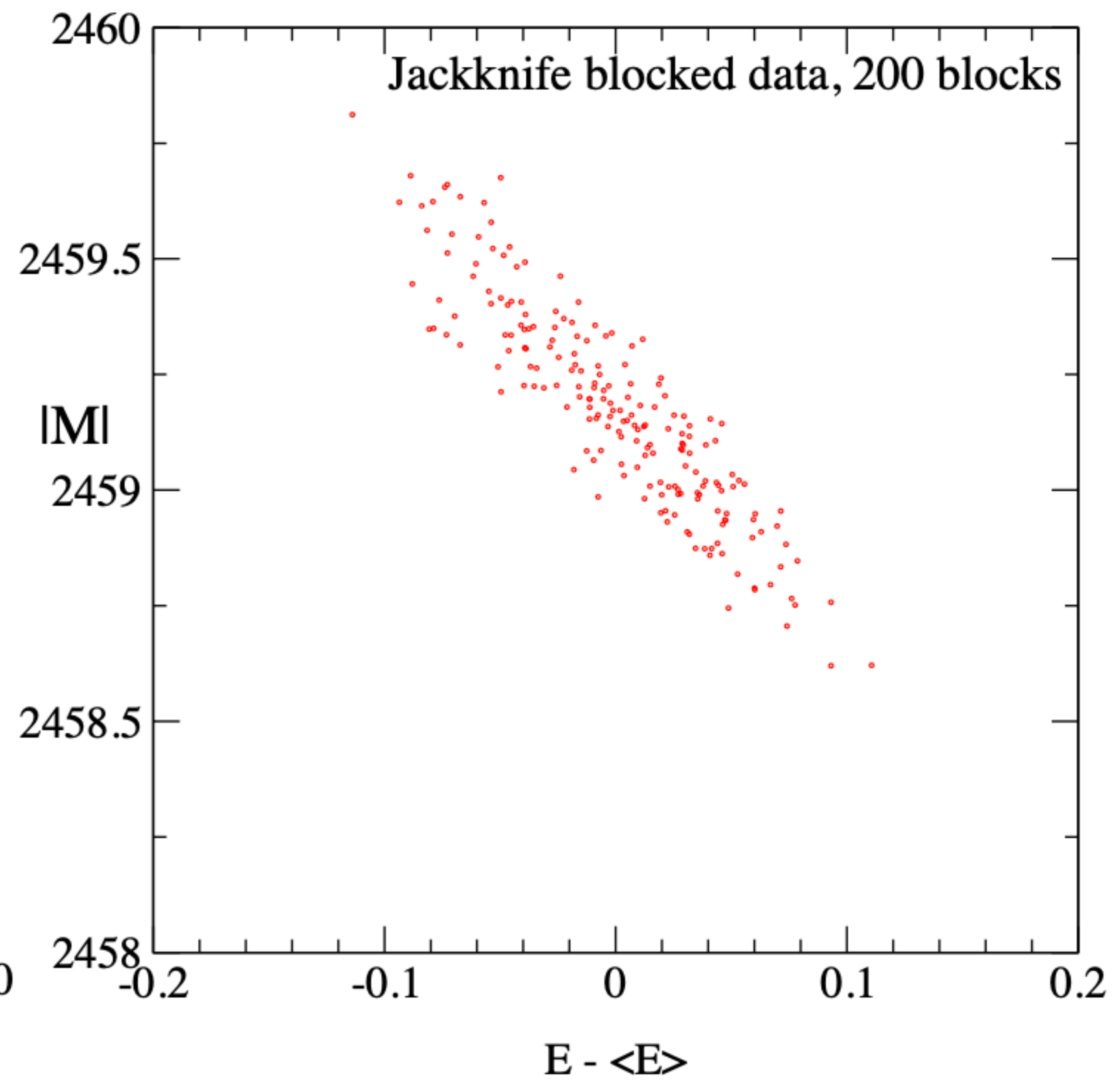
$$\Delta f(\mathbf{a})^2 = \frac{N-1}{N}\sum_n (\widehat{f(\mathbf{a})}_n - f(\mathbf{a}))^2 \sim |f'(\mathbf{a})|^2 \, \Delta\mathbf{a}^2$$

The Jackknife samples accumulate around the central value of the sample

1- Get Jackknife samples from raw data

2- Perform full analysis based on these samples





2-pt correlation fitting: Jackknife

What if I have to perform fits to these samples?

Our penalty function varies

$$\widehat{\chi}^2_n = \sum_{i,j} \left(\widehat{C\left(t_i\right)}_n - f\left(\mathbf{a}^\star, t_i\right) \right) \Sigma^{-1}_{ij} \left(\left(\widehat{C\left(t_j\right)}_n - f\left(\mathbf{a}^\star, t_j\right) \right) \right.$$

We "freeze" the covariance to the one of the full sample. It reduces the bias

These sample penalty functions relate to the full penalty function as

Jackknife $$\sum_n \widehat{\chi}^2_n = \frac{d-k}{(N-1)} + \chi^2$$

Original $$\sum_n \chi^2_n = (N-1)(d-k) + \chi^2$$

So, what about the parameter values and errors

On a single fit to data, the minimizer provides central values AND errors $\chi^2 \to \mathbf{a}^\star$

When using resampling methods, we forget about the errors from the minimizer $\widehat{\chi}^2_n \to \widehat{\mathbf{a}^\star}_n$

Central value is obtained as the mean of the Jackknifes $$\langle \mathbf{a}^\star \rangle = \frac{1}{N} \sum_{i=1}^{N} \widehat{\mathbf{a}^\star}_i$$

Covariances are obtained from the master formula

$$Cov(\mathbf{a}^\star(i), \mathbf{a}^\star(j)) = \frac{N-1}{N} \sum_{n=1}^{N} \left(\widehat{\mathbf{a}^\star(i)}_n - \langle \mathbf{a}^\star(i) \rangle \right) \left(\widehat{\mathbf{a}^\star(j)}_n - \langle \mathbf{a}^\star(j) \rangle \right)$$

2-pt correlation fitting: Bootstrap

This time, we do resampling with repetition, where K is not necessarily N

$$\widehat{C(t)}_n = \frac{1}{K}\sum_{i\neq n}^{K} C(t)_i$$ *This values are taken randomly from the sample, repetition is allowed*

The errors are similar to the raw sample case

$$\Sigma_{ij} = \frac{1}{M}\sum_{n=1}^{M}\left(\widehat{C\left(t_i\right)}_n - \langle C\left(t_i\right)\rangle\right)\left(\widehat{C\left(t_j\right)}_n - \langle C\left(t_j\right)\rangle\right)$$

The variance over the bootstrap is the variance of the mean value $\Sigma_{ii} = \sigma_i^2 = \sigma_{mean}^2$

The bootstrap allows for calculations of confidence intervals (these are biased estimators)

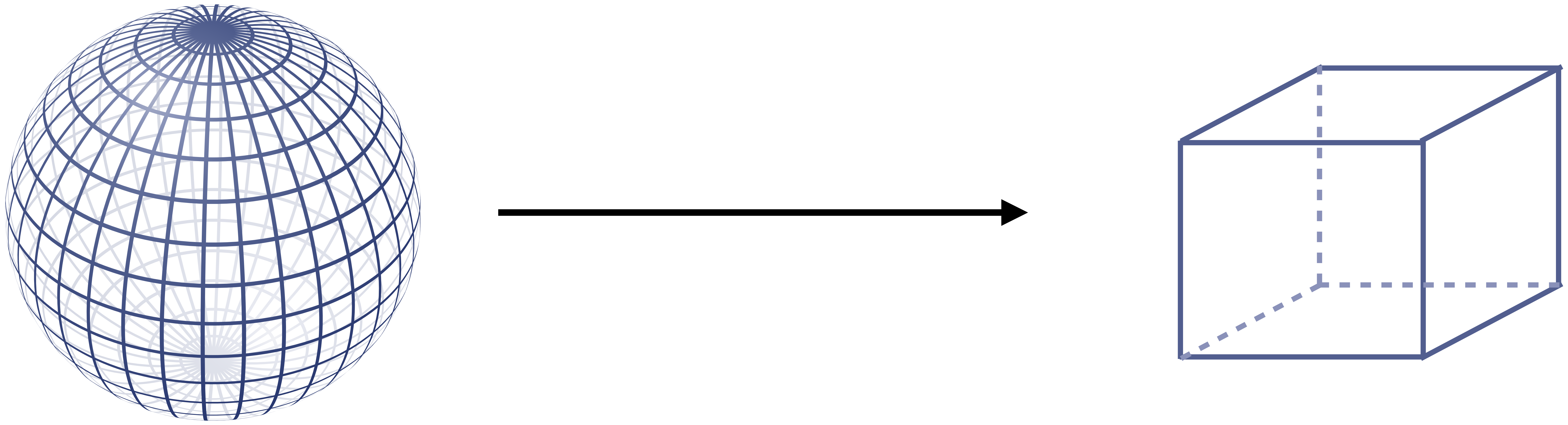
Questions? — Some water?

Next: Finite-volume symmetry!

Finite-volume symmetry: Cubic vs Spherical

Our universe is spherical, we have continuous, scalar rotational invariance

Our lattices are boxes in L^3, we cannot leave the box invariant with any type of rotation

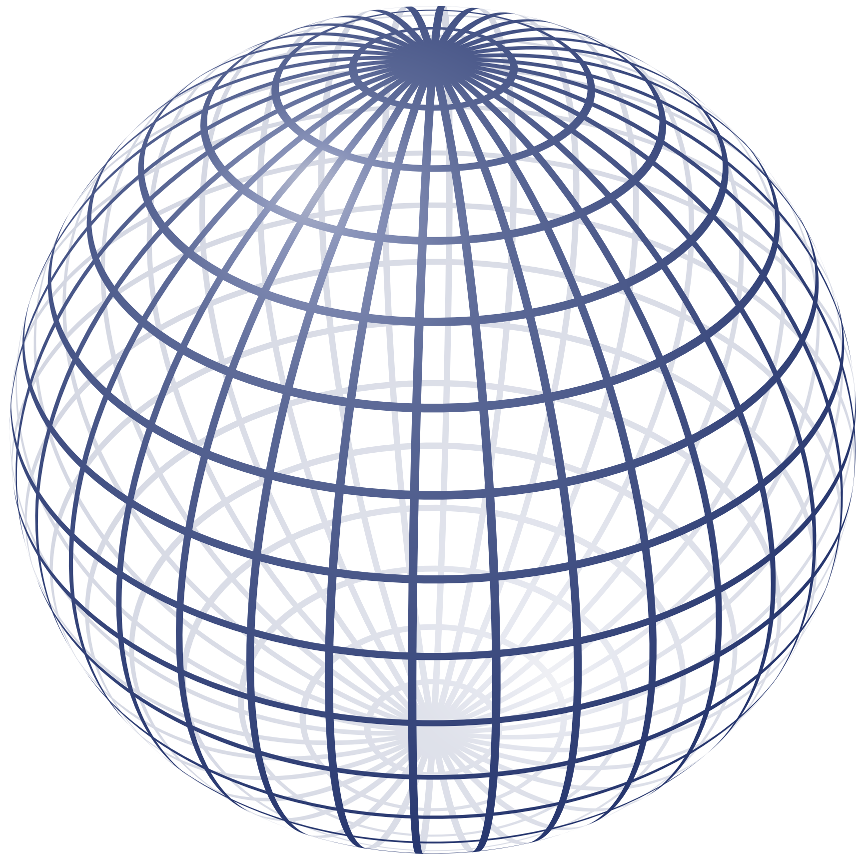


$O(3)$ $\qquad$ O_h

We are "losing" symmetries when moving from one to the other

What is being affected?

Finite-volume symmetry: Cubic vs Spherical



How do we classify particles in QM?

J^P **correspond to irreducible representations of the group** $O(3)$

J is the generator of rotations

the projection of angular momentun onto some axis, J_z **labels rows of the representation**

$O(3)$

Single particle states are classified by their irrepts in the RIHL $|p, m\rangle \otimes |j, \mu\rangle \equiv |m, j; p, \mu\rangle$

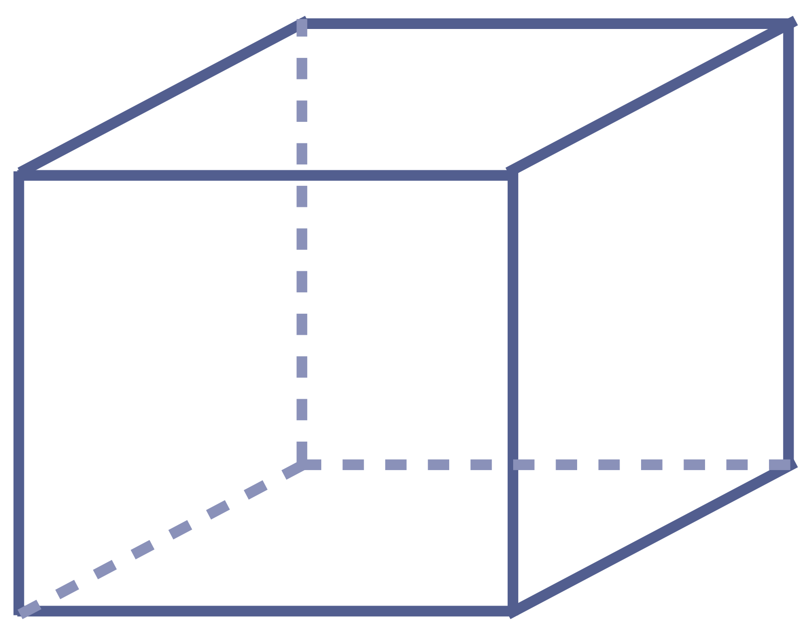
Two-particles states are typically described in either helicity or LS basis

Helicity basis $|JM; \mu_1\mu_2; \gamma\rangle$

LS basis $$|JM; LS; \gamma\rangle = \sum_{m_1, m_2} \langle LSM_LM_s \mid JM\rangle \langle s_1s_2m_1m_2 \mid SM_S\rangle \underline{|LM_L; m_1m_2; \gamma\rangle}$$

Helicity basis

Finite-volume symmetry: Cubic vs Spherical



O_h

On a typical lattice, the group of rotational symmetry is the cubic point group O_h

Therefore, the states of our hamiltonian will be described by its irreducible representations

For consistency, we describe these irreps as Λ^P, where P is the same parity operation as in the continuum

The operators/interpolators we build must respect these same symmetries

States with different J_z in the continuum appear in different irreps on the lattice

Finite-volume symmetry: Groups

A group G must fulfill the following properties:

If g_1, g_2 belong to G, then $g_1 g_2$ belongs too

The identity belongs to G

Every element must have an inverse

If $g_1 g_2 = g_2 g_1 \,\forall g_1\, g_2 \in G$, then the group is called Abelian

Our discrete groups, however, will not be abelian

a d-dimensional representation Γ of a group: a set of $d \times d$ matrices each acting on $g_i \in G$ such that
$\Gamma(g_1 g_2) = \Gamma(g_1)\Gamma(g_2)$

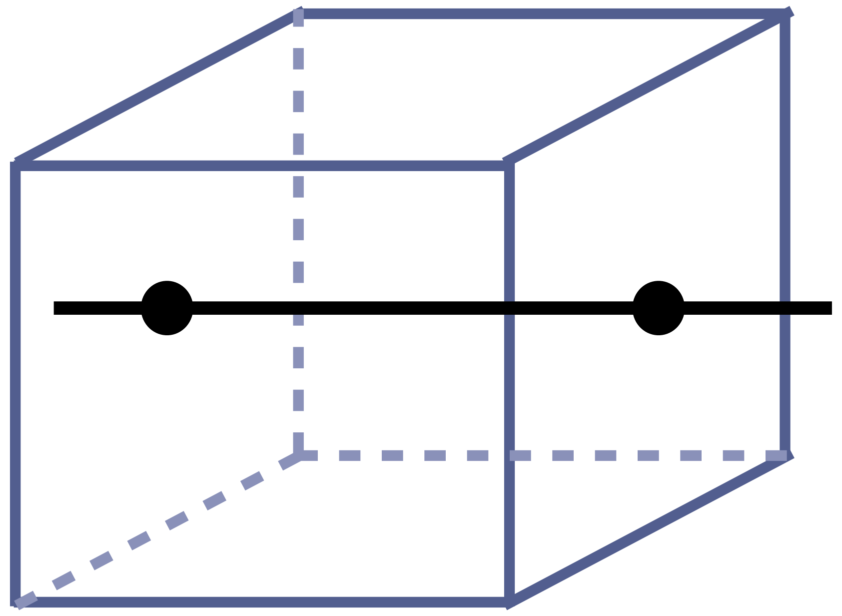
A set of matrices that respect the same operations as the group is a representation of it

If we can block diagonalize all matrices with the same transformation, then we can reduce the group representation

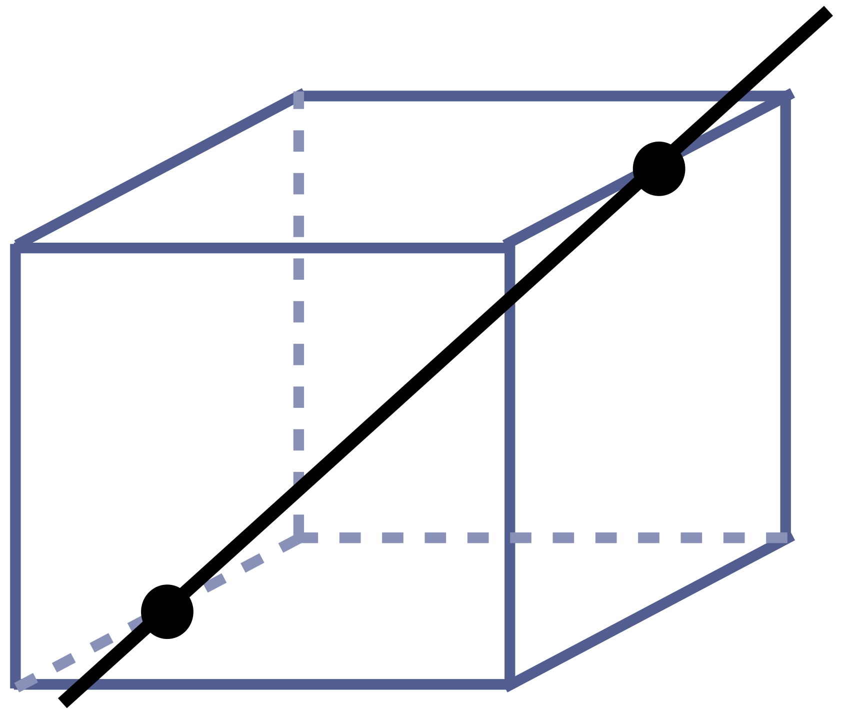
$$\Gamma(g) = \begin{pmatrix} \Gamma^{(1)}(g) & 0 \\ 0 & \Gamma^{(2)}(g) \end{pmatrix} = \underbrace{\Gamma^{(1)}(g) \oplus \Gamma^{(2)}(g)}_{\text{Reduced}}$$

Finite-volume symmetry

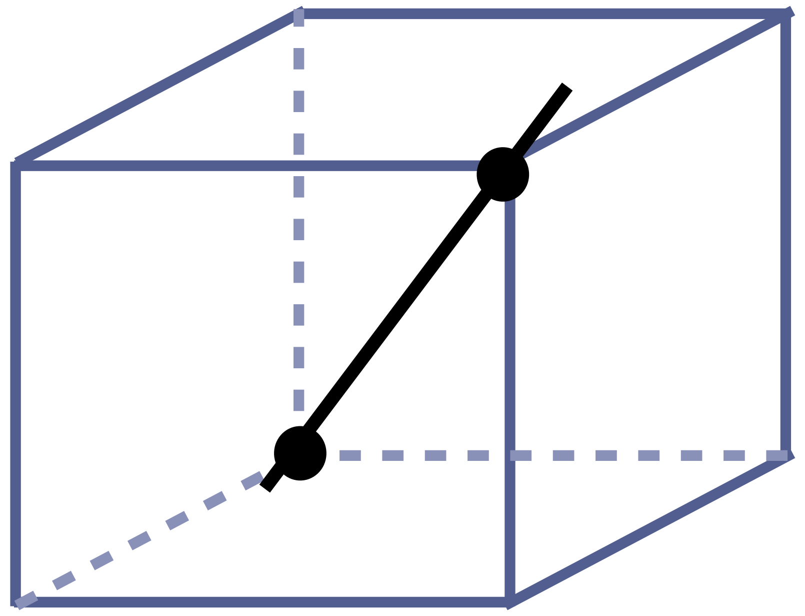
Symmetry operations on the octahedral group O



C_4



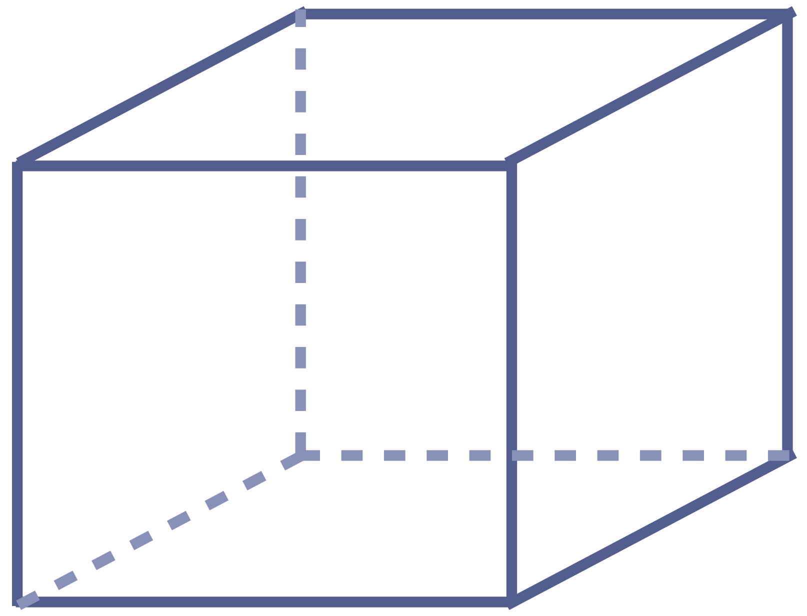
C_2



C_3

Operation	No.	Class Label
identity	1	$\mathbf{1}$
90° about axes through centres of opposite faces	6	C_4
180° about the same axes	3	C_4^2
120° about diagonals connecting opposite vertices	8	C_3
180° about axes through centers of opposite edges	6	C_2
	24	

Finite-volume symmetry: In-flight lattices

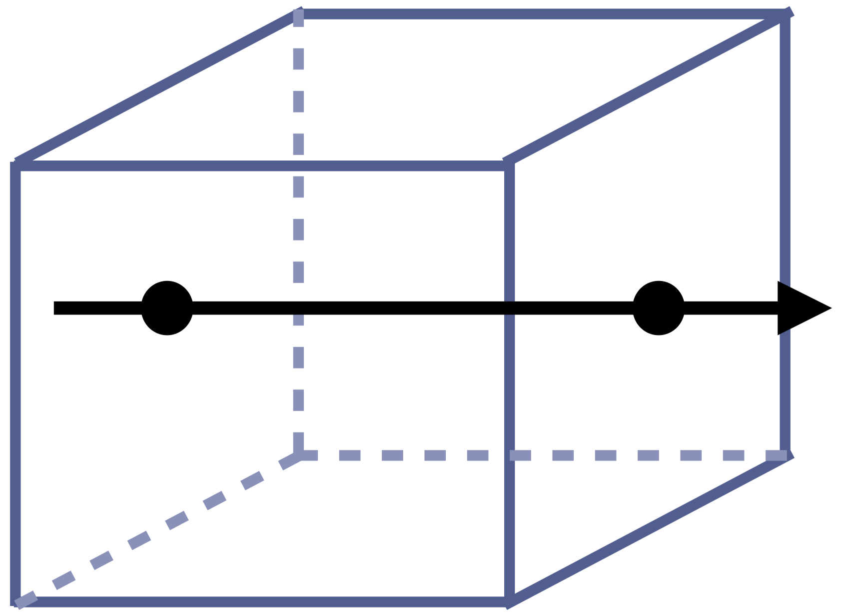


O_h

O_h is the symmetry group of a lattice at rest, only

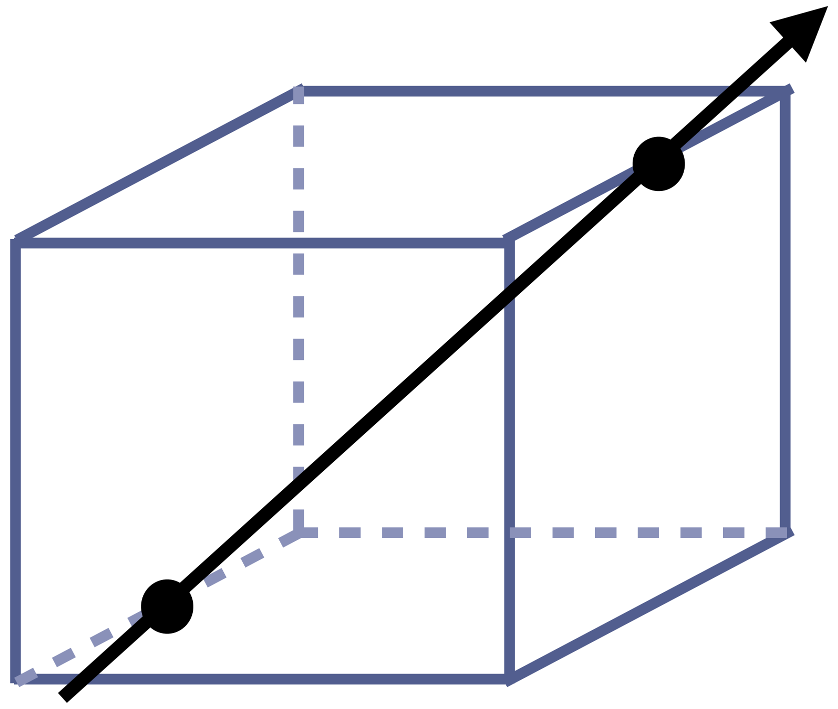
Lattice in flight (momenta $\neq 0$) have different reduced symmetry groups (subgroups of O_h)

$p = (n, 0, 0)$



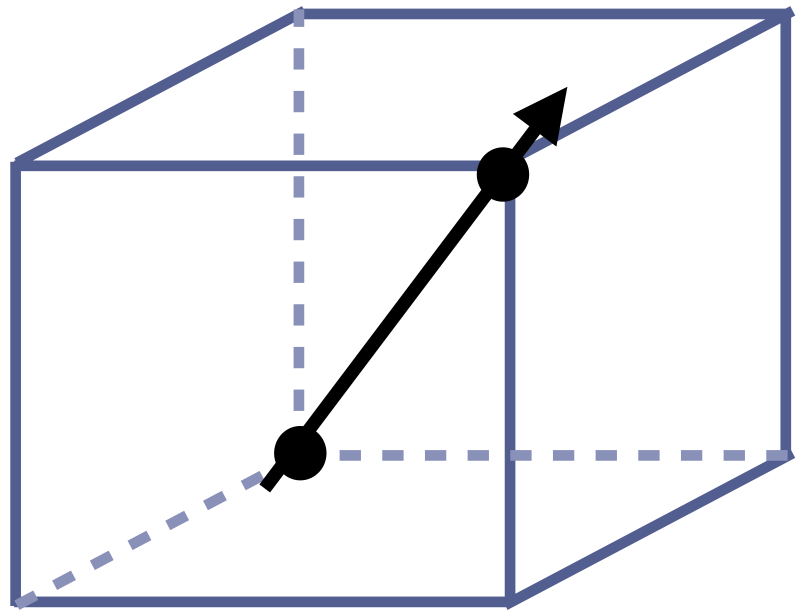
C_{4v}

$p = (0, n, n)$



C_{2v}

$p = (n, n, n)$



C_{3v}

Finite-volume symmetry: Properties

Vectors of matrices from different irreps are orthogonal

$$\sum_g \Gamma_i(g)_{mn}\Gamma_j(g)_{mn} = \delta_{ij}$$

Vectors from same irrep but different matrix elements are also orthogonal

$$\sum_g \Gamma_i(g)_{mn}\Gamma_j(g)_{m'n'} = \delta_{mm'}\delta_{nn'}$$

Vectors from the same rep and same matrix elements have magnitude h/l_i

$$\sum_g \Gamma_i(g)_{mn}\Gamma_i(g)_{mn} = h/\ell_i$$

where h **is the order of the group and** l_i **the dimension of** Γ_i

Now, the character of representation is

$$\chi(g) = \mathrm{Tr}(\Gamma(g)) \quad \forall g \in G$$

For an irrep, the characters of all matrices belonging to the same class are identical

In a group, number of irreps = number of classes

Properties:

$$\sum_g [\chi_i(g)]^2 = h \qquad \sum_g \chi_i(g)\chi_j(g) = h\delta_{ij}$$

Finite-volume symmetry

Remember, number of irreps = number of classes, there are 5 irreps for O $\longrightarrow$ A_1, A_2, E, T_1, T_2

Schur lemma $|G| = \sum_i \dim(\Gamma_i)^2$ $\longrightarrow$ $24 = \underline{\quad\quad\quad\quad\quad}$

$A_1 \quad A_2 \quad E \quad T_1 \quad T_2$

Finite-volume symmetry

Remember, number of irreps = number of classes, there are 5 irreps for O ⟶ A_1, A_2, E, T_1, T_2

Schur: $$|G| = \sum_i \dim\left(\Gamma_i\right)^2 \longrightarrow 24 = \underbrace{1^2}_{A_1} + \underbrace{1^2}_{A_2} + \underbrace{2^2}_{E} + \underbrace{3^2}_{T_1} + \underbrace{3^2}_{T_2}$$

Finite-volume symmetry

Remember, number of irreps = number of classes, there are 5 irreps for O $\longrightarrow$ A_1, A_2, E, T_1, T_2

Schur: $$|G| = \sum_i \dim(\Gamma_i)^2 \longrightarrow 24 = \underbrace{1^2 + 1^2 + 2^2 + 3^2 + 3^2}_{A_1 \quad A_2 \quad E \quad T_1 \quad T_2}$$

The cubic point group O_h also includes spatial inversions

$$O_h = O \otimes \{\mathbf{1}, \mathbf{1}_s\} \qquad \mathbf{1}_S \begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$

This increases the number of classes and dimensionality to 48

$$48 = \underbrace{1^2 + 1^2 + 1^2 + 1^2 + 2^2 + 2^2 + 3^2 + 3^2 + 3^2 + 3^2}_{A_{1g} \quad A_{1u} \quad A_{2g} \quad A_{2u} \quad E_g \quad E_u \quad T_{1g} \quad T_{1u} \quad T_{2g} \quad T_{2u}}$$

Finite-volume symmetry

We tabulate the irreps by class on a character table

$\mathbf{O}$	$\mathbf{1}$	$8C_3$	$6C_2$	$6C_4$	$3\left(C_4\right)^2$
A_1	$+1$	$+1$	$+1$	$+1$	$+1$
A_2	$+1$	$+1$	-1	-1	$+1$
E	$+2$	-1	0	0	$+2$
T_1	$+3$	0	-1	$+1$	-1
T_2	$+3$	0	$+1$	-1	-1

The entries consist of characters, the trace of the matrices representing group elements of the column's class in the given row's group representation.

Finite-volume symmetry

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$$\chi(g) = \mathrm{Tr}(\Gamma(g)) \quad \forall g \in G$$

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T_2	$+3$	0	$+1$	-1	-1

Dimension!!

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Finite-volume symmetry

We tabulate the irreps by class on a character table

Number of non-identical transformations!!

$\mathbf{O}$	$\mathbf{1}$	$8C_3$	$6C_2$	$6C_4$	$3(C_4)^2$
A_1	$+1$	$+1$	$+1$	$+1$	$+1$
A_2	$+1$	$+1$	-1	-1	$+1$
E	$+2$	-1	0	0	$+2$
T_1	$+3$	0	-1	$+1$	-1
T_2	$+3$	0	$+1$	-1	-1

The entries consist of characters, the trace of the matrices representing group elements of the column's class in the given row's group representation.

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A_2	$+1$	$+1$	-1	-1	$+1$
E	$+2$	-1	0	0	$+2$
T_1	$+3$	0	-1	$+1$	-1
T_2	$+3$	0	$+1$	-1	-1

Orthogonality!!

The entries consist of characters, the trace of the matrices representing group elements of the column's class in the given row's group representation.

Finite-volume symmetry: explicit irreps ($d = 3$)

Lets define some of the specific irreps of the operations we introduced

$$\mathbf{1}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} \longrightarrow \mathbf{1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Rotation of $\pm\pi/2$ about x,y,z axes $6C_4$

Simple vector (x, y, z)

$$C_x(1)\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} x \\ \pm z \\ \mp y \end{pmatrix} \longrightarrow C_x(1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \pm 1 \\ 0 & \mp 1 & 0 \end{pmatrix}$$

$$C_y(1)\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} \mp z \\ y \\ \pm x \end{pmatrix} \longrightarrow C_y(1) = \begin{pmatrix} 0 & 0 & \mp 1 \\ 0 & 1 & 0 \\ \pm 1 & 0 & 0 \end{pmatrix}$$

$$C_z(1)\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} \pm y \\ \mp x \\ z \end{pmatrix} \longrightarrow C_z(1) = \begin{pmatrix} 0 & \pm 1 & 0 \\ \mp 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

T_1

What about (yz, xz, xy) ??

$$C_x(1)\begin{pmatrix} yz \\ xz \\ xy \end{pmatrix} \rightarrow \begin{pmatrix} -yz \\ \mp xy \\ \pm yz \end{pmatrix} \longrightarrow C_yz(1) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & \mp 1 \\ 0 & \pm 1 & 0 \end{pmatrix}$$

$$C_y(1)\begin{pmatrix} yz \\ xz \\ xy \end{pmatrix} \rightarrow \begin{pmatrix} \pm xy \\ -xz \\ \mp yz \end{pmatrix} \longrightarrow C_y(1) = \begin{pmatrix} 0 & 0 & \pm 1 \\ 0 & -1 & 0 \\ \mp 1 & 0 & 0 \end{pmatrix}$$

$$C_z(1)\begin{pmatrix} yz \\ xz \\ xy \end{pmatrix} \rightarrow \begin{pmatrix} \mp xz \\ \pm yz \\ -xy \end{pmatrix} \longrightarrow C_xy(1) = \begin{pmatrix} 0 & \mp 1 & 0 \\ \pm 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

T_2

Finite-volume symmetry: explicit irreps ($d = 3$)

T_1 **representations:**

$$\mathbf{1} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$8C_3$

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

More possible sign combinations!!

$6C_2$

$$\begin{pmatrix} 0 & \pm1 & 0 \\ \pm1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & \pm1 \\ 0 & -1 & 0 \\ \pm1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & \pm1 \\ 0 & \pm1 & 0 \end{pmatrix}$$

$6C_4$

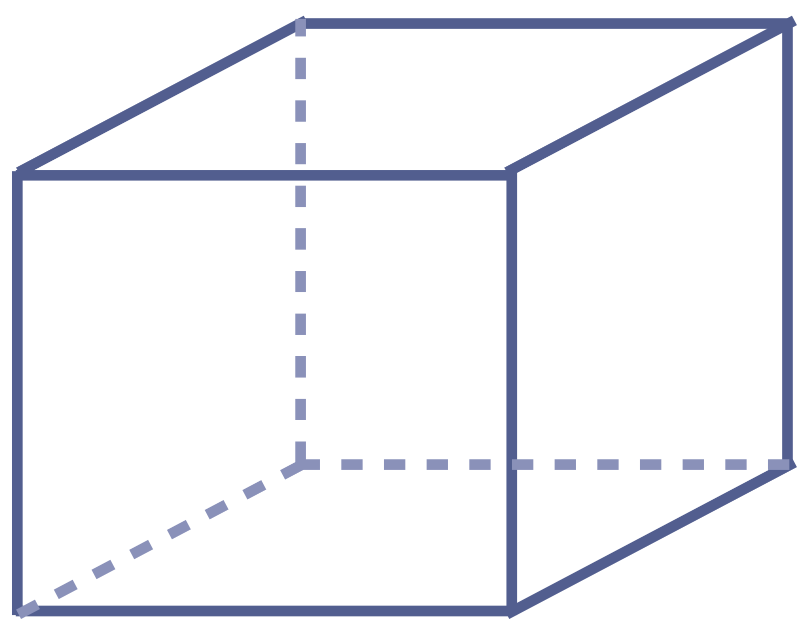
$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \pm1 \\ 0 & \mp1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & \mp1 \\ 0 & 1 & 0 \\ \pm1 & 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & \pm1 & 0 \\ \mp1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$3\,(C_4)^2$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Finite-volume symmetry: Recap

Symmetry operations on the octahedral group O



O

Operation	No.	Class Label
identity	1	$\mathbf{1}$
90° about axes through centres of opposite faces	6	C_4
180° about the same axes	3	C_4^2
120° about diagonals connecting opposite vertices	8	C_3
180° about axes through centers of opposite edges	6	C_2
	24	

Character table

$\mathbf{O}$	$\mathbf{1}$	$8C_3$	$6C_2$	$6C_4$	$3\,(C_4)^2$
A_1	$+1$	$+1$	$+1$	$+1$	$+1$
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E	$+2$	-1	0	0	$+2$
T_1	$+3$	0	-1	$+1$	-1
T_2	$+3$	0	$+1$	-1	-1

Finite-volume symmetry: Subductions

So, how does angular momentum subduce into O irreps?

	A_1	A_2	E	T_1	T_2
$J=0$	1				
$J=1$				1	
$J=2$			1		1
$J=3$		1		1	1
$J=4$	1		1	1	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

We can invert the table

Λ	Dimension	J
A_1	1	$0, 4, \ldots$
A_2	1	$3, 5, \ldots$
E	2	$2, 4, \ldots$
T_1	3	$1, 3, \ldots$
T_2	3	$2, 3, \ldots$

Finite-volume symmetry: Subductions

So, how does angular momentum subduce into O irreps?

	A_1	A_2	E	T_1	T_2	*# Rows*
$J=0$	1					*1*
$J=1$				1		*3*
$J=2$			1		1	*5*
$J=3$		1		1	1	*7*
$J=4$	1		1	1	1	*9*
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	

We can invert the table

Λ	Dimension	J
A_1	1	$0, 4, \ldots$
A_2	1	$3, 5, \ldots$
E	2	$2, 4, \ldots$
T_1	3	$1, 3, \ldots$
T_2	3	$2, 3, \ldots$

Questions? — Some water?

Next day: Subductions and the GEVP