Three particle scattering amplitudes from finite-volume simulations

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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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- Experiments are not

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?

### Discrete energy spectrum

- $E_0(L)$
- $E_1(L)$
- $E_2(L)$

### Scattering amplitudes

- $i M_{n\rightarrow m}$

S. Sharpe, “3-particle quantization condition” 03/20/2015, YITP workshop, Kyoto
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]
Problems considered today

Theoretically understood; numerical implementations mature. Will sketch as warm-up problem.

Formalism under development—will present new solution based on generalizing Lüscher’s formalism. Practical applicability under investigation.
Outline

- Motivations
- Status of multi particle quantization conditions
- Set-up and main ideas
- Recap of 2-particle quantization condition
- 3-particle quantization condition (in terms of $K_{df,3}$)
- Utility of 3-particle result: truncation
- Infinite volume relation between $K_{df,3}$ and $M_3$
- Conclusions and outlook
HALQCD method

- There is an alternative approach, followed by the HALQCD collaboration [Aoki et al.], using the Bethe-Salpeter wave-function calculated with lattice QCD to determine scattering amplitudes.
- Extended from 2 particle to 3 (and higher) particle case in non-relativistic domain.
- Potentially more powerful than the Lüscher-like methods I discuss today, but based on certain assumptions.
Motivations
1. Studying resonances

- Most hadrons are resonances
  - Resonances are not asymptotic states; show up in behavior of scattering amplitudes
  - FV methods determine scattering amplitudes indirectly
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\[ m_\pi = 391 \text{ MeV} \]

[ρ resonance in ππ phase shift]

\[ \rho \text{ resonance in } \pi\pi \text{ phase shift} \]

[Dudek et al., 2013]
1. Studying resonances

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

- Many resonances have three particle decay channels
  \[ \omega(782) \rightarrow \pi \pi \pi \quad K^* \rightarrow K \pi \pi \quad N(1440) \rightarrow N \pi \pi \]
1. Studying resonances

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

- Many resonances have three particle decay channels
  
  \[
  \omega(782) \rightarrow \pi\pi\pi \quad K^* \rightarrow \pi\pi K \quad N \rightarrow N\pi\pi
  \]

Need three-particle methods to systematically predict resonance properties from first principles.
2. 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.
2. Determining interactions

- For nuclear physics need **NN** and **NNN** interactions
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- Meson interactions needed for understanding pion & kaon condensates
  - $$\pi\pi$$, $$K\bar{K}$$, $$\pi\pi\pi$$, $$\pi K\bar{K}$$, etc.

Need three-particle methods to systematically determine 3-particle interactions from first principles
3. Decay amplitudes

- Calculating weak decay amplitudes allows tests of SM
- Many amplitudes involve 3 (or more) particles
  - $K \rightarrow \pi\pi, \pi\pi\pi$
  - $D \rightarrow \pi\pi, K\bar{K}, \eta\eta, 4\pi, \ldots$
  - $\ldots$
3. Decay amplitudes

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  - $\ldots$

Need 3, 4, $\ldots$ particle methods to determine such decay amplitudes from first principles
Status of multi particle quantization conditions
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 $P$, 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 $1\to2$ weak amplitude (e.g. $K\to\pi\pi$) and infinite volume decay amplitude determined [Lellouch & Lüscher 00]

• LL formula generalized to general $P$, to multiple (2 body) channels, to arbitrary currents, general BCs & arbitrary spin (e.g. $\gamma^*\pi\to\rho\to\pi\pi$, $\gamma^*N\to\Delta\to\pi N$, $\gamma D\to NN$) [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; Briceño & Hansen 15;...

• Leading order QED effects on quantization condition determined [Beane & Savage 14]
State of the art

[Dudek, Edwards, Thomas & Wilson 14]

Coupled two-body channels

$m_\pi \sim 391\,\text{MeV}$
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 $M_2$ and 3-body scattering quantity $K_{df,3}$; relation between $K_{df,3}$ & $M_3$ via integral equations now known

- [Meißner, Rios & Rusetsky 14] determined volume dependence of 3-body bound state in unitary limit
Status for 3 particles

- [Beane, Detmold & Savage 07 and Tan 08] particles in NRQM, and argued it applied also in QFT

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- [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] bound state in unitary limit
Set-up & main ideas
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:
    $$\frac{1}{L^3} \sum \vec{k}$$
    $$\vec{k} = \frac{2\pi}{L} \vec{n}$$

- Consider identical particles with physical mass $m$, interacting \textit{arbitrarily} except for a $\mathbb{Z}_2$ (G-parity-like) symmetry
  - Only vertices are $2 \rightarrow 2$, $2 \rightarrow 4$, $3 \rightarrow 3$, $3 \rightarrow 1$, $3 \rightarrow 5$, $5 \rightarrow 7$, etc.
  - Even & odd particle-number sectors decouple
Methodology

• Calculate (for some $P=2\pi n_P/L$)

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

• Poles in $C_L$ occur at energies of finite-volume spectrum

• For 2 & 3 particle states, $\sigma \sim \pi^2$ & $\pi^3$, respectively

• E.g. for 2 particles:

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

Boxes indicated summation over finite-volume momenta

Infinite-volume vertices

Full propagators Normalized to unit residue at pole
$C_L(E, \vec{P}) = \sigma^\dagger_3 + \sigma_3 + \cdots$

Boxes indicate summation over finite-volume momenta

Infinite-volume vertices

Full propagator
Key step 1

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

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

\[
\frac{1}{L^3} \sum_k g(k) = \int \frac{d^3k}{(2\pi)^3} g(k) + \sum_{l \neq 0} \int \frac{d^3k}{(2\pi)^3} e^{iLl \cdot k} g(k)
\]

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]

\[
\left( \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_k - \int \frac{d^4k}{(2\pi)^4} \right) \frac{1}{k^2 - m^2 + i\epsilon} \frac{1}{(P - k)^2 - m^2 + i\epsilon} g(k) \\
= \int d\Omega_q^* d\Omega_q^{*\prime} f^* (\hat{q}^*) \mathcal{F} \ (q^*, q^{*\prime}) g^* (\hat{q}^{*\prime}) + \text{exp. suppressed}
\]

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

Kinematic function

f & g evaluated for ON-SHELL momenta

Depend only on direction in CM
Key step 2

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

\[
\left( \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^4k}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2 + i\epsilon} g(k) = \int d\Omega_{q^*} d\Omega_{\tilde{q}^*} f^*(\tilde{q}^*) \mathcal{F} (q^*, \tilde{q}^*) g^*(\tilde{q}^*) + \text{exp. suppressed}
\]

- Example

\[ P = (E, \vec{P}) \]

\[ \sigma^\dagger \]

- Focus on this loop

q* is relative momentum of pair on left in CM

f & g evaluated for ON-SHELL momenta

Depend only on direction in CM

"sum=integral + [sum-integral]" if integrand has pole, with [KSS]
Key step 2

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

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

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

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

\[
\mathcal{F} \equiv \eta \left[ \frac{Rq^*}{8\pi E^*} \delta_{\ell_1\ell_2} \delta_{m_1m_2} + \frac{i}{2\pi E L} \sum_{\ell,m} x^{-\ell} \mathcal{Z}_{\ell m}^P [1; x^2] \int d\Omega Y_{\ell_1,m_1}^* Y_{\ell,m}^* Y_{\ell_2,m_2} \right]
\]

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

\[ Z_{4,0} & \text{ and } Z_{6,0} \text{ for } P=0 \]  

[Luu & Savage, `11]

\[ \bar{q}^2 = x^2 = (q^*L/2\pi)^2 \]

FIG. 29. The functions \( Z_{4,0}(1; \bar{q}^2) \) (left panel) and \( Z_{6,0}(1; \bar{q}^2) \) (right panel).
Key step 2

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

\[
\left( \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^4k}{(2\pi)^4} \right) \frac{f(k)}{k^2 - m^2 + i\epsilon} \frac{1}{(P - k)^2 - m^2 + i\epsilon} g(k) \\
= \int d\Omega_{q^*} d\Omega_{q^{*\prime}} f^* (\hat{q}^*) \mathcal{F} (q^*, q^{*\prime}) g^* (\hat{q}^{*\prime})
\]

- Diagrammatically

Diagram showing off-shell and on-shell states with finite-volume residue.
Variant of key step 2

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

\[
\left( \int \frac{dk_0}{2\pi L^3} \sum_k \frac{PV}{f(k)} \frac{1}{k^2 - m^2 + i\varepsilon} \frac{1}{(P-k)^2 - m^2 + i\varepsilon} \right) = \int d\Omega_{q^*} d\Omega_{q'^*} f^*(\hat{q}^*) F_{PV}(q^*,q'^*) g^*(\hat{q}'^*)
\]

- Key properties of $F_{PV}$ (discussed below): real and no unitary cusp at threshold
Variant of key step 2

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

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

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

- Key properties of $F_{PV}$ (discussed below): real and no unitary cusp at threshold

- Example of appearance in 3-particle analysis:
Key step 3

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

\[ \sigma^\dagger \]
Key step 3

- 2 out of 6 time orderings:

\[ E - \omega' - \omega_2 - \omega_3 - \omega_4 - \omega_5 \]
\[ E - \omega_1 - \omega_2 - \omega_5 \]
\[ \sum_{j=1,6} \omega_j \]

On-shell energy \( \omega_j = \sqrt{k_j^2 + M^2} \)
Key step 3

- 2 out of 6 time orderings:

- If restrict $M < E^* < 5M$ then only 3-particle “cuts” have singularities, and these occur only when all three particles to go on-shell.
Combining key steps 1-3

- For each diagram, determine which momenta must be summed, and which can be integrated.

- In our 3-particle example, find:

![Diagram showing momenta summation and integration](image)
Combining key steps 1-3

- For each diagram, determine which momenta must be summed, and which can be integrated.

- In our 2-particle example, find:

  Can replace sum with integral here

  But not here
Combining key steps 1-3

- For each diagram, determine which momenta must be summed, and which can be integrated

- In our 2-particle example, find:

  Can replace sum with integral here

  ![Diagram](image)

  But not here

- Then repeatedly use sum = integral + “sum-integral” to simplify
Key issues 4-6

- Dealing with cusps, avoiding divergences in 3-particle scattering amplitude, and dealing with breaking of particle interchange symmetry

- Discuss later!
2-particle quantization condition

Following method of [Kim, Sachrajda & SS 05]
Apply previous analysis to 2-particle correlator \((0 < E^* < 4M)\)

\[
C_L(E, \vec{P}) = \sigma \uparrow \sigma + \sigma \uparrow \sigma \ \ \ \text{these loops are now integrated}
\]

Collect terms into infinite-volume Bethe-Salpeter kernels

\[
C_L(E, \vec{P}) = \sigma \uparrow \sigma + \sigma \uparrow \sigma + \sigma \uparrow \sigma + \cdots
\]
• Apply previous analysis to 2-particle correlator

• Collect terms into infinite-volume Bethe-Salpeter kernels

\[
C_L(E, \vec{P}) = \sigma^\dagger \sigma \quad \Rightarrow \quad \text{Leading to}
\]

\[
C_L(E, \vec{P}) = \sigma^\dagger \sigma + \sigma^\dagger iB \sigma
\]

+ \sigma^\dagger iB iB \sigma + \cdots
Next use sum identity

\[ C_L(E, \vec{P}) = \sigma^\dagger \sigma + \sigma^\dagger iB \sigma + \cdots + \sigma^\dagger iB \sigma + \cdots \]

And regroup according to number of “F cuts”

\[ C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + \left\{ \sigma^\dagger + \sigma^\dagger iB + \cdots \right\}_F = \left\{ \sigma + \sigma^\dagger iB + \sigma + \cdots \right\} + \cdots \]

Matrix elements:
Next use sum identity

\[ C_L(E, \vec{P}) = \sigma^\dagger \sigma + \sigma^\dagger \begin{array}{c} iB \\ \end{array} \sigma + \sigma^\dagger \begin{array}{c} iB \\ \end{array} \sigma + \cdots \]

And keep regrouping according to number of “F cuts”

\[ C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + \begin{array}{c} A \\ \end{array} \begin{array}{c} A' \\ \end{array} + \begin{array}{c} A \\ \end{array} \left\{ \begin{array}{c} iB \\ \end{array} + \begin{array}{c} iB \\ \end{array} + \begin{array}{c} iB \\ \end{array} + \cdots \right\} \begin{array}{c} A' \\ \end{array} + \cdots \]

two F cuts

the infinite-volume, on-shell 2→2 scattering amplitude
Next use sum identity

\[ C_L(E, \vec{P}) = \sigma^\dagger \sigma + \sigma^\dagger iB \sigma + \cdots \]

Alternate form if use PV-tilde prescription:

\[ C_L(E, \vec{P}) = C_{\infty}^{PV}(E, \vec{P}) + F_{\overline{PV}} \]

\[ + A_{PV} \{ iB + iB + iB + \cdots \} A'_{\overline{PV}} + \cdots \]

\[ iK \]

the infinite-volume, on-shell 2\rightarrow2 K-matrix
Final result:

\[ C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + \sum_{n=0}^{\infty} A' iF [iM_{2\to2F}]^n A \]

Correlator is expressed in terms of infinite-volume, physical quantities and kinematic functions encoding the finite-volume effects.
- Final result:

\[
C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + \sum_{n=0}^{\infty} A' i F [i M_{2 \rightarrow 2} i F]^n A
\]

- \(C_L(E, \vec{P}) = C_\infty(E, \vec{P}) + A' i F \frac{1}{1 - i M_{2 \rightarrow 2} i F} A\)

- \(C_L(E, \vec{P})\) diverges whenever \(i F \frac{1}{1 - i M_{2 \rightarrow 2} i F}\) diverges
• Final result:

\[ C_L (E, \vec{P}) = C_\infty (E, \vec{P}) \]

\[ + \frac{1}{1 - iM_{2\rightarrow2}iF} A \]

\[ = C_\infty (E, \vec{P}) + \sum_{n=0}^{\infty} A' iF[iM_{2\rightarrow2}iF]^n A \]

\[ \Rightarrow \quad \Delta_{L, \vec{P}} (E) = \det [(iF)^{-1} - iM_{2\rightarrow2}] = 0 \]
Final result:

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

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

\[ \Rightarrow \quad \Delta_{L, \vec{P}}(E) = \det \left[ (F_{PV})^{-1} + \mathcal{K}_2 \right] = 0 \]
2-particle quantization condition

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

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

- $\mathcal{K}_2, F_{PV}$ are matrices in $l,m$ space

- $\mathcal{K}_2$ 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 $l_{\text{max}}$

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

Equivalent to generalization of s-wave Lüschner equation to moving frame [Rummukainen & Gottlieb]
3-particle quantization condition

Following [Hansen & SS 14]
Final result

- Spectrum is determined (for given $L, P$) by solutions of

$$\Delta_{L, P}(E) = \det \left[ F_3^{-1} + \mathcal{K}_{df, 3} \right] = 0$$

- Superficially similar to 2-particle form ...

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

- ... but $F_3$ contains both kinematical, finite-volume quantities ($F_{PV}$ & $G$) and the dynamical, infinite-volume quantity $\mathcal{K}_2$
Final result

• Spectrum is determined (for given $L, P$) by solutions of

$$\Delta_{L,P}(E) = \det \left[ F_3^{-1} + \mathcal{K}_{df,3} \right] = 0$$

$$F_3 = \frac{F_{PV}}{2\omega L^3} \left[ -\frac{2}{3} + \frac{1}{1 + (1 + \mathcal{K}_2 G)^{-1} \mathcal{K}_2 F_{PV}^{\sim}} \right]$$

$$G_{p,\ell',m';k,\ell,m} = \left( \frac{k^*}{q_p^*} \right)^{\ell'} \frac{4\pi Y_{\ell',m'}(k^*) H(p) H(k) Y_{\ell,m}^{*}(\hat{p}^*)}{2\omega_{kp} (E - \omega_k - \omega_p - \omega_{kp})} \left( \frac{p^*}{q_k^*} \right)^{\ell} \frac{1}{2\omega_k L^3}$$

• Superficially similar to 2-particle form ...

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

• ...but $F_3$ contains both kinematical, finite-volume quantities ($F_{PV}$ & $G$) and the dynamical, infinite-volume quantity $\mathcal{K}_2$
Final result

\[ \Delta_{L,P}(E) = \det \left[ F_3^{-1} + \mathcal{K}_{df,3} \right] = 0 \]

\[ F_3 = \frac{F_{PV}}{2\omega L^3} \left[ -\frac{2}{3} + \frac{1}{1 + (1 + \mathcal{K}_2 G)^{-1} \mathcal{K}_2 F_{PV}} \right] \]

- All quantities are (infinite-dimensional) matrices, e.g. \((F_3)_{klm;l'm'}\), with indices

  [finite volume “spectator” momentum: \(k=2\pi n/L\)] \(\times\) [2-particle CM angular momentum: \(l,m\)]

Three on-shell particles with total energy-momentum \((E, P)\)

- For large \(k\) other two particles are below threshold; must include such configurations by analytic continuation up to a cut-off at \(k \sim m\) [provided by \(H(k)\)]

S. Sharpe, “3-particle quantization condition” 03/20/2015, YITP workshop, Kyoto

47/88
Final result

\[ \Delta_{L,P}(E) = \det \left( F_3^{-1} + \mathcal{K}_{df,3} \right) = 0 \]

\[ F_3 = \frac{F_{\tilde{P}_{\tilde{V}}}}{2\omega L^3} \left[ -\frac{2}{3} + \frac{1}{1 + (1 + \mathcal{K}_2 G)^{-1} \mathcal{K}_2 F_{\tilde{P}_{\tilde{V}}}} \right] \]

- Important limitation: our present derivation requires that all two-particle sub-channels are non-resonant at the spectral energy under consideration

- Resonances imply that \( \mathcal{K}_2 \) has a pole, and this leads to additional finite volume dependence not accounted for in the derivation

- We only have an ugly solution—searching for something better
Final result

\[ \Delta_{L,P}(E) = \det \left[ F_3^{-1} + \mathcal{K}_{df,3} \right] = 0 \]

\[ F_3 = \frac{F_{PV}}{2\omega L^3} \left[ -\frac{2}{3} + \frac{1}{1 + (1 + \mathcal{K}_2 G)^{-1} \mathcal{K}_2 F_{PV}} \right] \]

- Successfully separated infinite volume quantities from finite volume kinematic factors, but….
  - What is \( \mathcal{K}_{df,3} \)?
  - How do we obtain this result?
  - How can it be made useful?
Key issue 4: dealing with cusps

- Can sum subdiagrams without 3-particle cuts into Bethe-Salpeter kernels

\[ C_L(E, \bar{P}) = \sum \text{subdiagrams} \]

\[ \Rightarrow \text{Skeleton expansion in terms of Bethe-Salpeter kernels} \]

\[ iB_2 \equiv \sum \text{subdiagrams} \]

\[ iB_3 \equiv \sum \text{subdiagrams} \]

S. Sharpe, “3-particle quantization condition” 03/20/2015, YITP workshop, Kyoto
Key issue 4: dealing with cusps

- Want to replace sums with integrals + F-cuts as in 2-particle analysis
- Straightforward implementation fails when have 3 particle intermediate states adjacent to $2\to2$ kernels

\[ C_L(E, \vec{P}) = \ldots \]
Cusp analysis (1)

- Aim: replace sums with integrals + finite-volume residue

- E.g.

\[(E, \vec{P}) \rightarrow \frac{1}{L^6} \sum_k \sum \vec{a} \]

\[= \frac{1}{L^6} \sum_k \sum \vec{a} \frac{A(\vec{k}, \vec{a}) B(\vec{k}, \vec{a})}{E - \omega_k - \omega_a - \omega_k a}\]

- Can replace sums with integrals for smooth, non-singular parts of summand

- Singular part of left-hand 3-particle intermediate state

\[\sqrt{k^2 + m^2} \quad \sqrt{a^2 + m^2} \quad \sqrt{(\vec{P} - \vec{k} - \vec{a})^2 + m^2}\]
Cusp analysis (2)

\[
\frac{1}{L^6} \sum \vec{k} \sum \vec{a} \frac{A(\vec{k}, \vec{a}) B(\vec{k}, \vec{a})}{E - \omega_k - \omega_a - \omega_{ka}}
\]

Step 1: treat sum over \(a\)

\[
\frac{1}{L^3} \sum \vec{a} \rightarrow \int \vec{a} + \left( \frac{1}{L^3} \sum \vec{a} - \int \vec{a} \right)
\]

Difference gives zeta-function \(F\) with \(A\) & \(B\) projected on shell [Lüscher,...]

\(F\) has multiple singularities, so leave \(k\) summed for \(F\)-term
Cusp analysis (2)

\[
\frac{1}{L^6} \sum \vec{k} \sum \vec{a} \frac{A(\vec{k}, \vec{a}) B(\vec{k}, \vec{a})}{E - \omega_{k} - \omega_{a} - \omega_{ka}}
\]

Step 1: treat sum over \( a \)

\[
\frac{1}{L^3} \sum \vec{a} \rightarrow \int \vec{a} + \left( \frac{1}{L^3} \sum \vec{a} - \int \vec{a} \right)
\]

Difference gives zeta-function \( F \) with \( A \) & \( B \) projected on shell [Lüscher,...]

Step 2: treat sum over \( k \)

- Want to replace sum over \( k \) with integral for \( \int \vec{a} \) term
- Only possible if integral over \( a \) gives smooth function
- \( i\varepsilon \) prescription and standard principal value (PV) lead to cusps at threshold \( \Rightarrow \) sum-integral \( \sim 1/L^4 \) [Polejaeva & Rusetsky]
- Requires use of modified \( \widetilde{PV} \) prescription

Result:

\[
\frac{1}{L^6} \sum \vec{k} \sum \vec{a} = \int \vec{k} \int \vec{a} + \sum \vec{k} \text{ “F term”}
\]

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Cusp analysis (3)

- Simple example:
  \[ f(c) = \int_0^\infty dx \frac{\sqrt{x} e^{-\frac{(x-c)}{c-x}}}{c-x} \]

- Far below threshold, \( \tilde{PV} \) smoothly turns back into PV.
Cusp analysis (4)

- Bottom line: must use $\tilde{P}V$ prescription for all loops

- This is why K-matrix $K_2$ appears in 2-particle summations

- $K_2$ is standard above threshold, and given below by analytic continuation (so there is no cusp)

- This prescription is that used previously when studying finite-volume effects on bound-state energies using two-particle quantization condition [Detmold, Savage,...]

- Far below threshold smoothly turns into $M_2^\ell$
Key issue 5: dealing with “switches”

\[ C_L(E, \vec{P}) = \ldots \]
Key issue 5: dealing with “switches”

\[ C_L(E, \vec{P}) = \begin{array}{c}
\bigoplus_{0 \text{ switches}} \bigoplus_{1 \text{ switch}} \bigoplus_{2 \text{ switches}} + \\
\end{array} \]

- 0 switches:
- 1 switch:
- 2 switches:

“switch state”
Key issue 5: dealing with “switches”

- With cusps removed, no-switch diagrams can be summed as for 2-particle case
- “Switches” present a new challenge
One-switch diagrams

\[ C_L^{(2)} = C \]

Can treat similarly to 2-particle case leading to a series of \( F_{PV} \)’s and \( K_2 \)’s

• End up with L-dependent part of \( C^{(2)} \) having at its core:

\[ \ell, m \quad k \quad iK_2 \quad \bar{p} \quad \ell', m' \quad iK_2 \]

On-shell

On-shell

• This is our first contribution to the infinite-volume 3 particle scattering amplitude
One-switch problem

- Amplitude is **singular** for some choices of $k$, $p$ in physical regime
  - Propagator goes on shell if top two (and thus bottom two) scatter elastically

- Not a problem per se, but leads to difficulties when amplitude is symmetrized
  - Occurs when include three-switch contributions

- Singularity implies that decomposition in $Y_{\ell m}$ will not converge uniformly
  - Cannot usefully truncate angular momentum expansion
One-switch solution

- Define divergence-free amplitude by subtracting singular part
  - Utility of subtraction noted in [Rubin, Sugar & Tiktopoulos, '66]

\[ iK_{df,3} \supset \ell, m \rightarrow \ell', m' \]

- Key point: \( K_{df,3} \) is local and its expansion in harmonics can be truncated
- Subtracted term must be added back---leads to G contributions to \( F_3 \)
- Can extend divergence-free definition to any number of switches

Always on-shell; can be below threshold

Off-shell except at pole

\[ \begin{align*}
G_{p,\ell',m';k,\ell,m} & = \left( \frac{k^*}{q_p^*} \right)^\ell \frac{4\pi Y_{\ell',m'}(\vec{k}^*) H(\vec{p}) H(\vec{k}) Y_{\ell,m}(\vec{p}^*)}{2\omega_{kp}(E - \omega_k - \omega_p - \omega_{kp})} \left( \frac{p^*}{q_k^*} \right)^\ell \frac{1}{2\omega_k L^3}
\end{align*} \]
Key issue 6: symmetry breaking

- Using $\widetilde{\text{PV}}$ prescription breaks particle interchange symmetry
- Top two particles treated differently from spectator
- Leads to very complicated definition for $K_{df,3}$, e.g.

\[ iK_{df,3} \]
Key issue 6: symmetry breaking

- Final definition of $K_{df,3}$ is, crudely speaking:
  - Sum all Feynman diagrams contributing to $M_3$
  - Use $\tilde{PV}$ prescription, plus a (well-defined) set of rules for ordering integrals
  - Subtract leading divergent parts
  - Apply a set of (completely specified) extra factors ("decorations") to ensure external symmetrization

- $K_{df,3}$ is an UGLY infinite-volume quantity related to scattering

- At the time of our initial paper, we did not know the relation between $K_{df,3}$ and $M_3$ & $M_2$, although we had reasons to think that such a relationship exists

- Now we know the relationship
Final result

\[
\Delta_{L,P}(E) = \det \left[ F_3^{-1} + K_{df,3} \right] = 0
\]

\[
F_3 = \frac{F_{PV}}{2\omega L^3} \left[ -\frac{2}{3} + \frac{1}{1 + (1 + K_2 G)^{-1} K_2 F_{PV}} \right]
\]

• Successfully separated infinite volume quantities from finite volume kinematic factors, but …

• But what is \( K_{df,3} \)? ✓

• How do we obtain this result? ✓

• How can it be made useful?
Utility of result:
truncation
Truncation in 2 particle case

\[ \Delta_{L,\vec{p}}(E) = \det \left[ \left( \frac{F}{P_V} \right)^{-1} + \mathcal{K}_2 \right] = 0 \]

- If \( \mathcal{M} \) (which is diagonal in \( l,m \)) vanishes for \( l > l_{\text{max}} \) then can show that need only keep \( l \leq l_{\text{max}} \) in \( F \) (which is not diagonal) and so have finite matrix condition which can be inverted to find \( \mathcal{M}(E) \) from energy levels.
Truncation in 3 particle case

\[ \Delta_{L,P}(E) = \det \left[ F_3^{-1} + K_{df,3} \right] = 0 \]

\[ F_3 = \frac{F_{PV}}{2\omega L^3} \left[ -\frac{2}{3} + \frac{1}{1+(1+K_2G)^{-1}K_2F_{PV}} \right] \]

- For fixed E & P, as spectator momentum \(|k|\) increases, remaining two-particle system drops below threshold, so \(F_{PV}\) becomes exponentially suppressed
  - Smoothly interpolates to \(F_{PV}=0\) due to H factors; same holds for G
- Thus \(k\) sum is naturally truncated (with, say, \(N\) terms required)
- \(l\) is truncated if both \(K_2\) and \(K_{df,3}\) vanish for \(l > l_{max}\)
- Yields determinant condition truncated to \([N(2l_{max}+1)]^2\) block
Truncation in 3 particle case

\[ \Delta_{L,P}(E) = \det \left[ F_{3}^{-1} + \mathcal{K}_{df,3} \right] = 0 \]

\[ F_{3} = \frac{F_{PV}^{\infty}}{2\omega L^{3}} \left[ -\frac{2}{3} + \frac{1}{1+(1+\mathcal{K}_{2}G)^{-1}\mathcal{K}_{2}F_{PV}} \right] \]

- Given prior knowledge of \( \mathcal{K}_{2} \) (e.g. from 2-particle quantization condition) each energy level \( E_{i} \) of the 3 particle system gives information on \( \mathcal{K}_{df,3} \) at the corresponding 3-particle CM energy \( E_{i}^{*} \)

- Probably need to proceed by parameterizing \( \mathcal{K}_{df,3 \rightarrow 3} \), in which case one would need at least as many levels as parameters at given energy

- Given \( \mathcal{K}_{2} \) and \( \mathcal{K}_{df,3} \) one can reconstruct \( \mathcal{M}_{3} \)

- The locality of \( \mathcal{K}_{df,3} \) is crucial for this program

- Clearly very challenging in practice, but there is an existence proof....
Isotropic approximation

- Assume $K_{df,3}$ depends only on $E^*$ (and thus is indep. of $k, l, m$)

- Also assume $K_2$ only non-zero for s-wave ($\Rightarrow l_{\text{max}}=0$) and known

- Truncated $[N \times N]$ problem simplifies: $K_{df,3}$ has only 1 non-zero eigenvalue, and problem collapses to a single equation:

\[
1 + F_3^{\text{iso}} K_{df,3}^{\text{iso}}(E^*) = 0
\]

Known in terms of two particle scattering amplitude

\[
F_3^{\text{iso}} \equiv \sum_{k,p} \frac{1}{2\omega_k L^3} \left[ F_{PV}^s \left( -\frac{2}{3} + \frac{1}{1 + [1 + K_{2}^{s} G^{s}]^{-1} K_{2}^{s} F_{PV}^s} \right) \right]_{k,p}
\]
Infinite volume relation between $K_{df,3}$ & $M_3$

[Hansen & SS 15, in preparation]
The issue

• Three particle quantization condition depends on $K_{df,3}$ rather than the three particle scattering amplitude $M_3$

• $K_{df,3}$ is an infinite volume quantity (loops involve integrals) but is not physical
  • Has a very complicated, unwieldy definition
  • Depends on the cut-off function $H$
  • However, it was forced on us by the analysis, and is some sort of local vertex

• To complete the quantization condition we must relate $K_{df,3}$ to $M_3$
The method

• Define a “finite volume scattering amplitude” $M_{L,3}$ which goes over to $M_3$ in an (appropriately taken) $L \to \infty$ limit

• Relate $M_{L,3}$ to $K_{df,3}$ at finite volume—which turns out to require a small generalization of the methods used to derive the quantization condition

• Take $L \to \infty$, obtaining nested integral equations
Modifying $C_L$ to obtain $\mathcal{M}_{L,3}$

\[
C_L(E, \tilde{P}) = C_\infty(E, \tilde{P}) + A_3' i F_3 \frac{1}{1 - i\mathcal{K}_{df,3\rightarrow3}} i F_3 A_3
\]

no poles

no poles

no poles
Modifying $C_L$ to obtain $M_{L,3}$

Step 1: “amputate”
Modifying $C_L$ to obtain $M_{L,3}$

Step 2: Drop disconnected diagrams
Modifying $C_L$ to obtain $M_{L,3}$

\[ iM_{L,3} \equiv S \left\{ \begin{array}{c}
\text{Step 3: Symmetrize}
\end{array} \right\} \]

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$\mathcal{M}_{L,3}$ in terms of $\mathcal{K}_{df,3}$

$$i\mathcal{M}_{L,3 \rightarrow 3} \equiv S \left\{ \begin{array}{c}
    \text{terms involving } M_{\vec{k}} \\
    \text{terms involving } \mathcal{K}_{df,3} \\
    \text{higher-order terms} \\
    \end{array} \right\}$$

$$i\mathcal{M}_{L,3 \rightarrow 3} = i\mathcal{D}_L + S \left[ \mathcal{L}_L \ i\mathcal{K}_{df,3 \rightarrow 3} \ \frac{1}{1 - iF_3 \ i\mathcal{K}_{df,3 \rightarrow 3}} \ \mathcal{R}_L \right]$$

$$i\mathcal{D}_L \equiv S \left[ \frac{1}{1 - i\mathcal{M}_{L,2 \rightarrow 2} \ iG} \ i\mathcal{M}_{L,2 \rightarrow 2} \ iG \ i\mathcal{M}_{L,2 \rightarrow 2} [2\omega L^3] \right]$$

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\[ M_{L,3} \text{ in terms of } K_{df,3} \]

\[ iM_{L,3 \rightarrow 3} = iD_L + S \left[ L_L \frac{iK_{df,3 \rightarrow 3}}{1 - IF_3} \frac{1}{iK_{df,3 \rightarrow 3}} R_L \right] \]

\[ iD_L \equiv S \left[ \frac{1}{1 - iM_{L,2 \rightarrow 2}} IG iM_{L,2 \rightarrow 2} IG iM_{L,2 \rightarrow 2}[2\omega L^3] \right] \]

- \( L_L \) and \( R_L \) depend only on \( M_{L,2} \), \( G \) and \( F_{PV} \)
- \( M_{L,2} \) is “finite volume two particle scattering amplitude”

\[ iM_{L,2 \rightarrow 2} \equiv iK_{2 \rightarrow 2} \frac{1}{1 - IF_iK_{2 \rightarrow 2}^{PV}} \]
$\mathcal{M}_{L,3}$ in terms of $\mathcal{K}_{df,3}$

\[
i\mathcal{M}_{L,3} \rightarrow 3 = i\mathcal{D}_L + S \left[ \mathcal{L}_L \, i\mathcal{K}_{df,3} \rightarrow 3 \frac{1}{1 - iF_3 \, i\mathcal{K}_{df,3} \rightarrow 3} \, \mathcal{R}_L \right]
\]

\[
i\mathcal{D}_L \equiv S \left[ \frac{1}{1 - i\mathcal{M}_{L,2} \rightarrow 2 \, iG} \, i\mathcal{M}_{L,2} \rightarrow 2 \, iG \, i\mathcal{M}_{L,2} \rightarrow 2 [2 \omega L^3] \right]
\]

- **Key point:** the same (ugly) $\mathcal{K}_{df,3}$ appears in $\mathcal{M}_{L,3}$ as in $\mathcal{C}_L$

\[
\mathcal{C}_L(E, \vec{P}) = C_\infty(E, \vec{P}) + A'_3 \, iF_3 \frac{1}{1 - i\mathcal{K}_{df,3} \rightarrow 3 \, iF_3 \, A_3}
\]

- **Can use** $\mathcal{M}_{L,3}$ **to derive quantization condition**
Final step: taking $L \to \infty$

\[ i\mathcal{M}_{L,3 \to 3} = i\mathcal{D}_L + S \left[ \mathcal{L}_L \frac{1}{1 - iF_3} i\mathcal{K}_{df,3 \to 3} \mathcal{R}_L \right] \]

\[ i\mathcal{D}_L \equiv S \left[ \frac{1}{1 - i\mathcal{M}_{L,2 \to 2}} iG i\mathcal{M}_{L,2 \to 2} \mathcal{R}_L \right] \]

\[ iF_3 \equiv \frac{iF_{PV}}{2\omega L^3} \left[ \frac{1}{3} + \frac{1}{1 - i\mathcal{M}_{L,2 \to 2}} iG i\mathcal{M}_{L,2 \to 2} \mathcal{F}_{PV} \right] \]

- All equations involve matrices with indices $k, l, m$

Spectator momentum
\[ k = 2n \pi / L \]
Summed over $n$

Already in infinite volume variables
Final step: taking $L \to \infty$

\[
i \mathcal{M}_{L,3\to3} = i \mathcal{D}_L + S \left[ \mathcal{L}_L \ i\mathcal{K}_{df,3\to3} \frac{1}{1 - iF_3} \ i\mathcal{K}_{df,3\to3} \ \mathcal{R}_L \right]
\]

\[
i \mathcal{D}_L \equiv S \left[ \frac{1}{1 - i \mathcal{M}_{L,2\to2}} \ iG \ i \mathcal{M}_{L,2\to2} \ iG \ i \mathcal{M}_{L,2\to2} \left[2\omega L^3\right] \right]
\]

\[
iF_3 \equiv \frac{iF_{PV}}{2\omega L^3} \left[ \frac{1}{3} + \frac{1}{1 - i \mathcal{M}_{L,2\to2}} iG \ i \mathcal{M}_{L,2\to2} \ iF_{PV} \right]
\]

- Sums over momenta $\to$ integrals (+ now irrelevant $1/L$ terms!)
- Must introduce pole prescription for sums to avoid singularities

\[
i \mathcal{M}_{3\to3} = \lim_{L \to \infty} \left|_{i\epsilon} i \mathcal{M}_{L,3\to3} \right|
\]
Final result: nested integral equations

(1) Obtain $L \to \infty$ limit of $D_L$

\[ iD^{(u,u)}(\vec{p}, \vec{k}) = iM_2(\vec{p})iG^{\infty}(\vec{p}, \vec{k})iM_2(\vec{k}) + \int_s \frac{1}{2\omega_s} iM_2(\vec{p})iG^{\infty}(\vec{p}, \vec{s})iD^{(u,u)}(\vec{s}, \vec{k}) \]

\[ G_{\ell' m';\ell m}^{\infty}(\vec{p}, \vec{k}) \equiv \left( \frac{k^*}{q_p^*} \right)^{\ell'} \frac{4\pi Y_{\ell' m'}(k^*) H(\vec{p})H(\vec{k})Y_{\ell m}^*(p^*)}{2\omega_k (E - \omega_k - \omega_p - \omega_{kp} + i\epsilon)} \left( \frac{p^*}{q_k^*} \right)^{\ell} \]

- Quantities are still matrices in $l,m$ space
- Presence of cut-off function means that integrals have finite range
- $D^{(u,u)}$ sums geometric series which gives physical divergences in $M_3$
Final result: nested integral equations

(2) Sum geometric series involving $\mathcal{K}_{df,3}$

$$i\mathcal{T}(\vec{p}, \vec{k}) = i\mathcal{K}_{df,3}(\vec{p}, \vec{k}) + \int_s \int_r i\mathcal{K}_{df,3}(\vec{p}, \vec{s}) \frac{i\rho(\vec{s})}{2\omega_s} i\mathcal{L}^{(u,u)}(\vec{s}, \vec{r}) i\mathcal{T}(\vec{r}, \vec{k}),$$

$$\mathcal{L}^{(u,u)}(\vec{p}, \vec{k}) = \left( \frac{1}{3} + i\mathcal{M}_2(\vec{p}) i\rho(\vec{p}) \right) (2\pi)^3 \delta^3(\vec{p} - \vec{k}) + i\mathcal{D}^{(u,u)}(\vec{p}, \vec{k}) i\rho(\vec{k}) \frac{2\omega_k}{2\omega_k},$$

- $\rho(k)$ is a phase space factor (analytically continued when below threshold)
- Requires $\mathcal{D}^{(u,u)}$ and $\mathcal{M}_2$
- Corresponds to summing the core geometric series, i.e.

$$i\mathcal{K}_{df,3 \to 3} \left. \frac{1}{1 - i F_3} \right| i\mathcal{K}_{df,3 \to 3}$$
Final result: nested integral equations

(3) Add in effects of external 2→2 scattering:

\[
\mathcal{M}_3(\vec{p}, \vec{k}) - S \left\{ D^{(u,u)}(\vec{p}, \vec{k}) \right\} = -S \left\{ \int_s \int_r L^{(u,u)}(\vec{p}, \vec{s}) T(\vec{s}, \vec{r}) R^{(u,u)}(\vec{r}, \vec{k}) \right\}
\]

- Sums geometric series on “outside” of \( K_{df,3} \)’s

\[
\lim_{L \to \infty} \left\{ \begin{array}{c}
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\text{ } \\
\end{array} \right\}
\]

- Can also invert and determine \( K_{df,3} \) given \( M_3 \) and \( M_2 \)
Conclusions & Outlook
Summary: successes

- Obtained a 3-particle quantization condition
- Confirmed that 3-particle spectrum determined by infinite-volume scattering amplitudes in a general relativistic QFT
- Truncation to obtain a finite problem occurs naturally
- Threshold expansion and other checks give us confidence in the expression
Summary: limitations

- Relation of $K_{df,3}$ to $M_3$ requires solving integral equations
- $K_2$ is needed below (as well as above) 2-particle threshold
- Formalism fails when $K_2$ is singular $\Rightarrow$ each two-particle channel must have no resonances within kinematic range
- Applies only to identical, spinless particles, with $Z_2$ symmetry
Many challenges remain!

- 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 $K \rightarrow \pi\pi\pi$)
  - Include $1 \rightarrow 2$, $2 \rightarrow 3$, … vertices
- Develop models of amplitudes so that new results can be implemented in simulations
- Onwards to 4 or more particles?!!
Many challenges remain!
Thank you!

Questions?