

# Finite volume quantization conditions for multiparticle states

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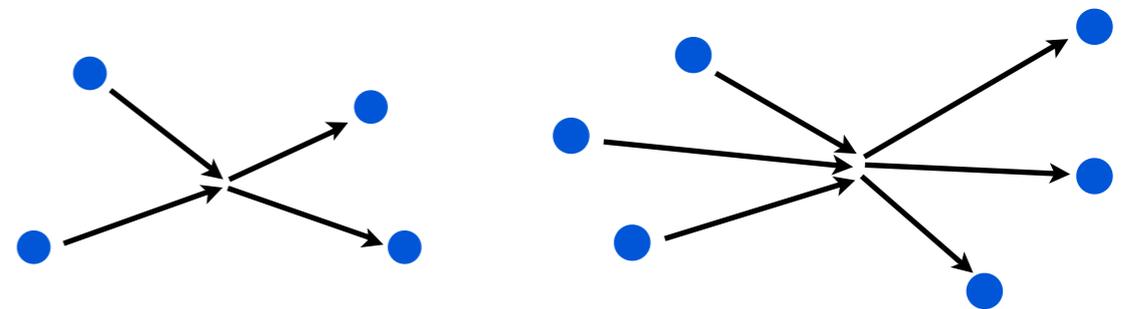


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# The fundamental issue

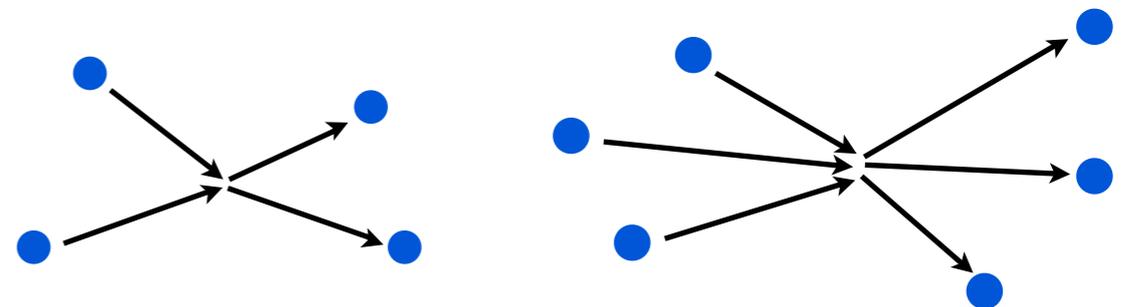
- Lattice simulations are done in finite volumes
- Experiments are not



How do we connect these?

# The fundamental issue

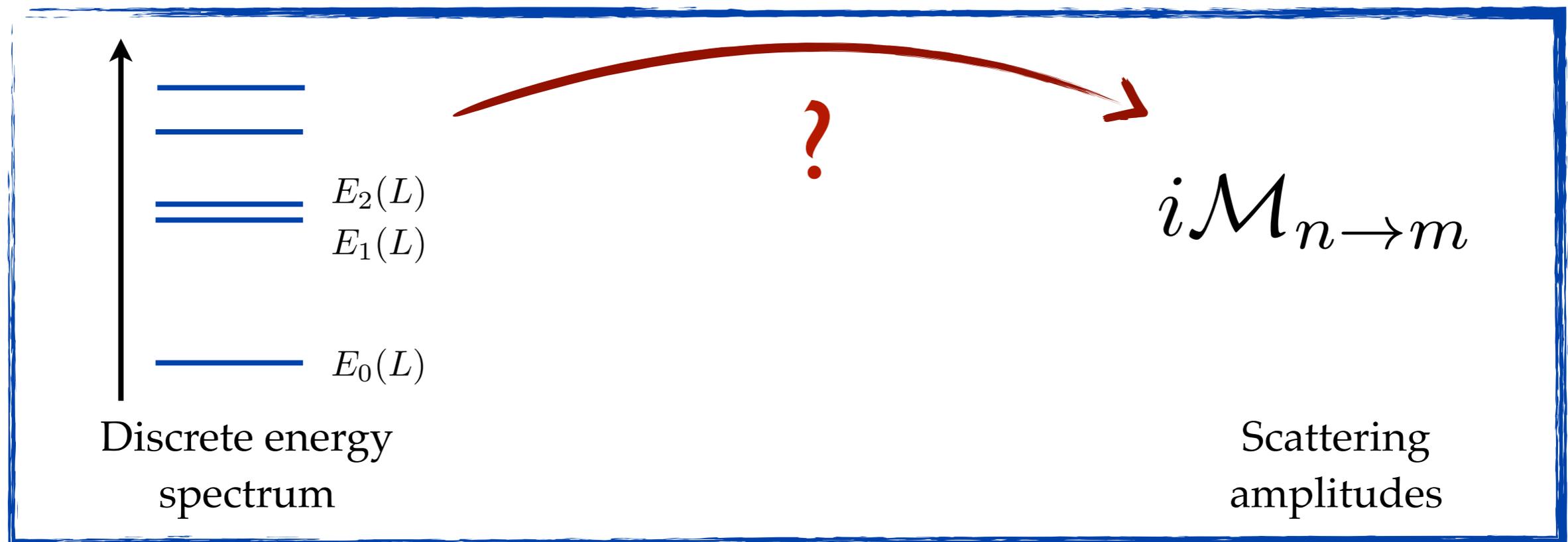
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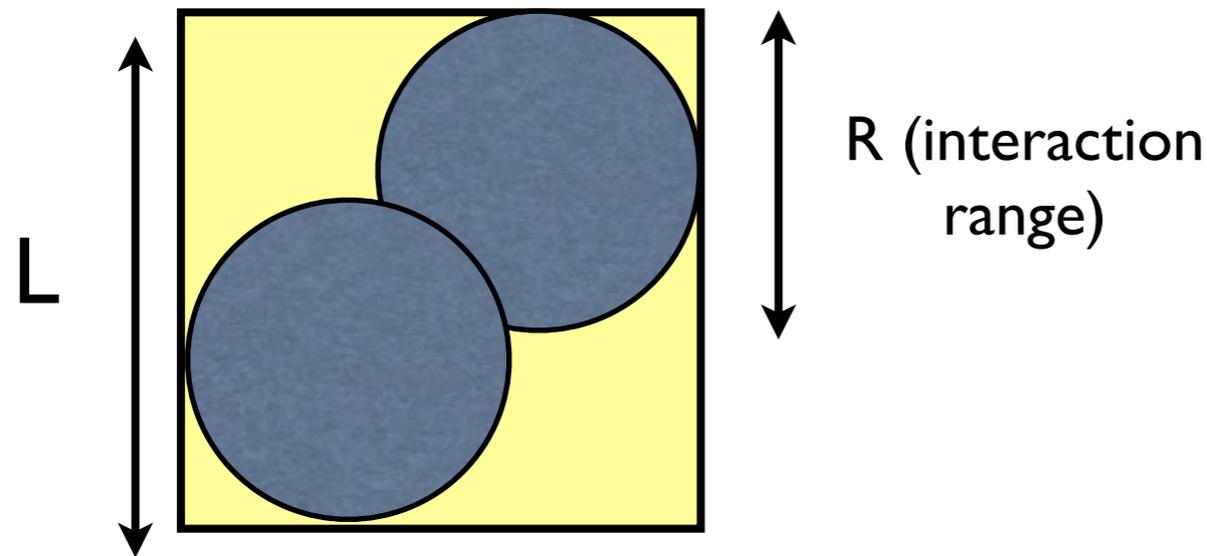
How do we connect these?

# The fundamental issue

- Lattice QCD can calculate energy levels of multiple particle systems in a box
- How are these related to scattering amplitudes?



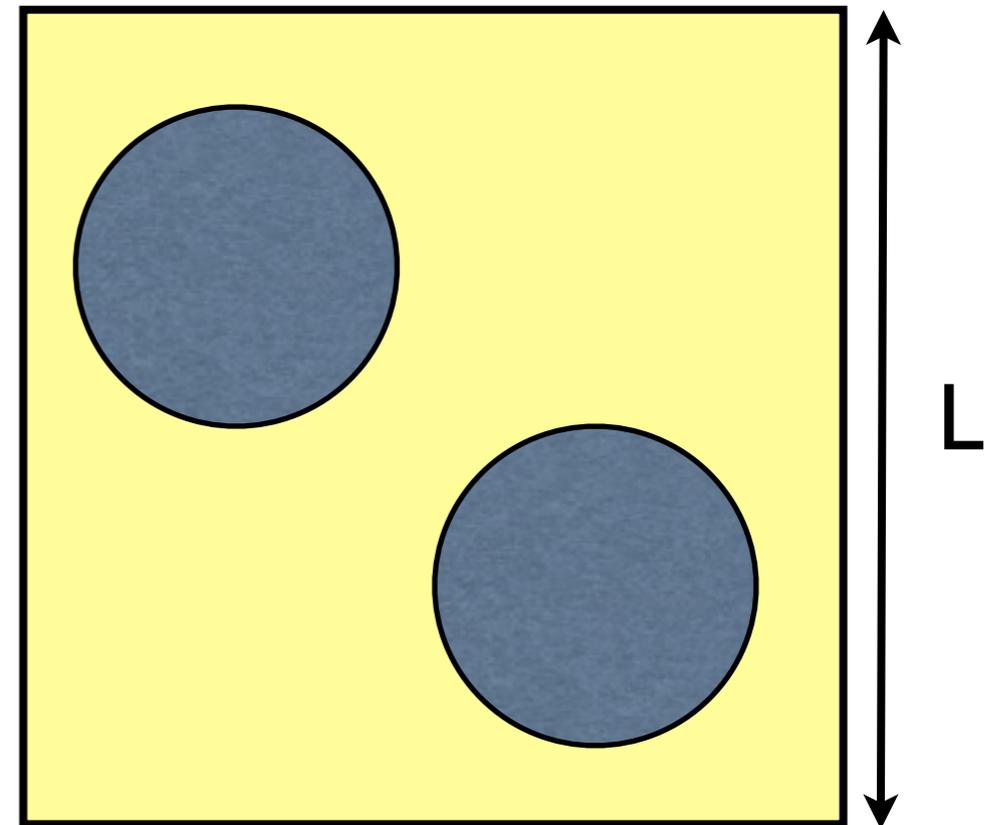
# When is spectrum related to scattering amplitudes?



$$L < 2R$$

No “outside” region.

Spectrum NOT related to scatt. amps.  
Depends on finite-density properties



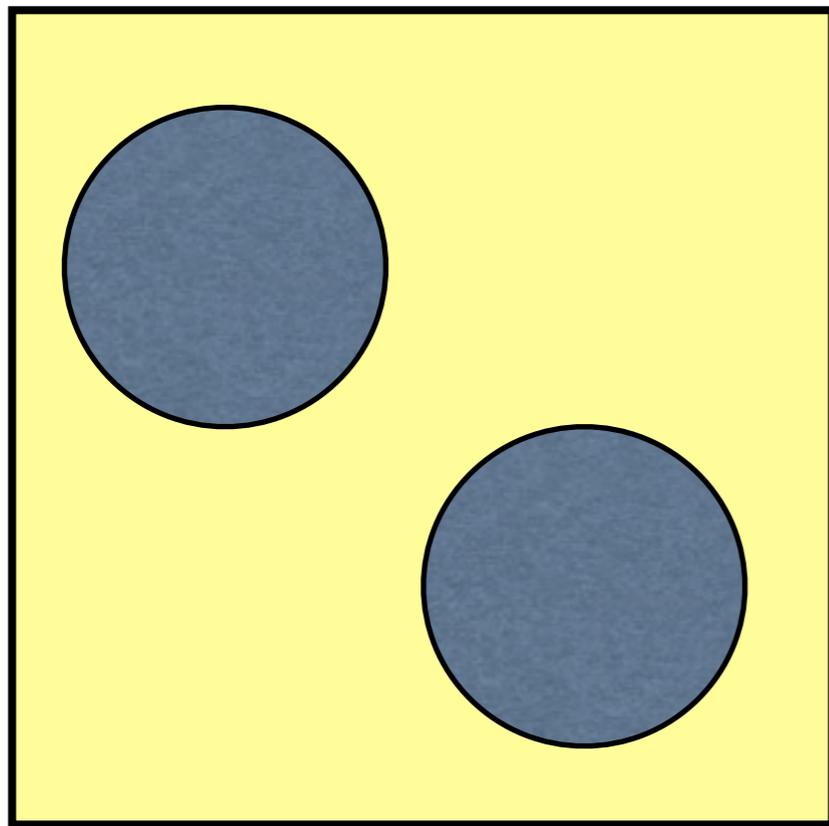
$$L > 2R$$

There is an “outside” region.  
Spectrum IS related to scatt. amps.  
up to corrections proportional to  
 $e^{-M_\pi L}$

[Lüscher]

# Systems considered today

## Quantization conditions

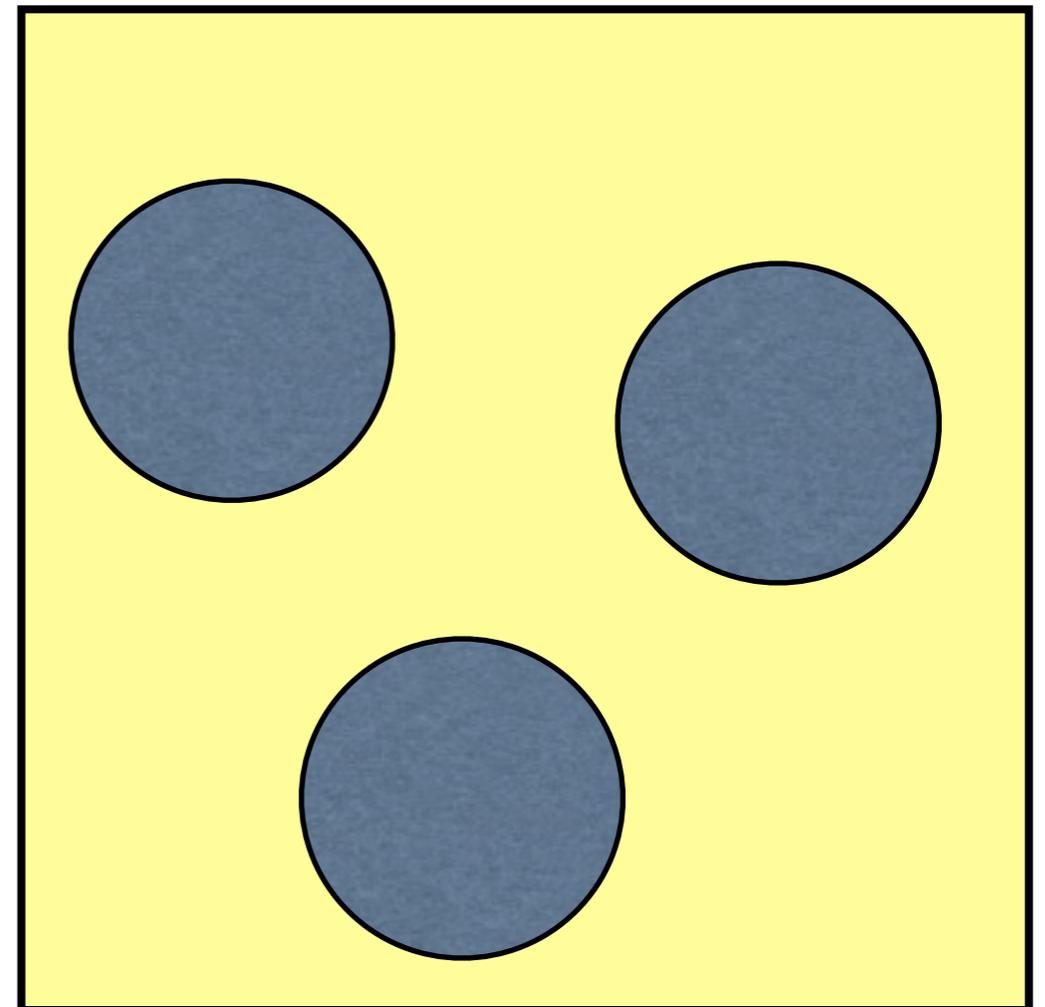


Theoretically understood;  
numerical implementations mature

[Mohler, Wilson]

What about including QED?

[Beane, Davoudi]



Formalism under development

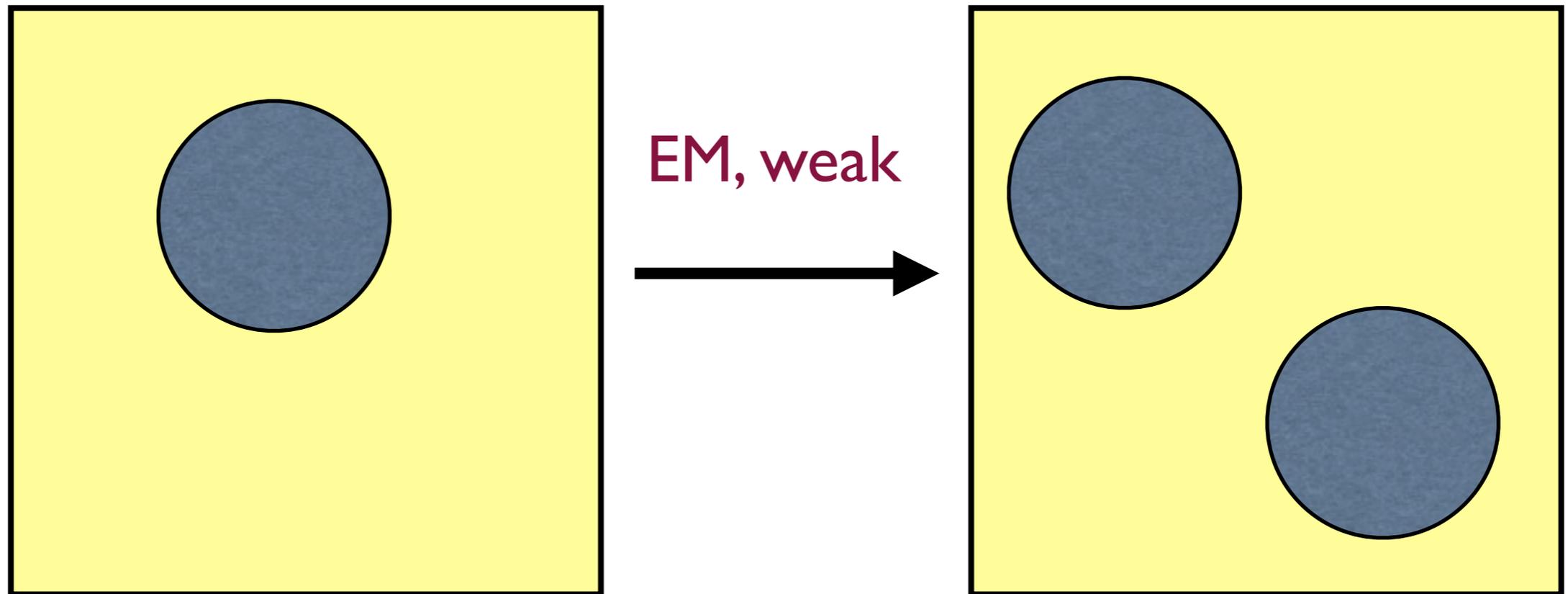
[Hansen]

How implement numerically?

[Doi]

# Systems considered today

## Transition amplitudes



Theoretically understood; [Agadjanov, Briceño]

numerical implementations expanding [Ishizuka, Kelly, Shultz]

# Outline

- Motivation
- Theoretical status
- Key theoretical ingredients
- 2-particle quantization condition
- Future directions & challenges

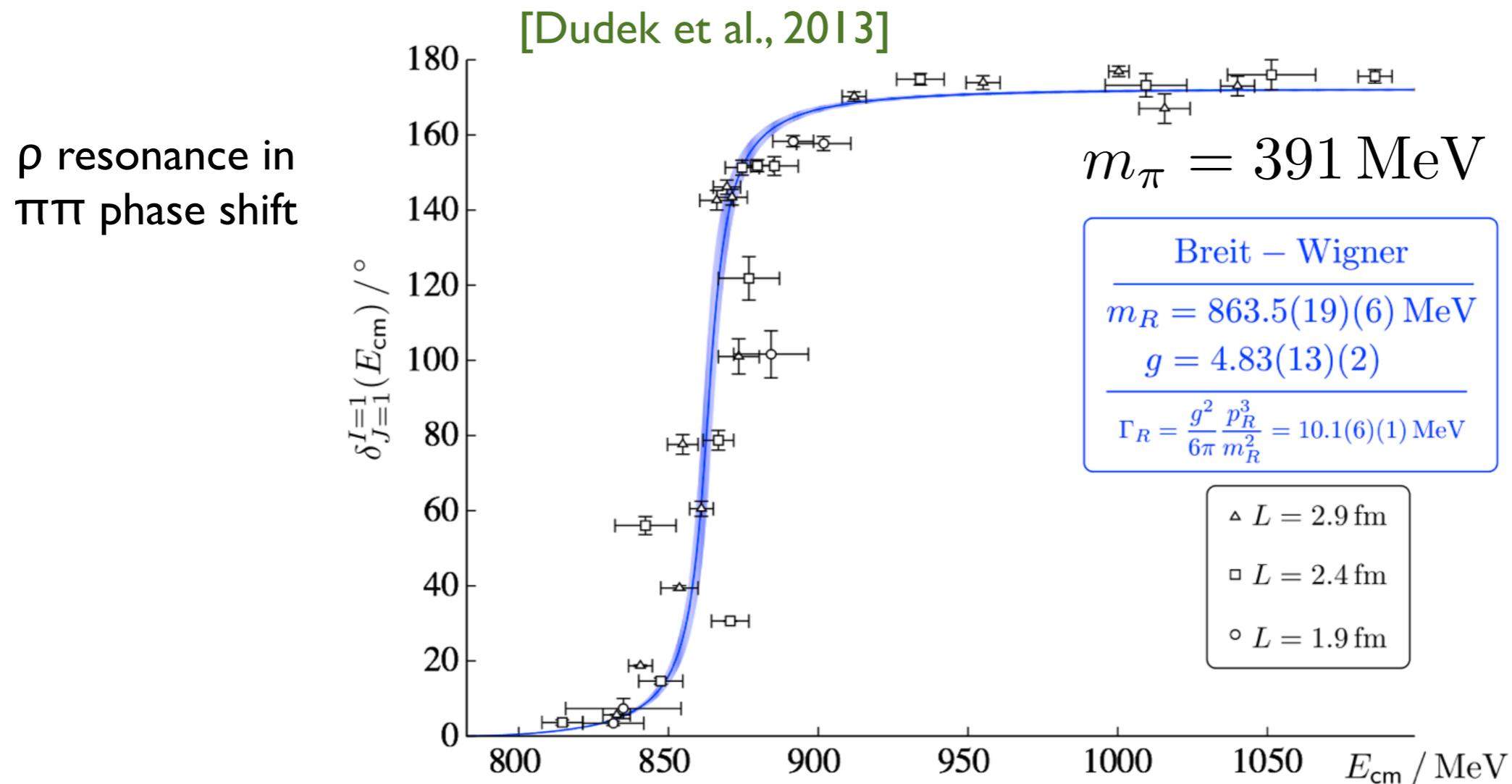
# Studying resonances

- **Most hadrons are resonances**
  - Resonances are not asymptotic states; show up in behavior of scatt. amplitudes
  - FV methods determine scattering amplitudes indirectly

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  - FV methods aim to determine scattering amplitudes indirectly
- Many resonances have three particle decay channels

$$\omega(782) \rightarrow \pi\pi\pi \quad K^* \longrightarrow K\pi\pi \quad N(1440) \rightarrow N\pi\pi$$

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$$\omega(782) \rightarrow \pi\pi\pi \quad K^* \longrightarrow K\pi\pi \quad N(1440) \rightarrow N\pi\pi$$

- Most resonances have multiple decay channels

$$a_0(980) \longrightarrow \eta\pi, K\bar{K} \quad f_0(980) \longrightarrow \pi\pi, K\bar{K}$$

# Determining interactions

- For nuclear physics need NN and NNN interactions
  - Input for effective field theory treatments of larger nuclei & nuclear matter
- Meson interactions needed for understanding pion & kaon condensates
  - $\pi\pi$ ,  $K\bar{K}$ ,  $\pi\pi\pi$ ,  $\pi K\bar{K}$ , etc.

# Calculating decay amplitudes

- Weak decay amplitudes allow tests of SM
  - $K \rightarrow \pi\pi, \pi\pi\pi$
  - $D \rightarrow \pi\pi, K\bar{K}, \eta\eta, 4\pi, \dots$
  - $B \rightarrow K\pi (+ \ell^+ \ell^-)$
  - ...
- EM transition amplitudes probe hadron structure

$$\rho \longrightarrow \pi\gamma^* \qquad N\gamma^* \longrightarrow \Delta \longrightarrow N\pi$$

# Theoretical status

# Status for 2 particles

- Long understood in NRQM [Huang & Yang 57, ...]
- Quantization formula in QFT for energies below inelastic threshold converted into NRQM problem and solved by [Lüscher 86 & 91]
- Solution generalized to arbitrary total momentum  $\mathbf{P}$ , multiple (2 body) channels, general BCs and arbitrary spins [Rummukainen & Gottlieb 85; Kim, Sachrajda & SS 05; Bernard, Lage, Meißner & Rusetsky 08; Hansen & SS 12; Briceño & Davoudi 12; ... ]
- Relation between finite volume  $1 \rightarrow 2$  weak amplitude (e.g.  $K \rightarrow \pi\pi$ ) and infinite volume decay amplitude determined [Lellouch & Lüscher 00]
- LL formula generalized to general  $\mathbf{P}$ , to multiple (2 body) channels, and to arbitrary currents and general BCs (e.g.  $\gamma^* \pi \rightarrow \rho \rightarrow \pi\pi$ ,  $\gamma^* N \rightarrow \Delta \rightarrow \pi N$ ,  $\gamma D \rightarrow NN$ ) [Kim, Sachrajda & SS 05; Christ, Kim & Yamazaki 05; Meyer 12; Hansen & SS 12; Briceño & Davoudi 12; Agadjanov, Bernard, Meißner & Rusetsky 14; Briceño, Hansen & Walker-Loud 14; ... ]
- Leading order QED effects on quantization condition determined [Beane & Savage 14]

# Status for 3 particles

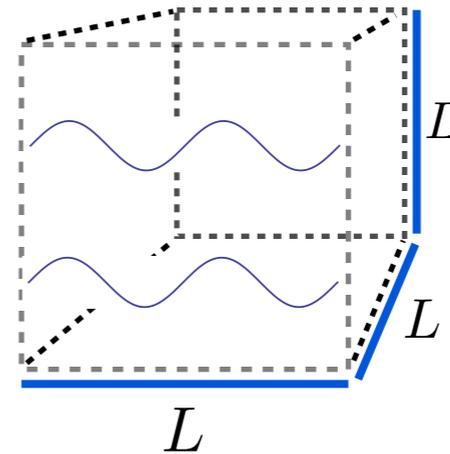
- [Beane, Detmold & Savage 07 and Tan 08] derived threshold expansion for  $n$  particles in NRQM, and argued it applied also in QFT
- [Polejaeva & Rusetsky 12] showed in NREFT that 3 body spectrum determined by infinite-volume scattering amplitudes, using integral equation
- [Briceño & Davoudi 12] used a dimer approach in NREFT, with s-wave interactions only, to determine relation between spectrum and a finite volume quantity, itself related to infinite-volume amplitudes by an integral equation
- [Hansen & SS 14, 15] derived quantization condition in (fairly) general, relativistic QFT relating spectrum and  $\mathcal{M}_2$  and 3-body scattering *quantity*  $K_{df,3}$ ; relation between  $K_{df,3}$  &  $\mathcal{M}_3$  via integral equations now known
- [Meißner, Rios & Rusetsky 14] determined volume dependence of 3-body bound state in unitary limit

# Some key theoretical ingredients

Following method of [Kim, Sachrajda & SS 05]

# Set-up

- Work in continuum (assume that LQCD can control discretization errors)
- Cubic box of size  $L$  with periodic BC, and infinite (Minkowski) time



- Spatial loops are sums:  $\frac{1}{L^3} \sum_{\vec{k}}$   $\vec{k} = \frac{2\pi}{L} \vec{n}$
- Easily extend to other BC (e.g. twisted)

- Consider general QFT with arbitrary vertices

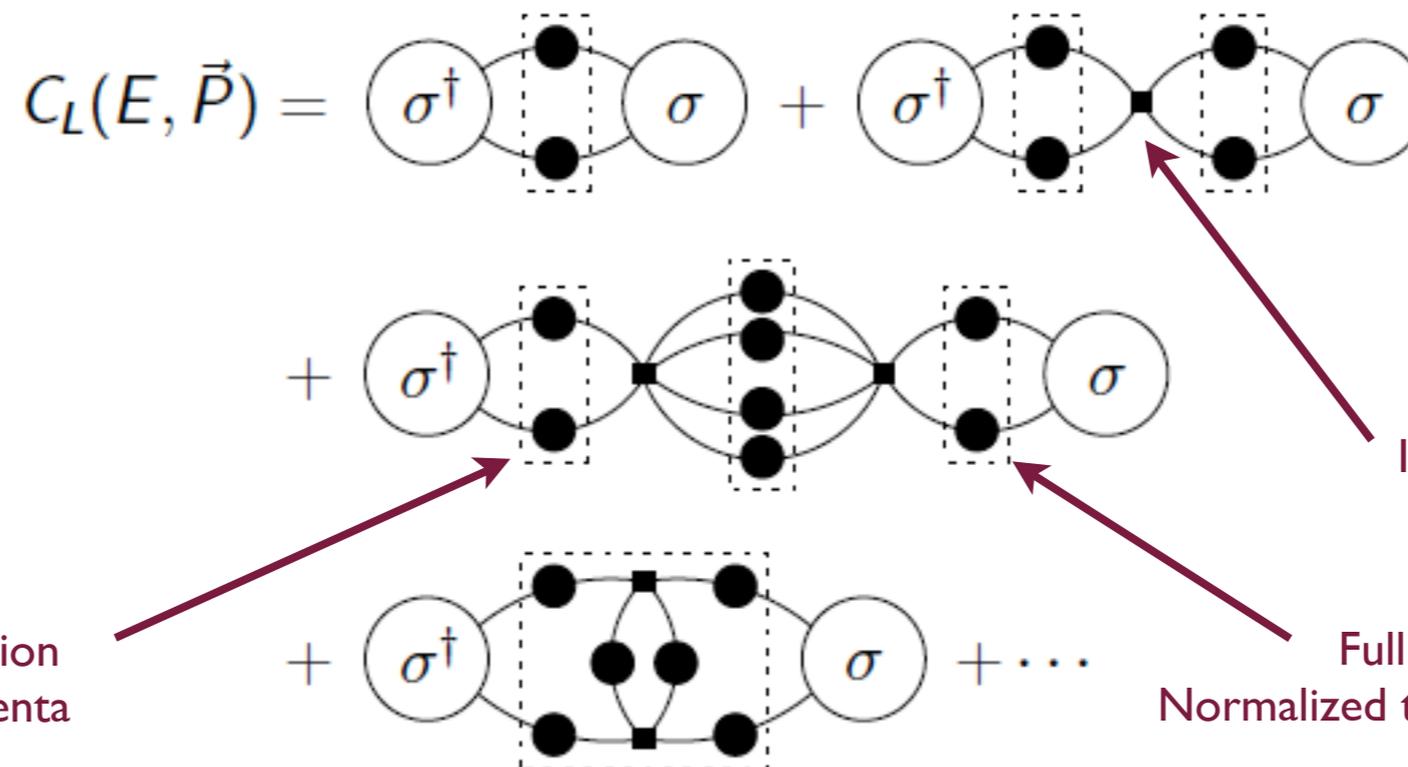
# Methodology

- Calculate (for some  $\mathbf{P}=2\pi\mathbf{n}_P/L$ )

$$C_L(E, \vec{P}) \equiv \int_L d^4x e^{-i\vec{P}\cdot\vec{x}+iEt} \langle \Omega | T \sigma(x) \sigma^\dagger(0) | \Omega \rangle_L$$

CM energy is  
 $E^* = \sqrt{(E^2 - P^2)}$

- Poles in  $C_L$  occur at energies of finite-volume spectrum
- For 2 & 3 particle states,  $\sigma \sim \pi^2$  &  $\pi^3$ , respectively
- Use all-orders diagrammatic expansion, e.g.



Boxes indicated summation over finite-volume momenta

Infinite-volume vertices

Full propagators Normalized to unit residue at pole

# Key step 1

- Replace loop sums with integrals where possible
  - Drop exponentially suppressed terms ( $\sim e^{-ML}$ ,  $e^{-(ML)^2}$ , etc.) while keeping power-law dependence

$$\frac{1}{L^3} \sum_{\vec{k}} g(\vec{k}) = \int \frac{d^3k}{(2\pi)^3} g(\vec{k}) + \sum_{\vec{l} \neq \vec{0}} \int \frac{d^3k}{(2\pi)^3} e^{iL\vec{l} \cdot \vec{k}} g(\vec{k})$$

# Key step 1

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Exp. suppressed if  $g(k)$  is smooth  
and scale of derivatives of  $g$  is  $\sim 1/M$

# Key step 2

- Use “sum=integral + [sum-integral]” if integrand has pole, with [KSS]

$$\left( \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^4k}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2 + i\epsilon} \frac{1}{(P - k)^2 - m^2 + i\epsilon} g(k)$$

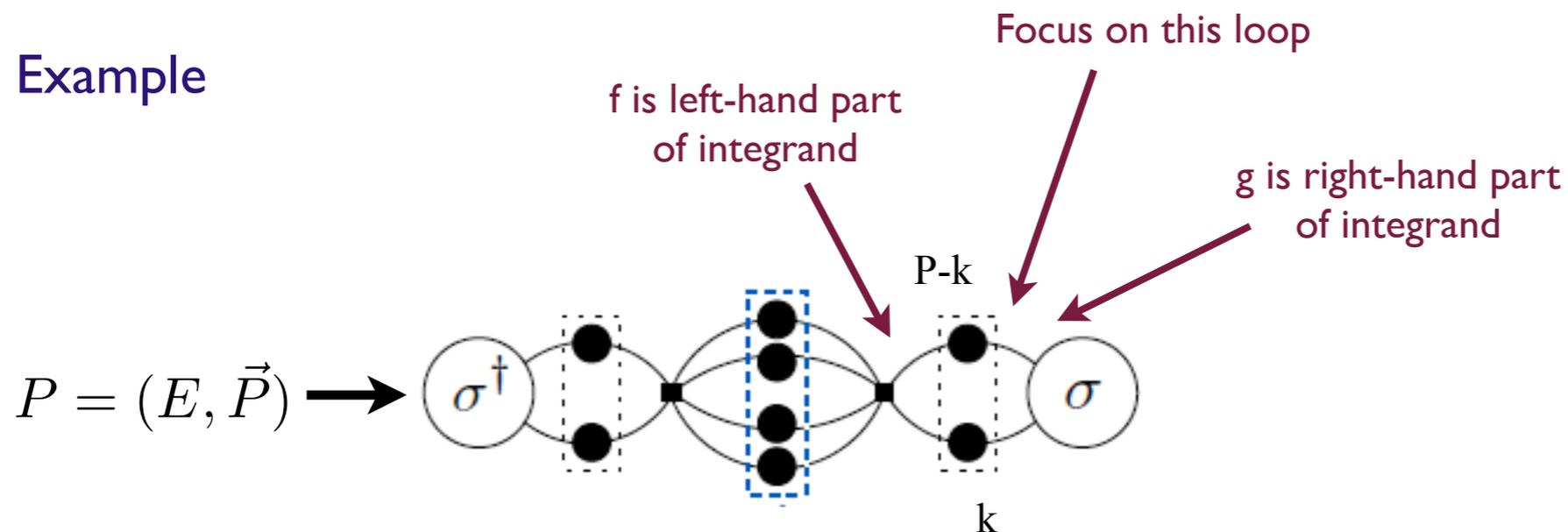
$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F}(q^*, q^{*'}) g^*(\hat{q}^{*'}) + \text{exp. suppressed}$$

$q^*$  is relative momentum  
of pair on left in CM

Kinematic function

$f$  &  $g$  evaluated for ON-SHELL momenta  
Depend only on direction in CM

- Example



# Key step 2

- Use “sum=integral + [sum-integral]” where integrand has pole, with [KSS]

$$\left( \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^4k}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2 + i\epsilon} \frac{1}{(P - k)^2 - m^2 + i\epsilon} g(k)$$

$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F}(q^*, q^{*'}) g^*(\hat{q}^{*'})$$

- Decomposed into spherical harmonics,  $\mathcal{F}$  becomes

$$F_{\ell_1, m_1; \ell_2, m_2} \equiv \eta \left[ \frac{\text{Re} q^*}{8\pi E^*} \delta_{\ell_1 \ell_2} \delta_{m_1 m_2} + \frac{i}{2\pi EL} \sum_{\ell, m} x^{-\ell} \mathcal{Z}_{\ell m}^P[1; x^2] \int d\Omega Y_{\ell_1, m_1}^* Y_{\ell, m}^* Y_{\ell_2, m_2} \right]$$

$x \equiv q^* L / (2\pi)$  and  $\mathcal{Z}_{\ell m}^P$  is a generalization of the zeta-function

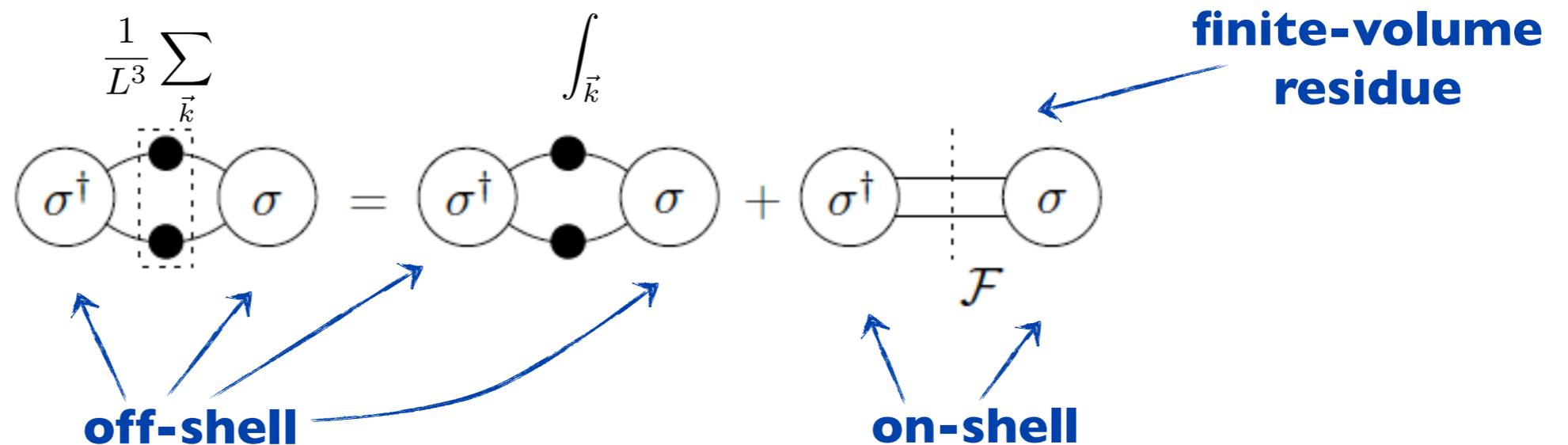
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$$\left( \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^4k}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2 + i\epsilon} \frac{1}{(P - k)^2 - m^2 + i\epsilon} g(k)$$

$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F}(q^*, q^{*'}) g^*(\hat{q}^{*'})$$

- Diagrammatically



# Variant of key step 2

- For generalization to 3 particles use (modified) PV prescription instead of  $i\epsilon$

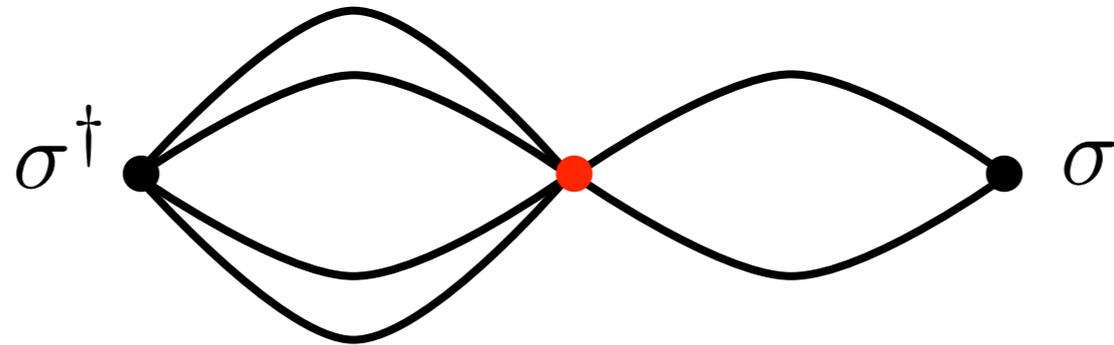
$$\left( \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} \overset{\widetilde{PV}}{-} \int \frac{d^4k}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2 + \cancel{i\epsilon}} \frac{1}{(P - k)^2 - m^2 + \cancel{i\epsilon}} g(k)$$

$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F}_{\widetilde{PV}}(q^*, q^{*'}) g^*(\hat{q}^{*'})$$

- Key properties of  $\mathbf{F}_{PV}$ : real and no unitary cusp at threshold [see Max's talk]

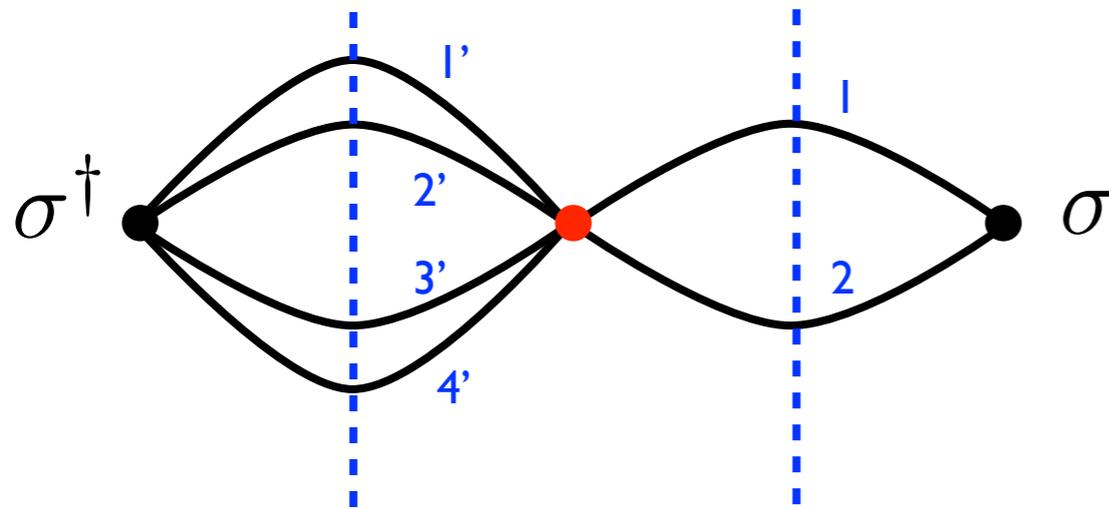
# Key step 3

- Identify potential singularities: can use time-ordered PT (i.e. do  $k_0$  integrals)
- Example



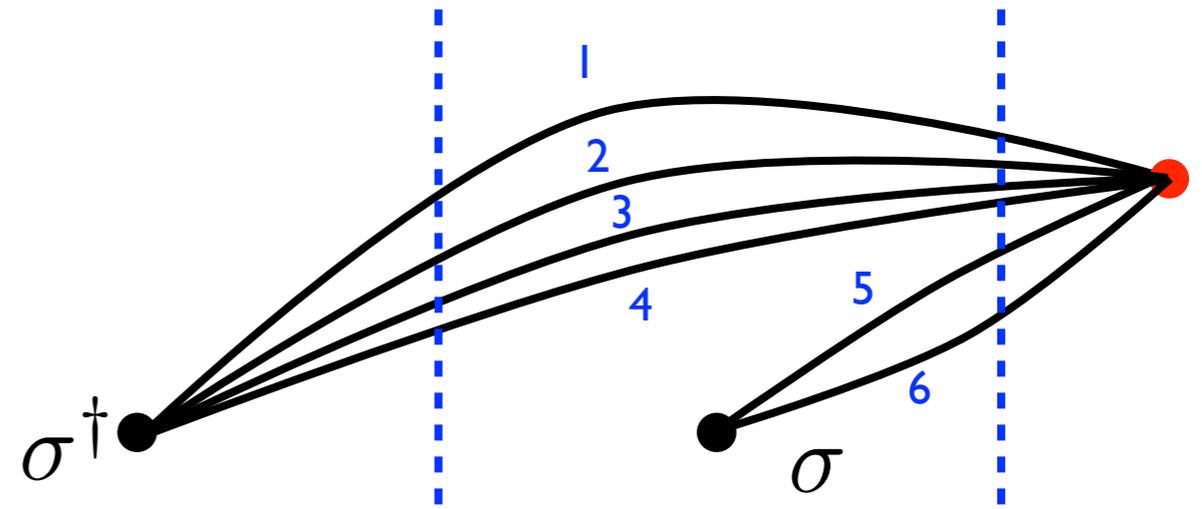
# Key step 3

- 2 out of 6 time orderings:



$$\frac{1}{E - \omega'_1 - \omega'_2 - \omega'_3 - \omega'_4}$$

$$\frac{1}{E - \omega_1 - \omega_2}$$



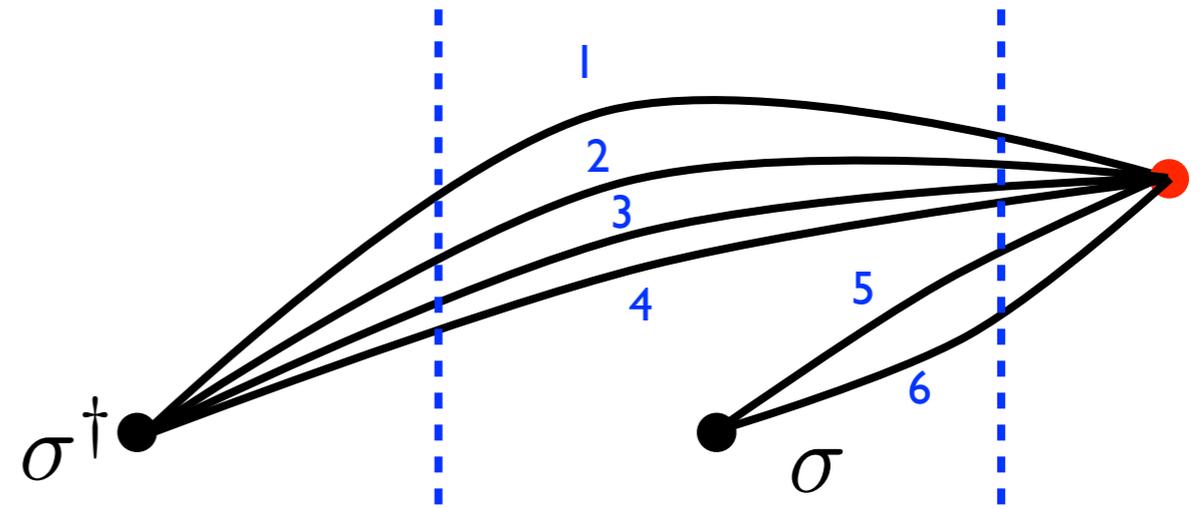
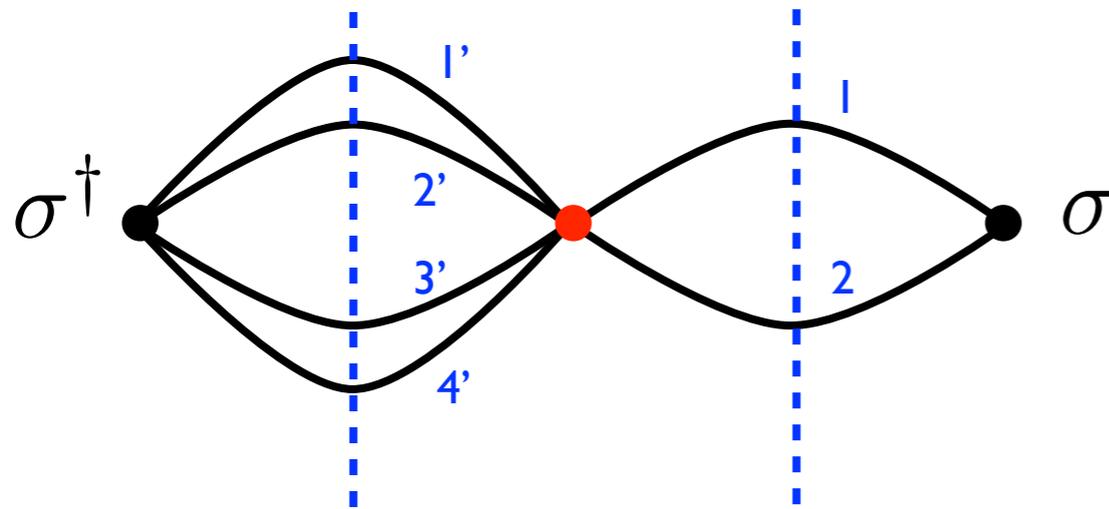
$$\frac{1}{E - \omega_1 - \omega_2 - \omega_3 - \omega_4}$$

$$\frac{1}{\sum_{j=1,6} \omega_j}$$

On-shell energy  $\omega_j = \sqrt{\vec{k}_j^2 + M^2}$

# Key step 3

- 2 out of 6 time orderings:



$$\frac{1}{E - \omega'_1 - \omega'_2 - \omega'_3 - \omega'_4}$$

$$\frac{1}{E - \omega_1 - \omega_2}$$

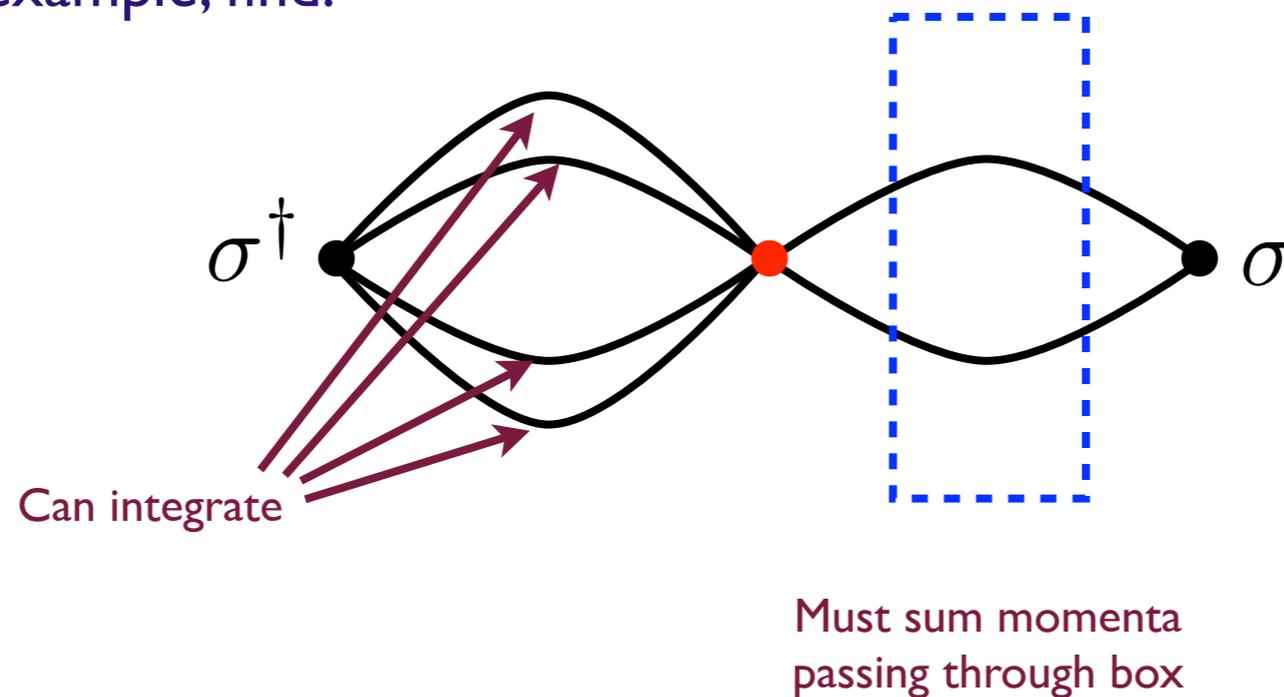
$$\frac{1}{E - \omega_1 - \omega_2 - \omega_3 - \omega_4}$$

$$\frac{1}{\sum_{j=1,6} \omega_j}$$

- If restrict  $0 < E^* < 4M$  then only 2-particle “cuts” have singularities, and these occur only when both particles go on-shell

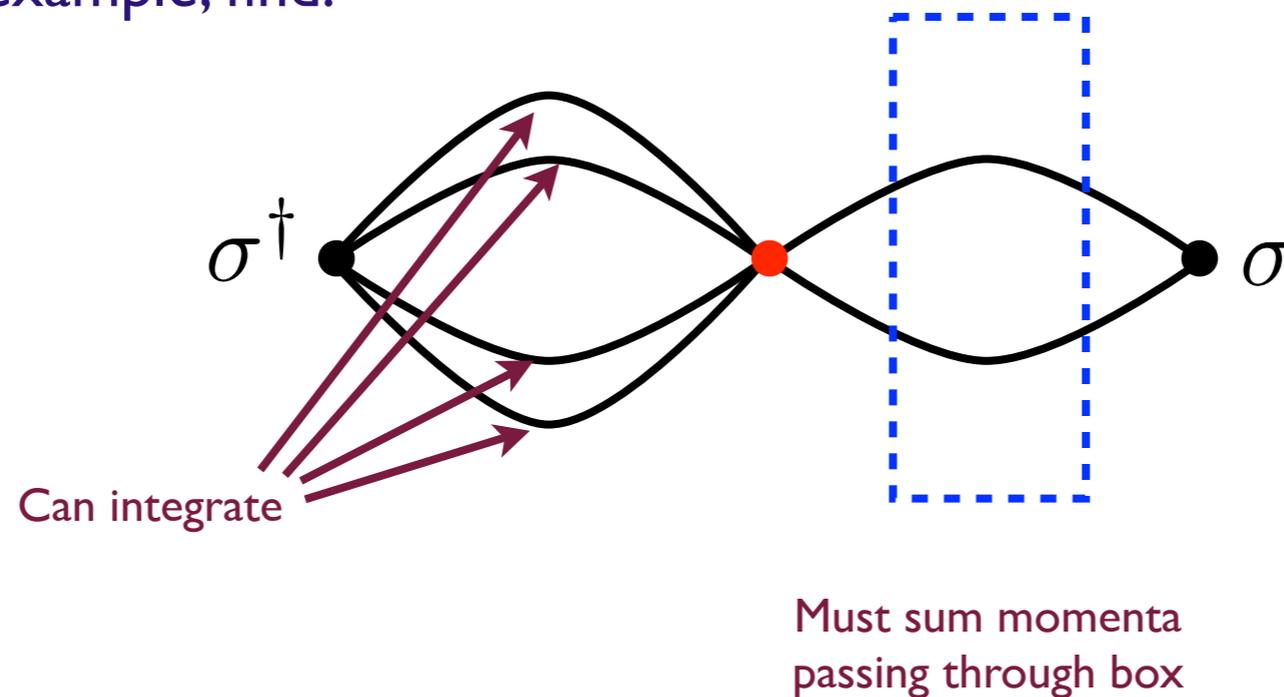
# Combining key steps 1-3

- For each diagram, determine which momenta must be summed, and which can be integrated
- In our example, find:



# Combining key steps 1-3

- For each diagram, determine which momenta must be summed, and which can be integrated
- In our example, find:



- Then repeatedly use  $\text{sum}=\text{integral} + \text{"sum-integral"}$  to simplify

# 2-particle quantization condition

Following method of [Kim, Sachrajda & SS 05]

- Apply previous analysis to 2-particle correlator ( $0 < E^* < 4M$ )

$$C_L(E, \vec{P}) = \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \dots$$

these loops are now integrated

- Collect terms into infinite-volume Bethe-Salpeter kernels

$$C_L(E, \vec{P}) = \text{diagram 1} + \text{diagram 2} + \dots$$

- Apply previous analysis to 2-particle correlator
- Collect terms into infinite-volume Bethe-Salpeter kernels

$$C_L(E, \vec{P}) = \text{diagram} + \text{diagram} \left\{ \text{diagram} + \text{diagram} + \text{diagram} + \dots \right\} \text{diagram} + \dots$$

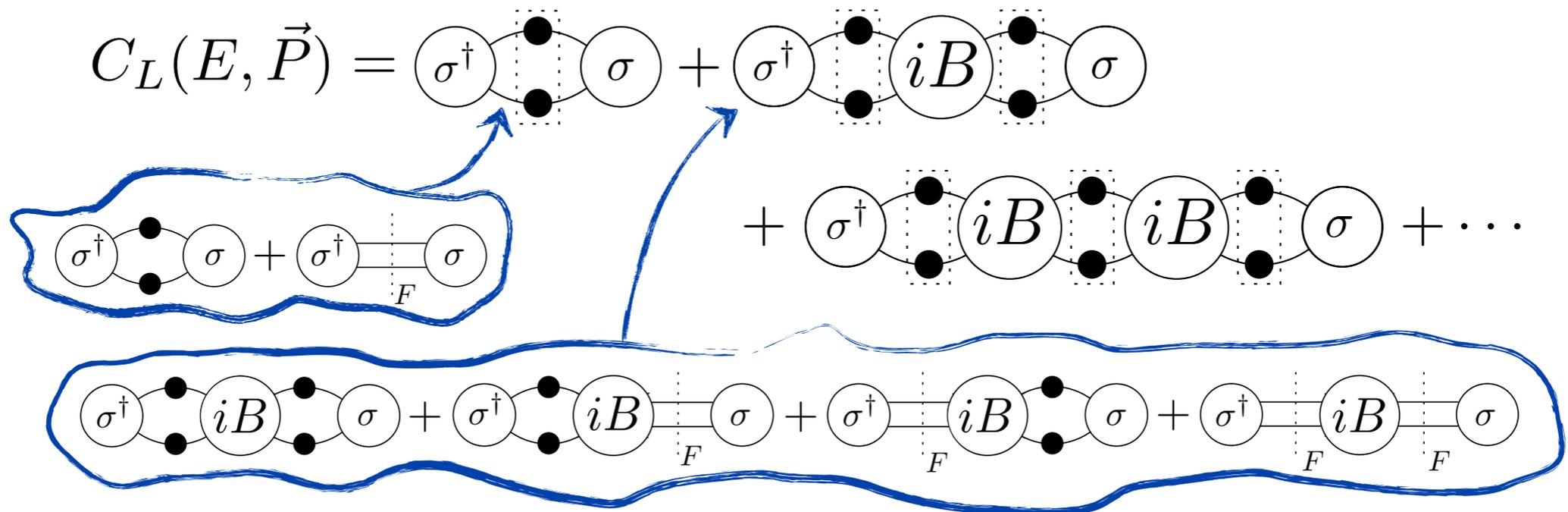
The diagram shows the expansion of the 2-particle correlator  $C_L(E, \vec{P})$ . The first term is a circle labeled  $\sigma^\dagger$  on the left and  $\sigma$  on the right, with two black dots between them. A dashed box encloses these two dots. The second term is a similar diagram, but the two dots are connected to a bracketed set of diagrams. The first diagram in the bracket is a single vertex. The second is a vertex with three internal lines. The third is a vertex with two internal lines. An arrow points from a cloud labeled  $iB$  to the bracketed set. The sequence ends with a plus sign and an ellipsis.

- Leading to

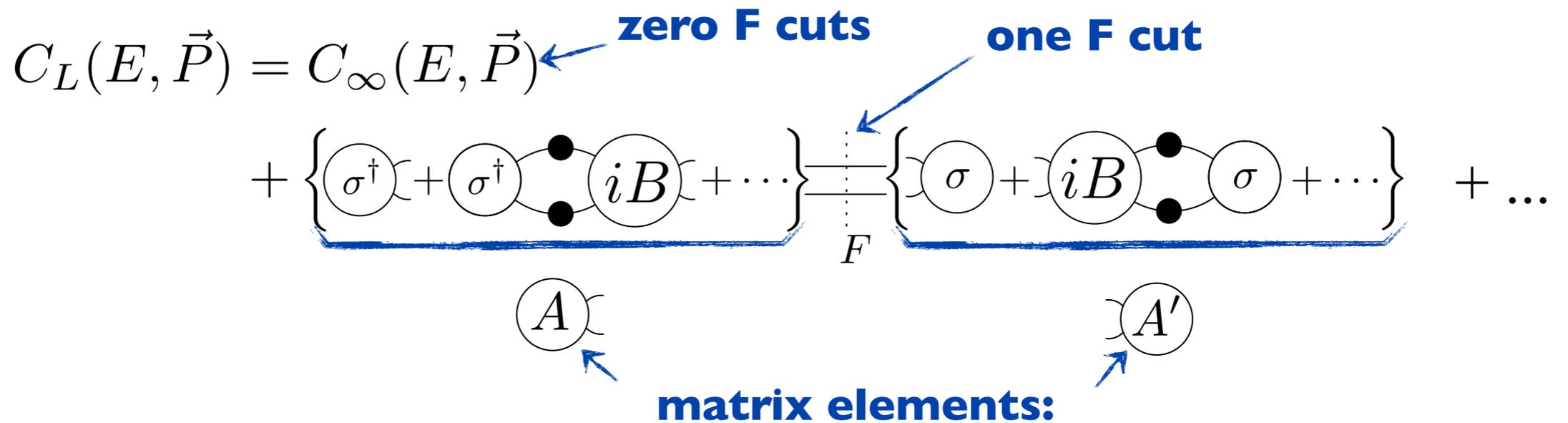
$$C_L(E, \vec{P}) = \text{diagram} + \text{diagram} + \text{diagram} + \dots$$

The diagram shows the resummed series for the 2-particle correlator. The first term is the same as in the previous equation. The second term is a diagram where the two dots are connected to a circle labeled  $iB$ , which is then connected to the  $\sigma$  particle. The third term is a diagram where the two dots are connected to a chain of two  $iB$  circles, which is then connected to the  $\sigma$  particle. The sequence ends with a plus sign and an ellipsis.

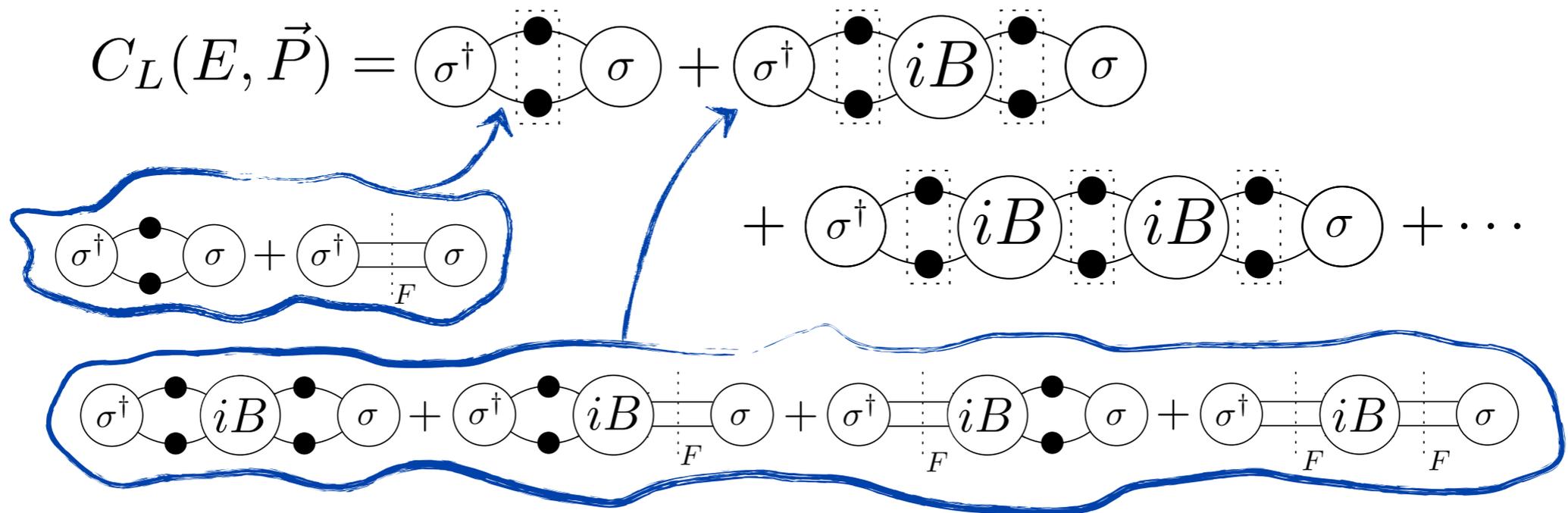
- Next use sum identity



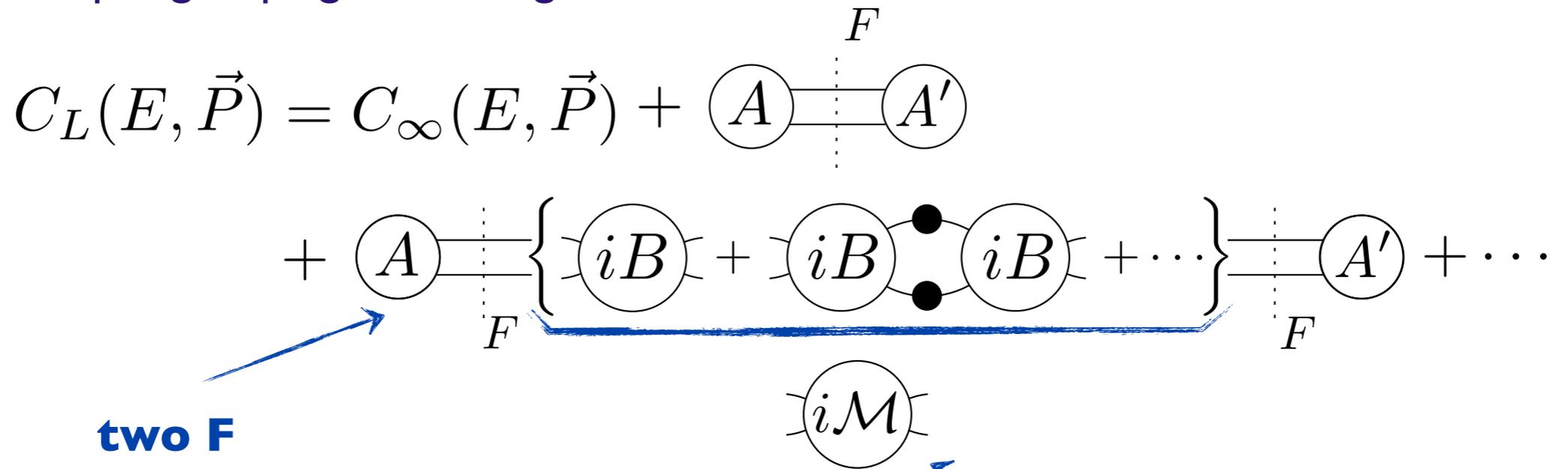
- And regroup according to number of “F cuts”



- Next use sum identity



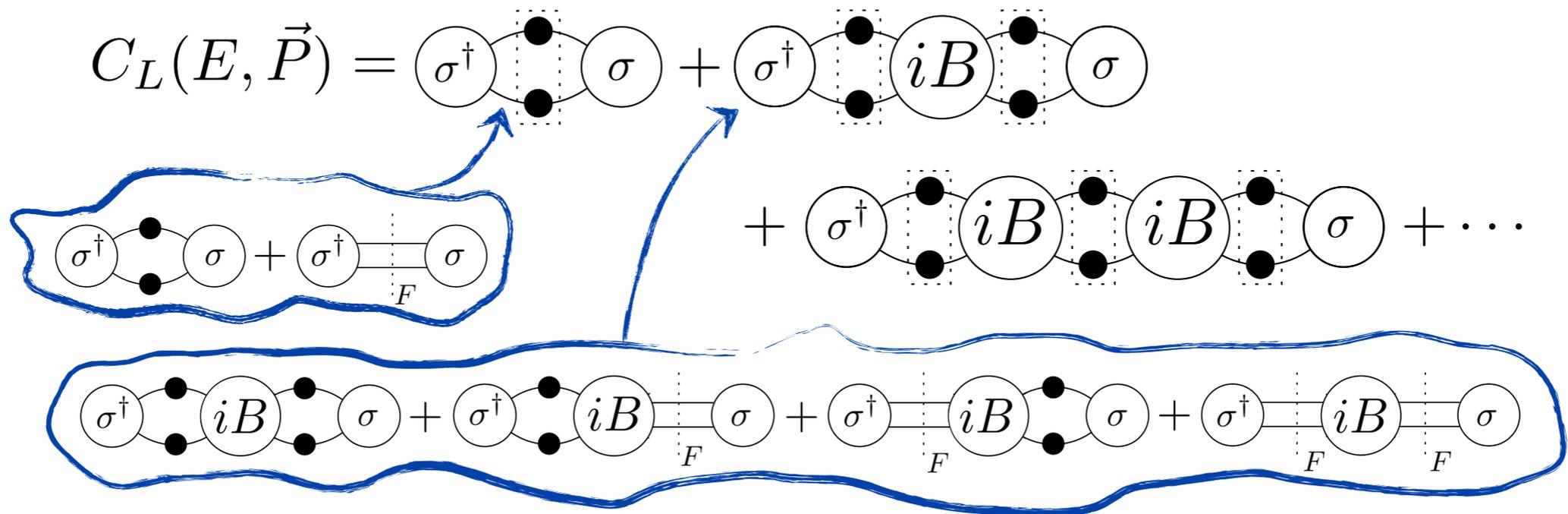
- And keep regrouping according to number of “F cuts”



two F cuts

the infinite-volume, on-shell 2→2 scattering amplitude

- Next use sum identity



- Alternate form if use PV-tilde prescription:

$$C_L(E, \vec{P}) = C_\infty^{\widetilde{PV}}(E, \vec{P}) + \begin{array}{c} F_{\widetilde{PV}} \\ \text{---} \\ A \text{---} A' \\ \text{---} \\ F_{\widetilde{PV}} \end{array} + \begin{array}{c} \text{---} \\ A_{\widetilde{PV}} \end{array} \left\{ \begin{array}{c} iB \\ \text{---} \\ \text{---} \end{array} + \begin{array}{c} \bullet \\ \bullet \\ \text{---} \\ iB \text{---} iB \\ \text{---} \\ \text{---} \end{array} + \dots \right\} \begin{array}{c} \text{---} \\ A'_{\widetilde{PV}} \\ \text{---} \\ F_{\widetilde{PV}} \end{array} + \dots$$

**the infinite-volume, on-shell  
2→2 K-matrix**

- Final result:

$$\begin{aligned}
 C_L(E, \vec{P}) &= C_\infty(E, \vec{P}) \\
 &+ \text{Diagram 1} + \text{Diagram 2} \\
 &+ \text{Diagram 3} + \dots
 \end{aligned}$$

The diagrams are Feynman-like diagrams representing terms in a series. Each diagram consists of a horizontal line with circles at the ends and intermediate points. Vertical dashed lines labeled 'F' connect these points to a common horizontal line below.   
 - Diagram 1: A circle labeled 'A' on the left, a circle labeled 'A'' on the right, and a vertical dashed line labeled 'F' between them.   
 - Diagram 2: A circle labeled 'A' on the left, a circle labeled 'iM' in the middle, and a circle labeled 'A'' on the right. Vertical dashed lines labeled 'F' connect 'A', 'iM', and 'A'' to a common horizontal line below.   
 - Diagram 3: A circle labeled 'A' on the left, two circles labeled 'iM' in the middle, and a circle labeled 'A'' on the right. Vertical dashed lines labeled 'F' connect 'A', each 'iM', and 'A'' to a common horizontal line below.

- $$C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + \sum_{n=0}^{\infty} A' iF [i\mathcal{M}_{2 \rightarrow 2} iF]^n A$$
- Correlator is expressed in terms of infinite-volume, physical quantities and kinematic functions encoding the finite-volume effects

- Final result:

$$\begin{aligned}
 C_L(E, \vec{P}) &= C_\infty(E, \vec{P}) \\
 &+ \begin{array}{c} \text{---} \circ A \text{---} \text{---} \circ A' \text{---} \\ \text{---} F \text{---} \end{array} + \begin{array}{c} \text{---} \circ A \text{---} \text{---} \circ i\mathcal{M} \text{---} \text{---} \circ A' \text{---} \\ \text{---} F \text{---} \quad \text{---} F \text{---} \end{array} \\
 &+ \begin{array}{c} \text{---} \circ A \text{---} \text{---} \circ i\mathcal{M} \text{---} \text{---} \circ i\mathcal{M} \text{---} \text{---} \circ A' \text{---} \\ \text{---} F \text{---} \quad \text{---} F \text{---} \quad \text{---} F \text{---} \end{array} + \dots
 \end{aligned}$$

- $$C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + \sum_{n=0}^{\infty} A' iF [i\mathcal{M}_{2 \rightarrow 2} iF]^n A$$

- $$C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + A' iF \frac{1}{1 - i\mathcal{M}_{2 \rightarrow 2} iF} A$$

↑ no poles, only cuts      ↑ matrices in l,m space      ← no poles, only cuts

- $$C_L(E, \vec{P}) \text{ diverges whenever } iF \frac{1}{1 - i\mathcal{M}_{2 \rightarrow 2} iF} \text{ diverges}$$

# 2-particle quantization condition

$$C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + A' iF \frac{1}{1 - i\mathcal{M}_{2 \rightarrow 2} iF} A$$

- At fixed  $L$  &  $\vec{P}$ , the finite-volume spectrum  $E_1, E_2, \dots$  is given by solutions to

$$\Delta_{L, \vec{P}}(E) = \det \left[ (iF)^{-1} - i\mathcal{M}_{2 \rightarrow 2} \right] = 0$$

- $\mathcal{M}$  is diagonal in  $l, m$ :  $i\mathcal{M}_{2 \rightarrow 2; l', m'; l, m} \propto \delta_{l, l'} \delta_{m, m'}$
- $F$  is off-diagonal, since the box violates rotation symmetry
- To make useful, truncate by assuming that  $\mathcal{M}$  vanishes above  $l_{max}$
- For example, if  $l_{max}=0$ , obtain

$$i\mathcal{M}_{2 \rightarrow 2; 00; 00}(E_n^*) = [iF_{00; 00}(E_n, \vec{P}, L)]^{-1}$$

Generalization of s-wave Lüscher equation to moving frame [Rummukainen & Gottlieb]

# Equivalent K-matrix form

$$C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + A' i F_{\widetilde{PV}} \frac{1}{1 + \mathcal{K}_2 F_{\widetilde{PV}}} A$$

- At fixed  $L$  &  $P$ , the finite-volume spectrum  $E_1, E_2, \dots$  is given by solutions to

$$\Delta_{L, \vec{P}}(E) = \det \left[ (F_{\widetilde{PV}})^{-1} + \mathcal{K}_2 \right] = 0$$

- $\mathcal{K}_2$  is diagonal in  $l, m$
- $F_{PV}$  is off-diagonal, since the box violates rotation symmetry
- To make useful, truncate by assuming that  $\mathcal{K}_2$  vanishes above  $l_{max}$
- For example, if  $l_{max}=0$ , obtain

$$i\mathcal{K}_{2;00;00}(E_n^*) = \left[ iF_{\widetilde{PV};00;00}(E_n, \vec{P}, L) \right]^{-1}$$

# Future directions & challenges

# Many challenges remain!

- Extend  $1 \rightarrow 2$  work to include arbitrary spin particles (so can use for N)
  - First step in NREFT taken for  $\gamma^* N \rightarrow \Delta \rightarrow \pi N$  [Agadjanov et al. 14]
- Develop general formalism for  $2 \rightarrow 2$  transitions (e.g. resonance form factors)
- Fully develop 3 body formalism
  - Allow two particle sub channels to be resonant
  - Extend to non-identical particles, particles with spin
  - Generalize LL factors to  $1 \rightarrow 3$  decay amplitudes (e.g. for  $K \rightarrow \pi\pi\pi$ )
  - ....
- Develop models of amplitudes so that new results can be implemented in simulations (e.g. following  $K\pi$ ,  $K\eta$  coupled channel analysis of [Dudek, Edwards, Thomas & Wilson 14])

# Many challenges remain!

- Onwards to 4 particles?!?



Thank you!  
Questions?

# Backup Slides

# 3-particle correlator

