

Finite volume quantization conditions for multiparticle states

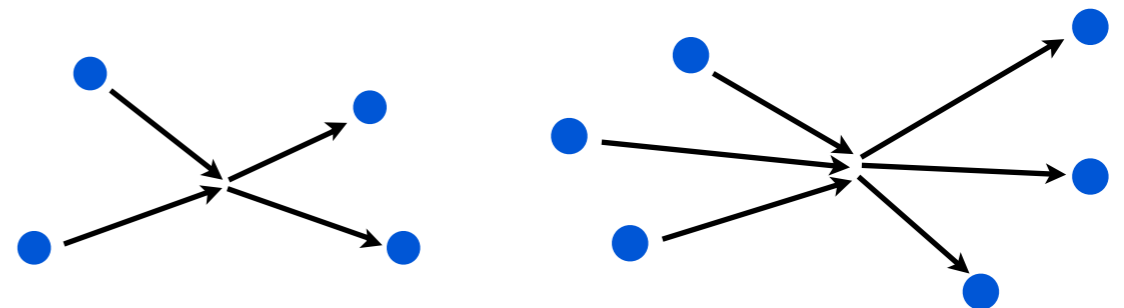


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The fundamental issue

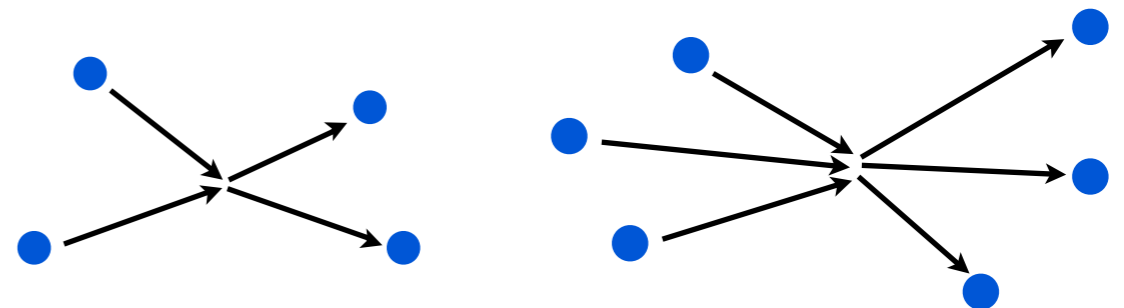
- Lattice simulations are done in finite volumes
- Experiments are not



How do we connect these?

The fundamental issue

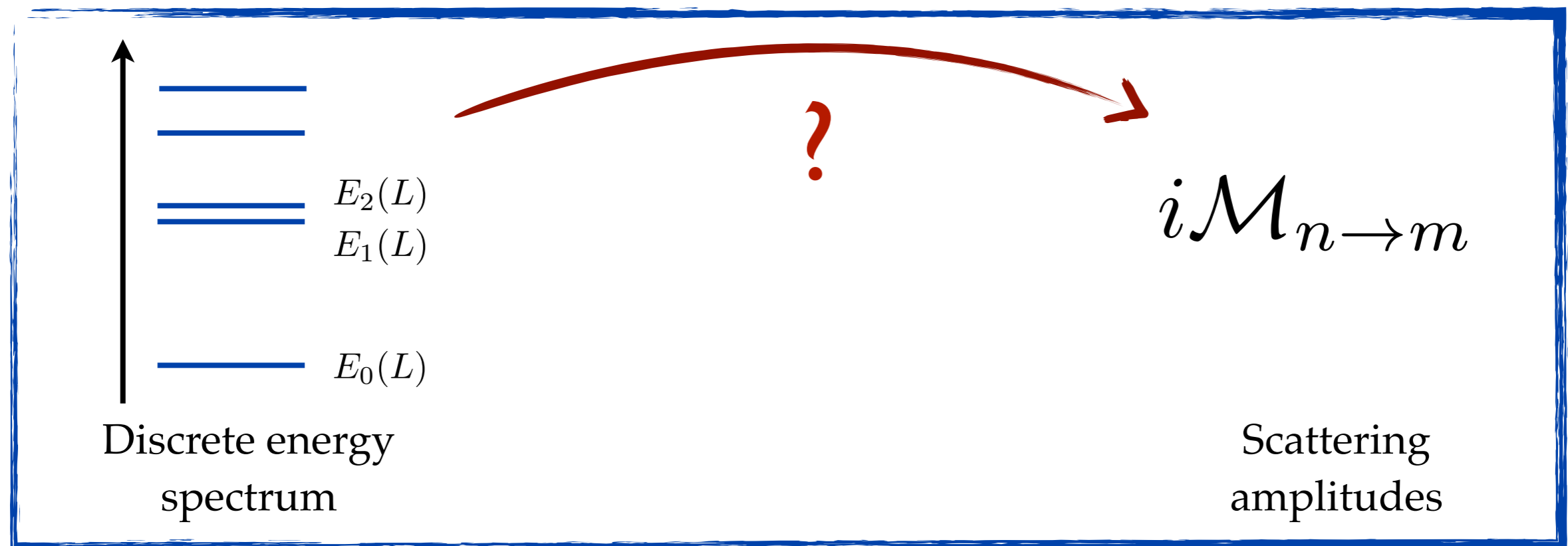
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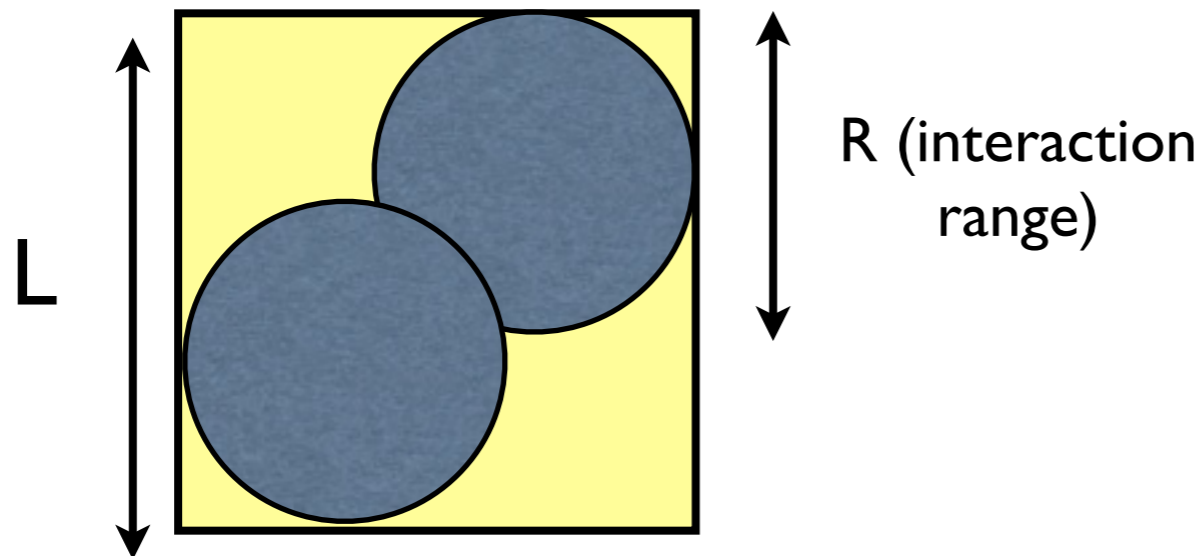
How do we connect these?

The fundamental issue

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



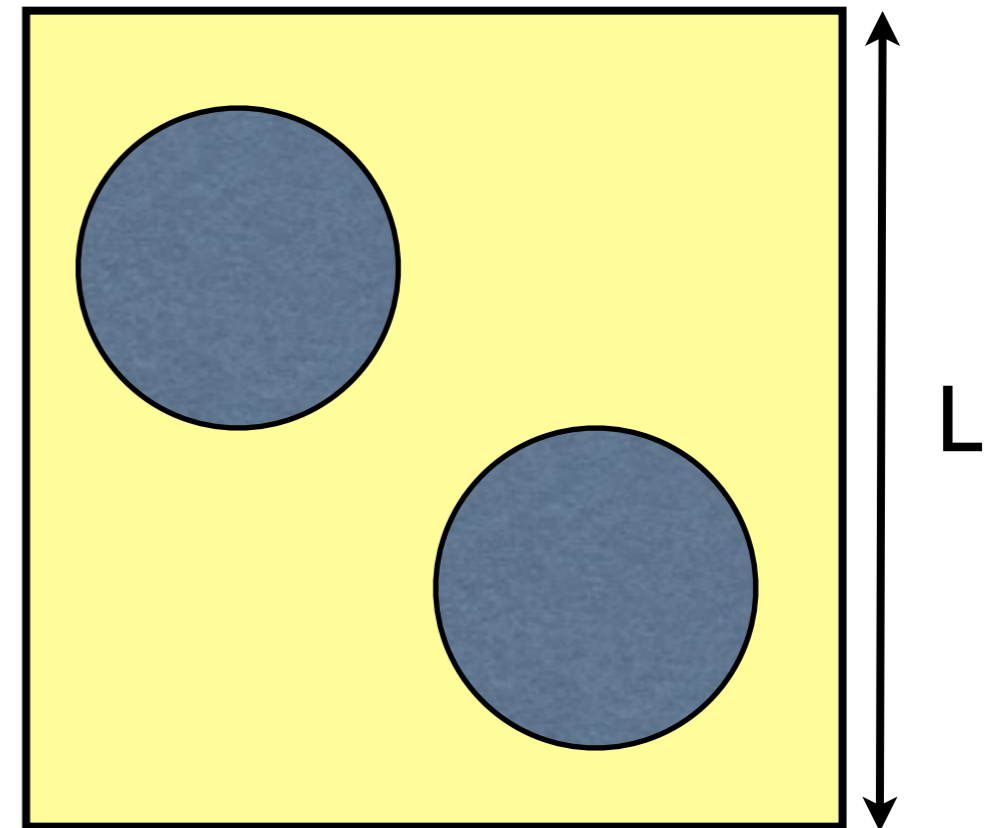
When is spectrum related to scattering amplitudes?



$$L < 2R$$

No “outside” region.

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



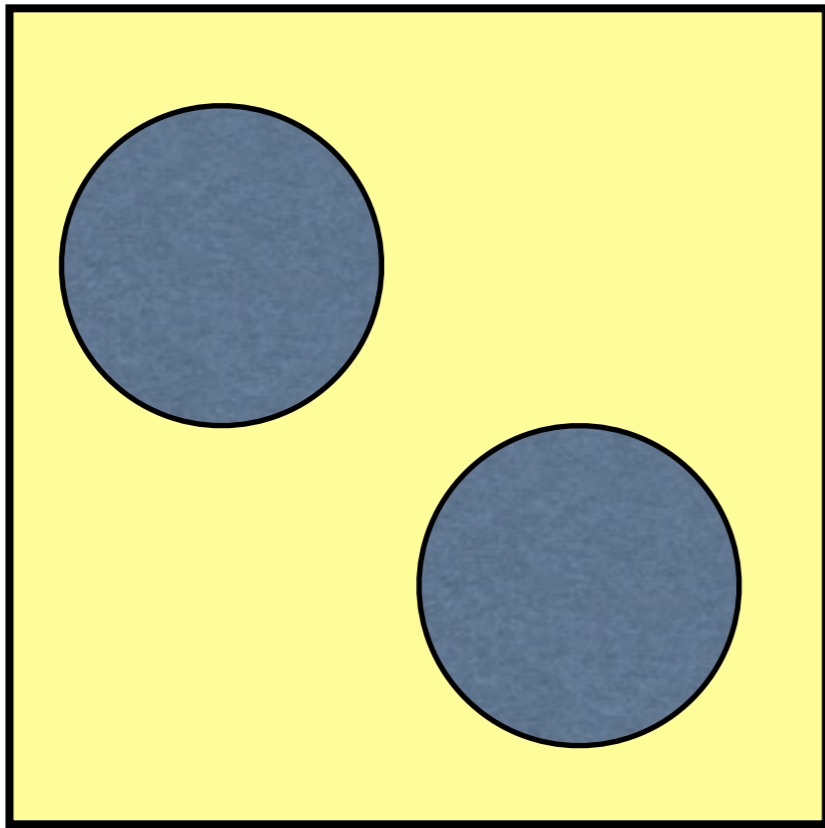
$$L > 2R$$

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

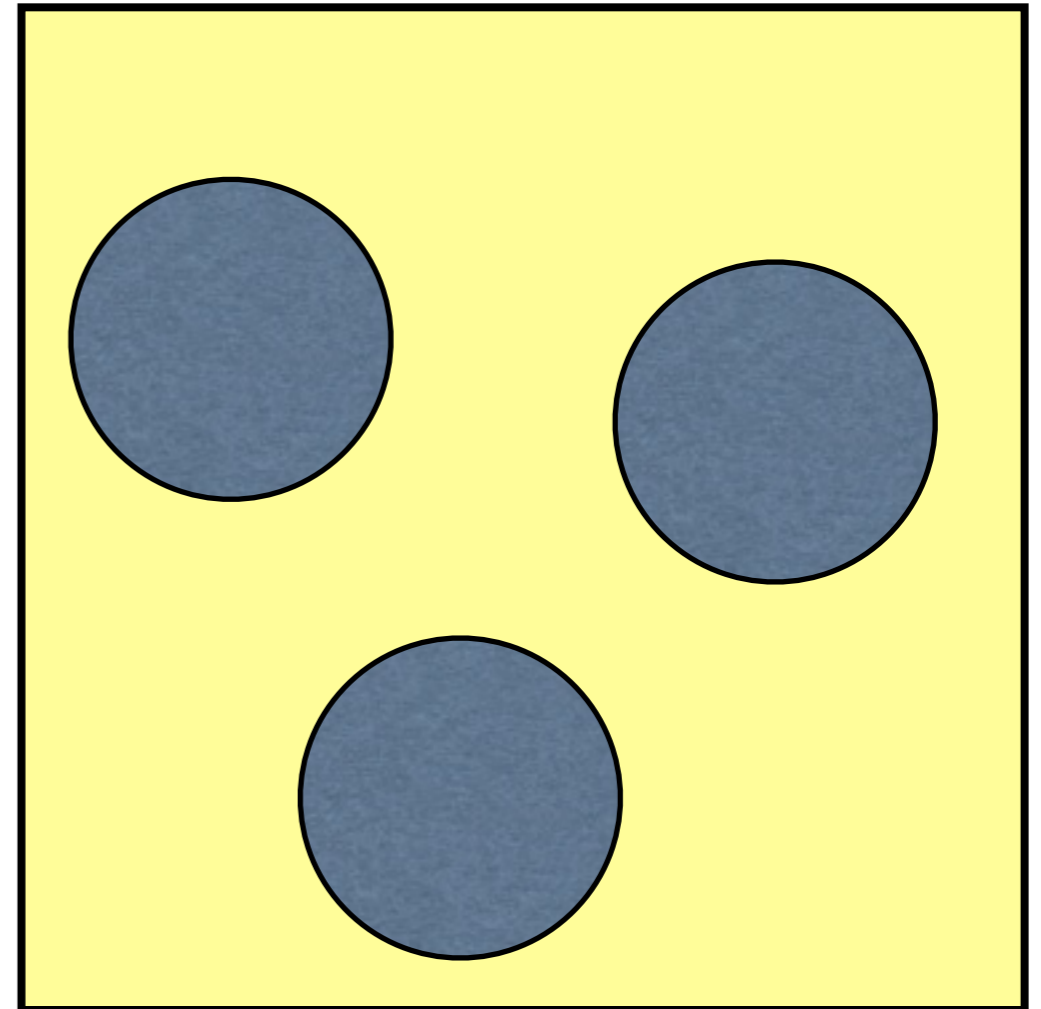


Theoretically understood;
numerical implementations mature

[Mohler, Wilson]

What about including QED?

[Beane, Davoudi]



Formalism under development

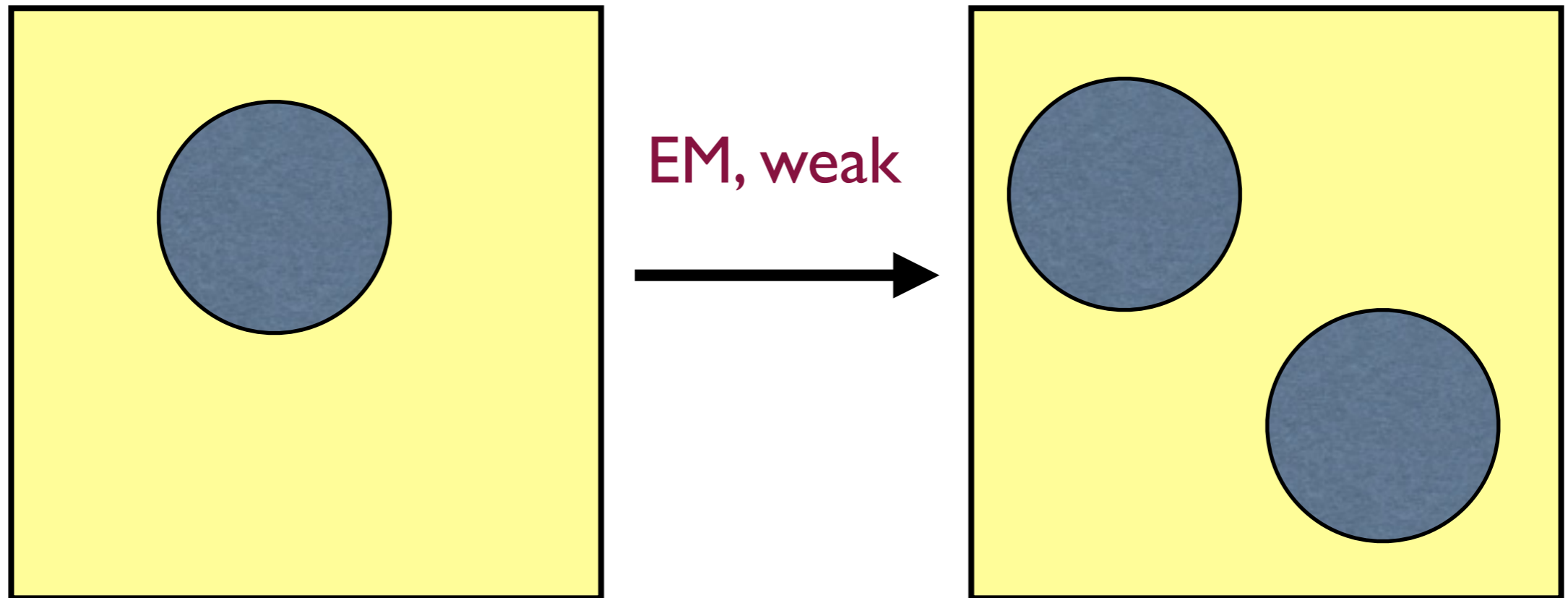
[Hansen]

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

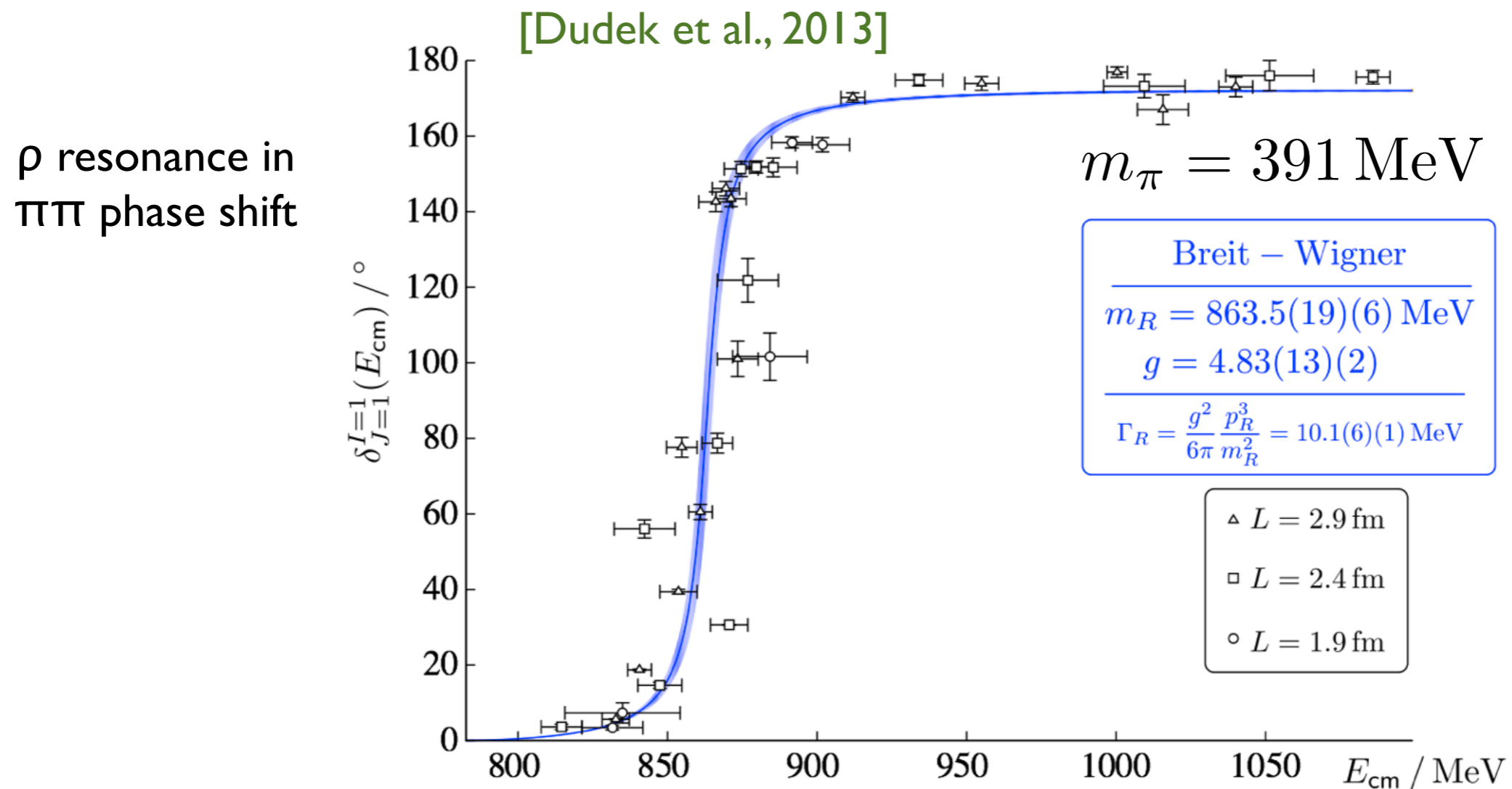
Studying resonances

- **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* $K_{\text{df},3}$; relation between $K_{\text{df},3}$ & \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]

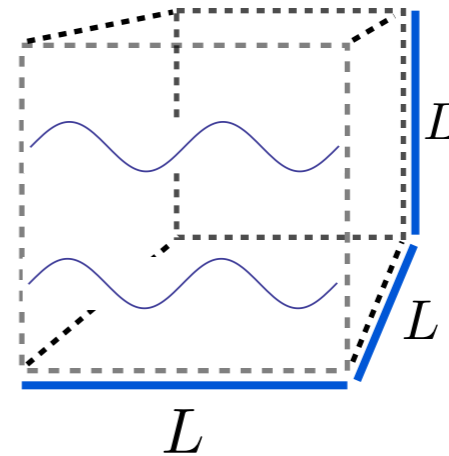
Set-up

- 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: $\frac{1}{L^3} \sum_{\vec{k}}$
- Easily extend to other BC (e.g. twisted)

- Consider general QFT with arbitrary vertices



$$\vec{k} = \frac{2\pi}{L} \vec{n}$$

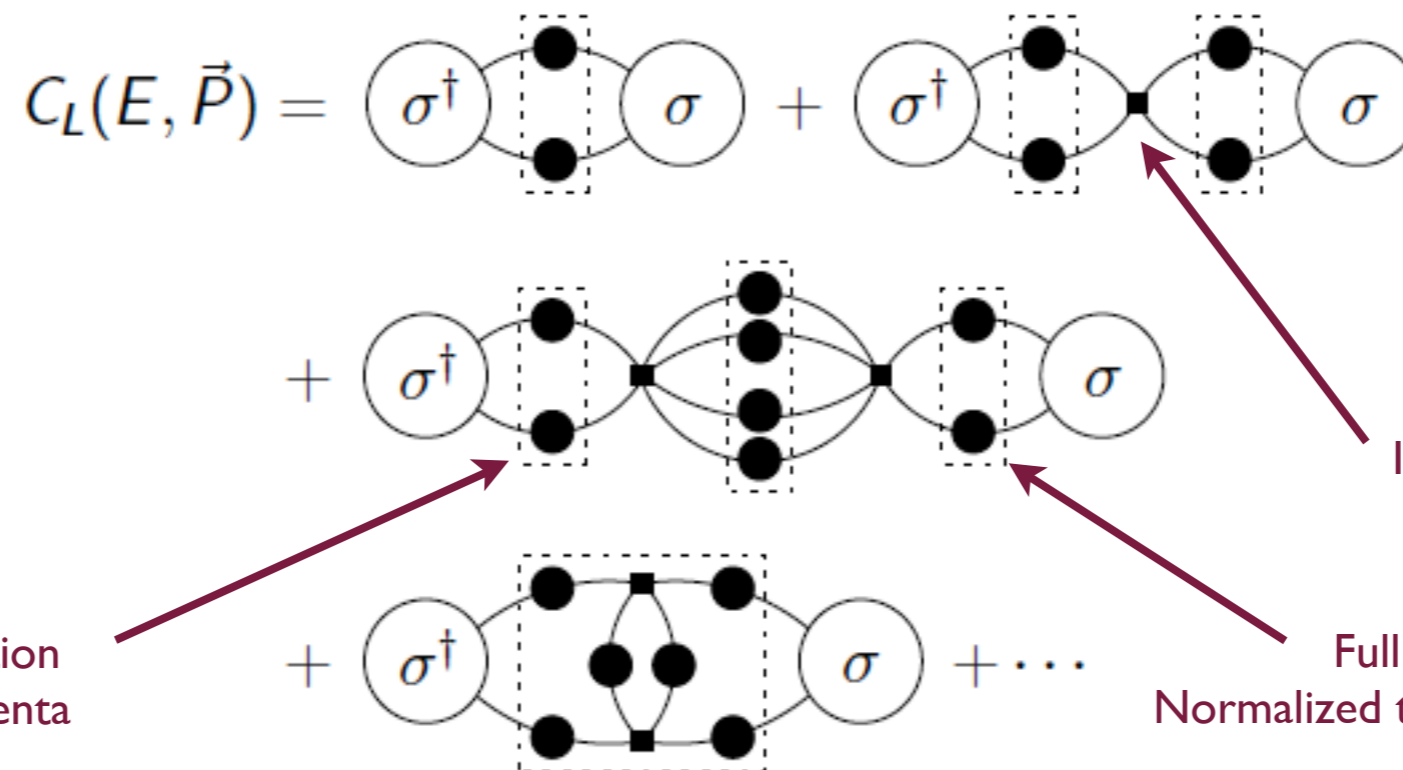
Methodology

- 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, $\sigma \sim \pi^2$ & π^3 , respectively
- Use all-orders diagrammatic expansion, e.g.



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

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]

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

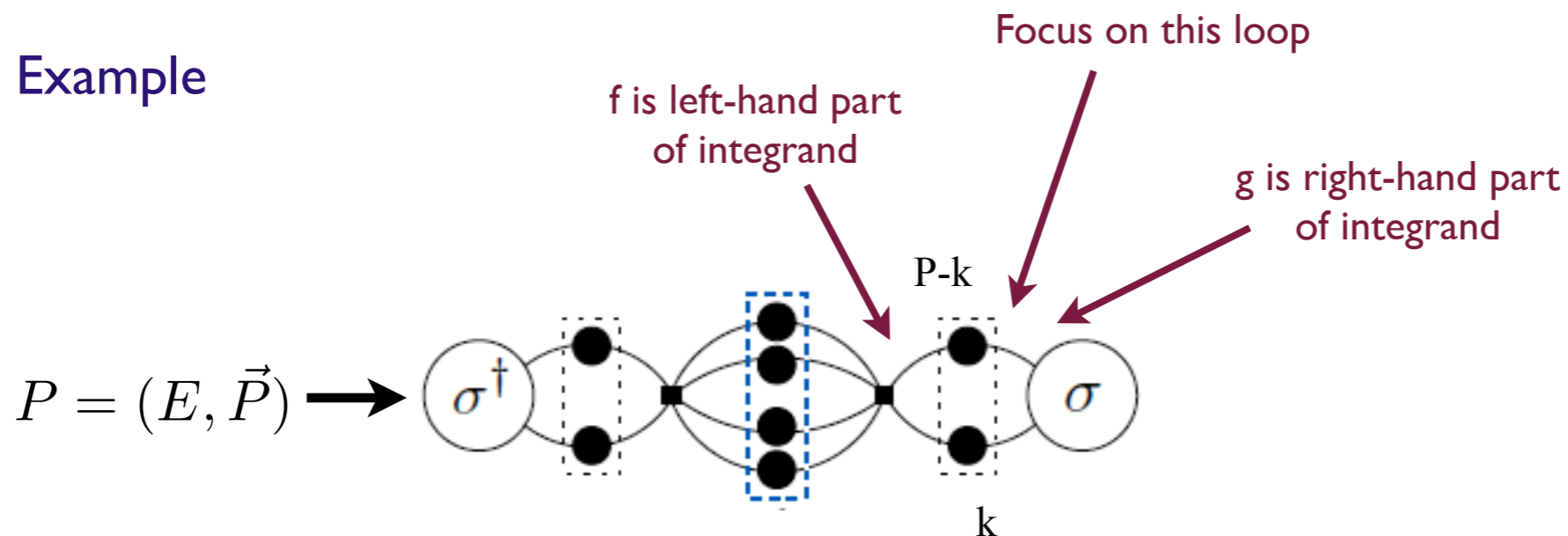
$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F}(q^*, q^{*'}) g^*(\hat{q}^{*'}) + \text{exp. suppressed}$$

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]

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

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

- 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

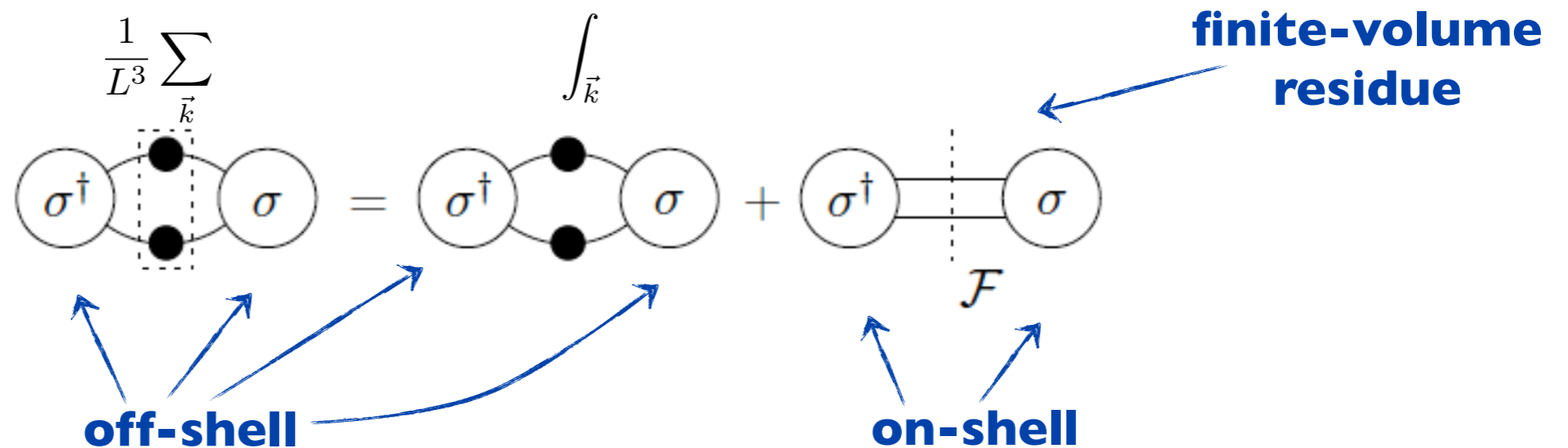
Key step 2

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

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

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

- Diagrammatically



Variant of key step 2

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

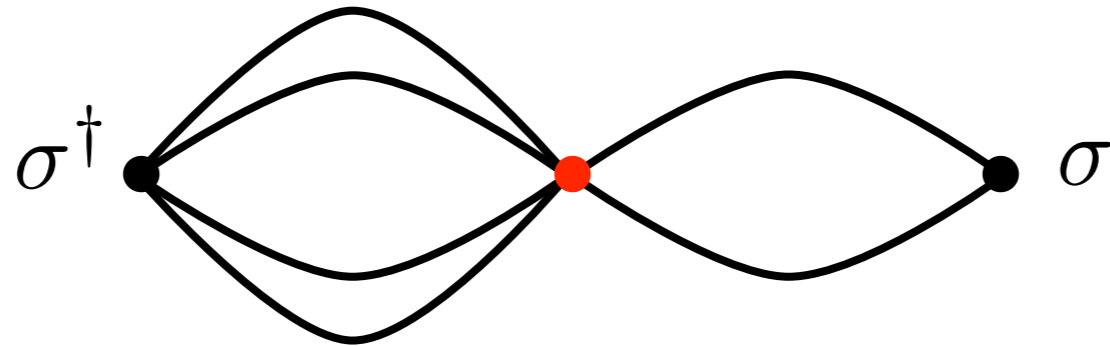
$$\left(\int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \widetilde{\textcolor{red}{PV}} \int \frac{d^4 k}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2 + \textcolor{red}{X}} \frac{1}{(P - k)^2 - m^2 + \textcolor{red}{X}} g(k)$$

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

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

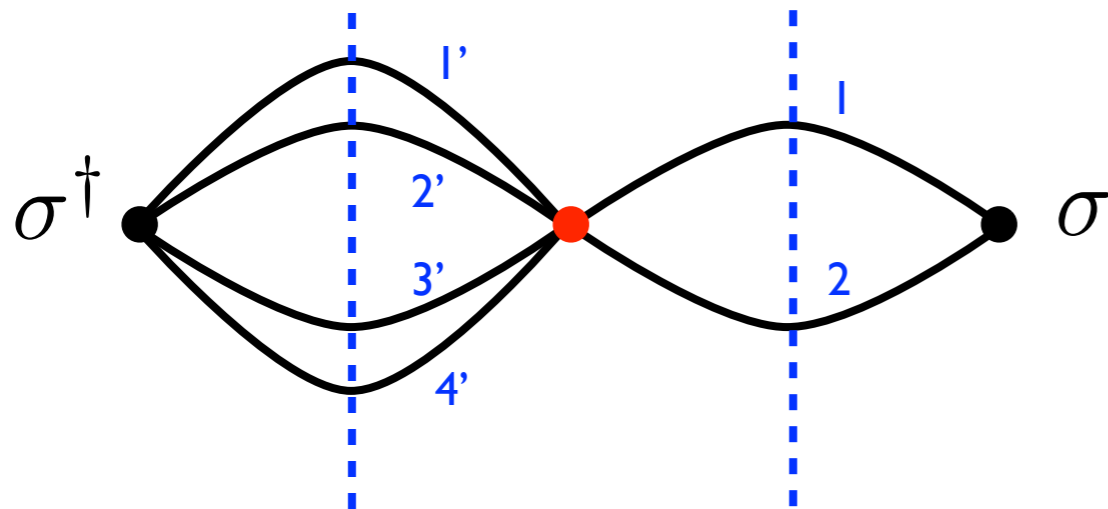
Key step 3

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



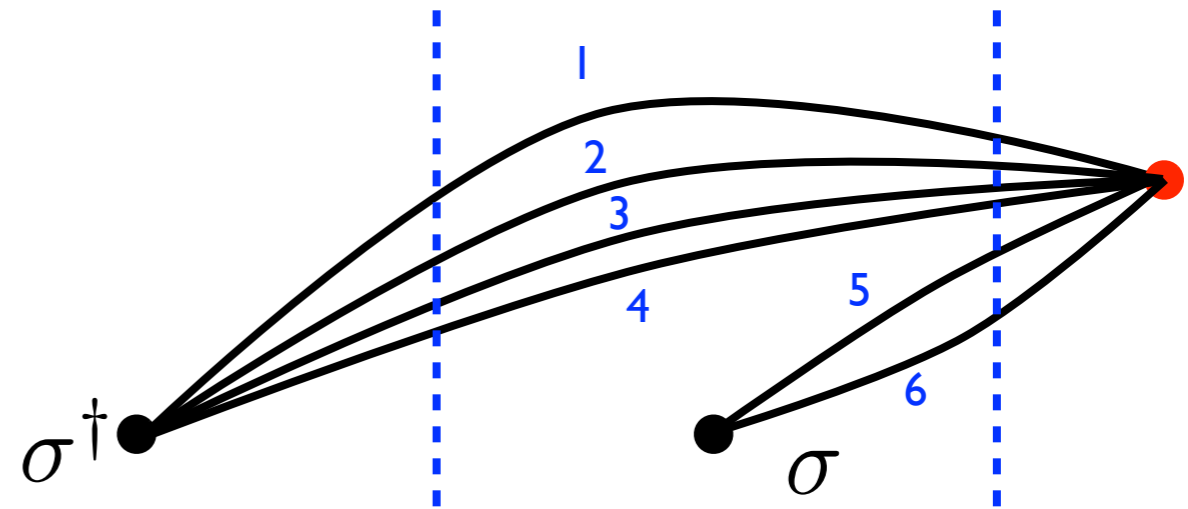
Key step 3

- 2 out of 6 time orderings:



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

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



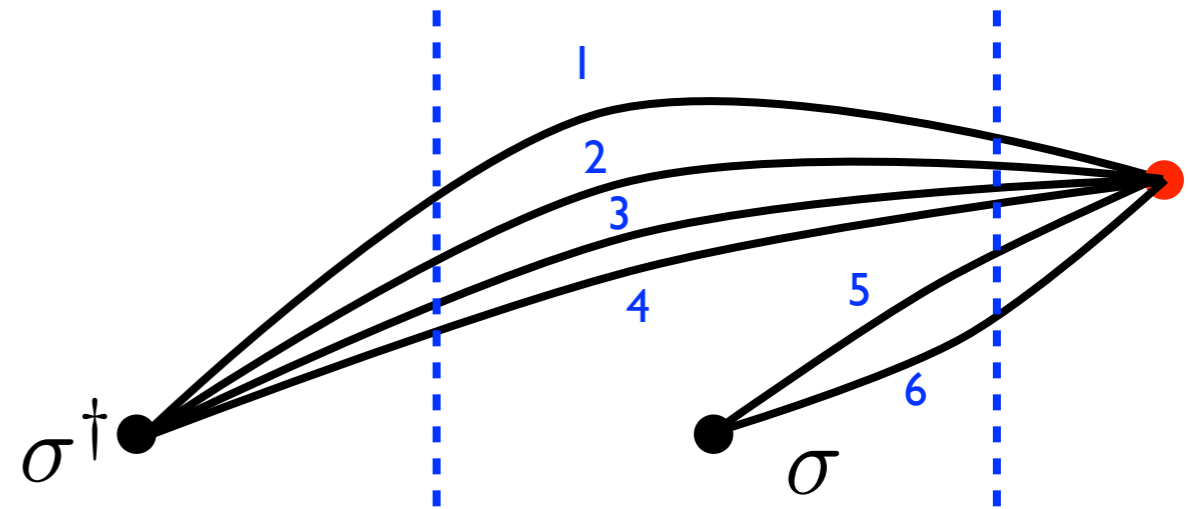
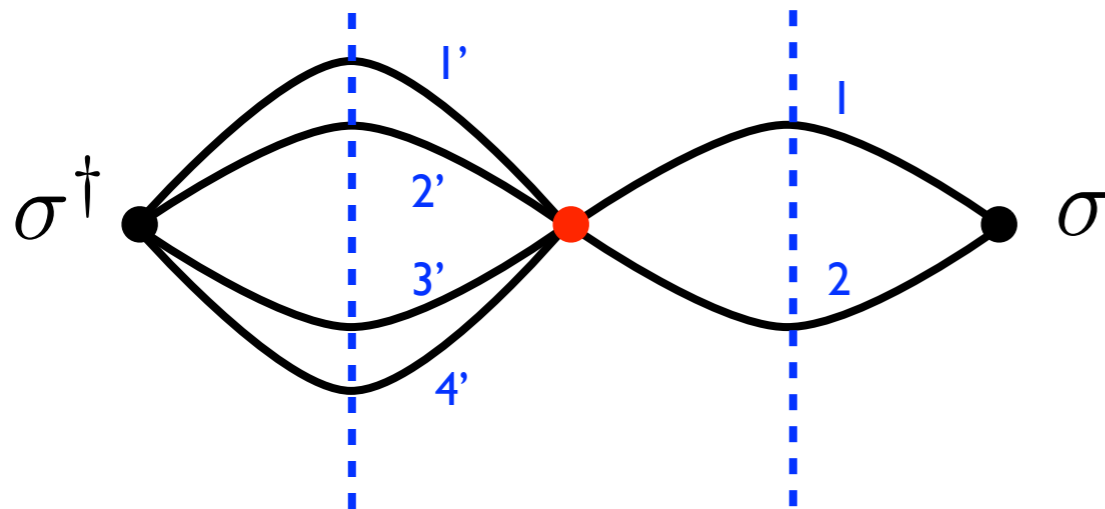
$$\frac{1}{E - \omega_1 - \omega_2 - \omega_3 - \omega_4}$$

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

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

Key step 3

- 2 out of 6 time orderings:



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

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

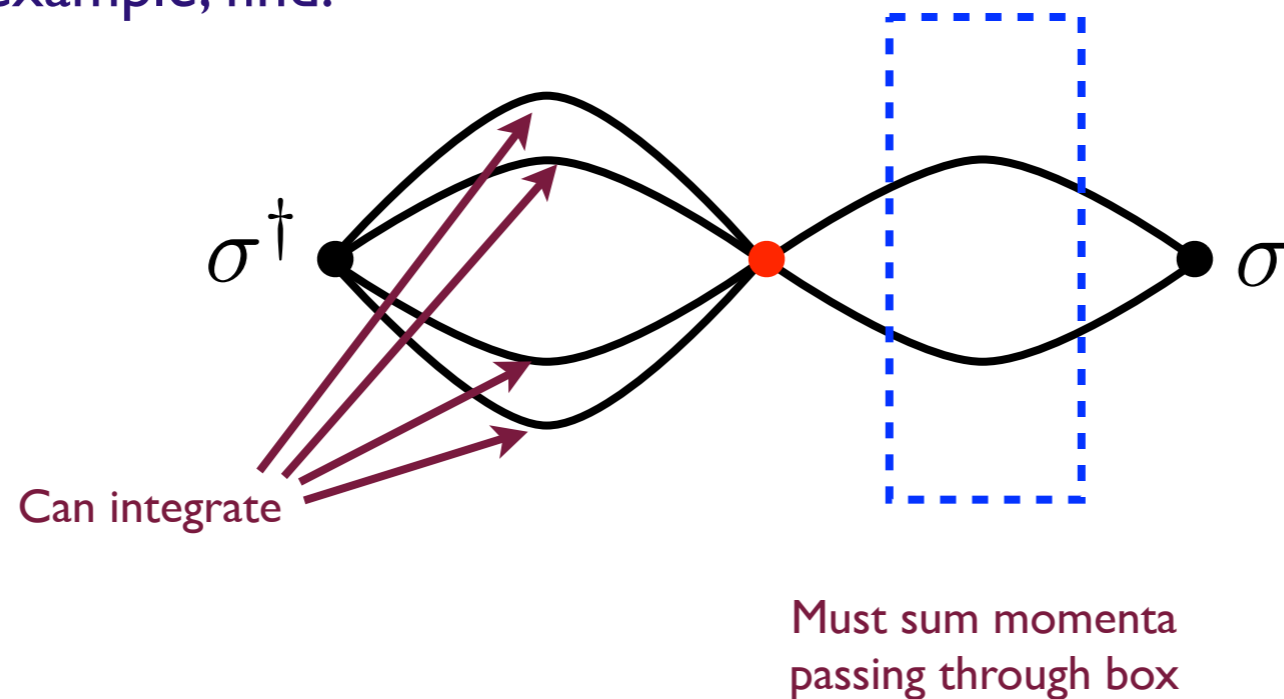
$$\frac{1}{E - \omega_1 - \omega_2 - \omega_3 - \omega_4}$$

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

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

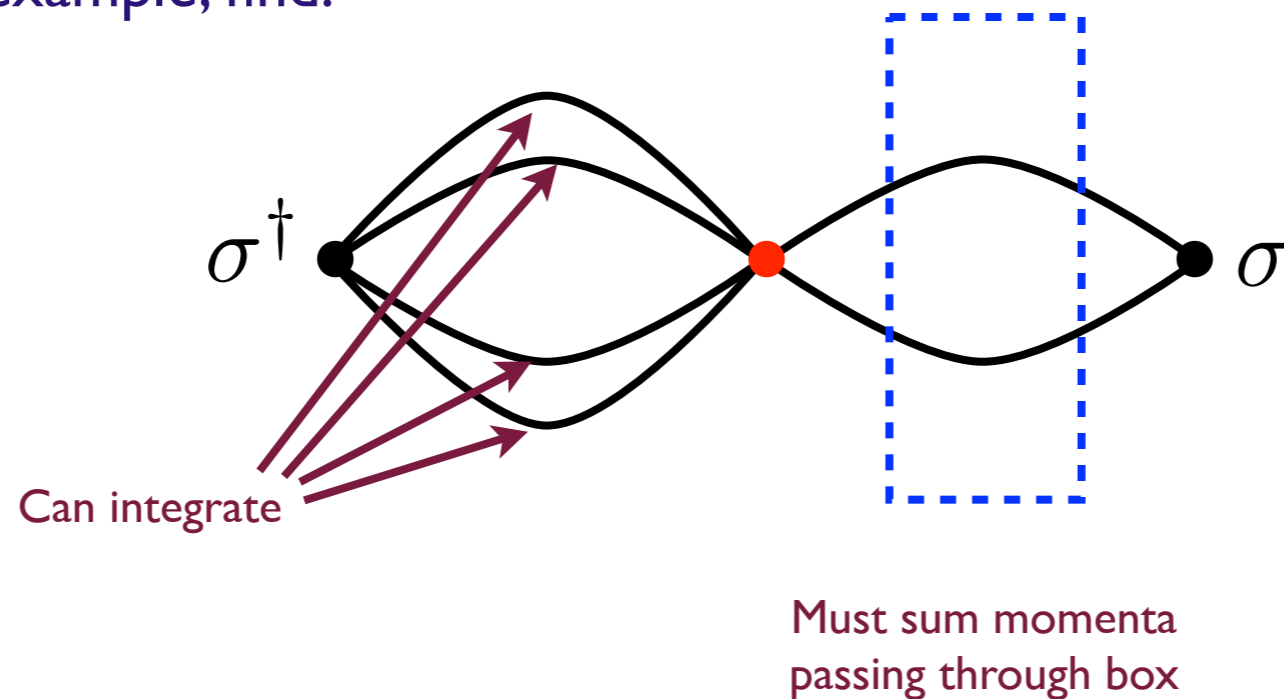
Combining key steps 1-3

- 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 with σ^\dagger and σ connected by two internal lines, with a dashed box around the internal lines. The second term is a similar diagram followed by a bracket containing a series of diagrams representing the Bethe-Salpeter kernel. A blue arrow points from a cloud-like shape labeled iB to the first diagram in the bracket. The diagrams in the bracket include a self-energy loop, a four-point interaction, and a two-point interaction. The series ends with an ellipsis, followed by another diagram with a dashed box and a final ellipsis.

- Leading to

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

The diagram shows the resummed form of the 2-particle correlator. The first term is the same as the first term in the previous equation. The second term is a diagram with two iB kernels inserted between the external lines. The third term is a diagram with three iB kernels inserted. The series ends with an ellipsis.

- Next use sum identity

$$C_L(E, \vec{P}) = \begin{array}{c} \text{diagram 1} + \text{diagram 2} \\ + \text{diagram 3} + \dots \end{array}$$

Diagram 1: σ^\dagger and σ connected by a dashed box with two black dots.

Diagram 2: σ^\dagger and σ connected by a dashed box with two black dots, and a circle labeled iB with two black dots.

Diagram 3: σ^\dagger and σ connected by a dashed box with two black dots, and two circles labeled iB with two black dots each.

Diagram 4: σ^\dagger and σ connected by a dashed box with two black dots, and a circle labeled iB with two black dots, and a dashed line labeled F connecting the iB circle to σ .

Diagram 5: σ^\dagger and σ connected by a dashed box with two black dots, and a circle labeled iB with two black dots, and a dashed line labeled F connecting the iB circle to σ .

Diagram 6: σ^\dagger and σ connected by a dashed box with two black dots, and a dashed line labeled F connecting σ^\dagger to a circle labeled iB with two black dots, which is then connected to σ .

Diagram 7: σ^\dagger and σ connected by a dashed box with two black dots, and a dashed line labeled F connecting σ^\dagger to a circle labeled iB with two black dots, which is then connected to a dashed line labeled F connecting to σ .

- Alternate form if use PV-tilde prescription:

$$C_L(E, \vec{P}) = C_\infty^{\widetilde{PV}}(E, \vec{P}) + \begin{array}{c} F_{\widetilde{PV}} \\ \text{diagram 1} \end{array} + \begin{array}{c} \text{diagram 2} \\ F_{\widetilde{PV}} \end{array} + \dots$$

Diagram 1: A and A' connected by a dashed line labeled $F_{\widetilde{PV}}$.

Diagram 2: A and A' connected by a dashed line labeled $F_{\widetilde{PV}}$, and a circle labeled iB with two black dots.

Diagram 3: A and A' connected by a dashed line labeled $F_{\widetilde{PV}}$, and two circles labeled iB with two black dots each.

Diagram 4: A and A' connected by a dashed line labeled $F_{\widetilde{PV}}$, and a circle labeled iK with two black 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 diagrams representing finite-volume corrections. Each diagram consists of a horizontal line with circles at the ends and vertices. Vertical dashed lines labeled F represent finite-volume insertions.

- Diagram 1: A circle labeled A on the left, connected by a horizontal line to a circle labeled A' on the right. A vertical dashed line labeled F is between them.
- Diagram 2: A circle labeled A on the left, connected by a horizontal line to a circle labeled $i\mathcal{M}$ in the middle, which is then connected to a circle labeled A' on the right. Two vertical dashed lines labeled F are between the circles.
- Diagram 3: A circle labeled A on the left, connected by a horizontal line to a circle labeled $i\mathcal{M}$, which is connected to another circle labeled $i\mathcal{M}$, which is then connected to a circle labeled A' on the right. Three vertical dashed lines labeled F are between the circles.

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

- Final result:

$$\begin{aligned}
 C_L(E, \vec{P}) &= C_\infty(E, \vec{P}) \\
 &+ \text{diagram with } A \text{ and } A' \text{ connected by } F \\
 &+ \text{diagram with } A \text{ and } A' \text{ connected by } F \text{ and } i\mathcal{M} \\
 &+ \text{diagram with } A \text{ and } A' \text{ connected by } F \text{ and two } i\mathcal{M} \text{ blocks} + \dots
 \end{aligned}$$

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

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

↑ 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 : $i\mathcal{M}_{2 \rightarrow 2; \ell', m'; \ell, m} \propto \delta_{\ell, \ell'} \delta_{m, m'}$
- 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 & \mathbf{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

