Multiparticle processes from the lattice



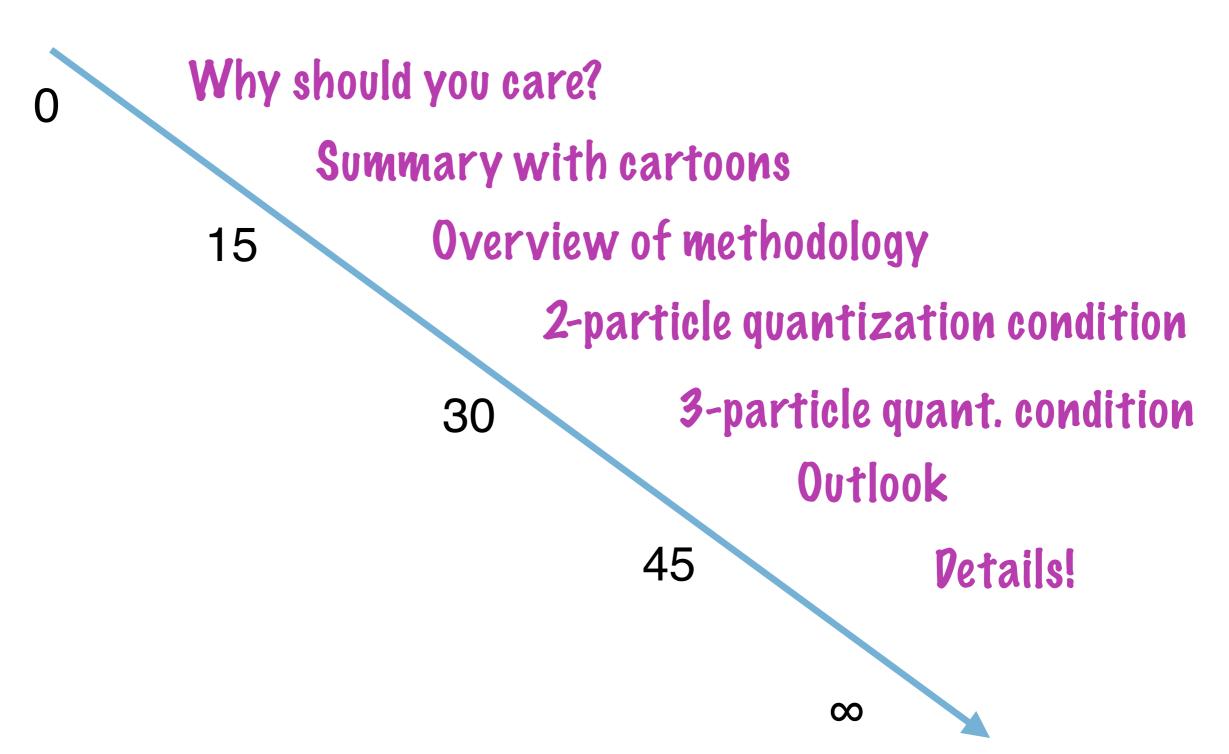
Steve Sharpe University of Washington



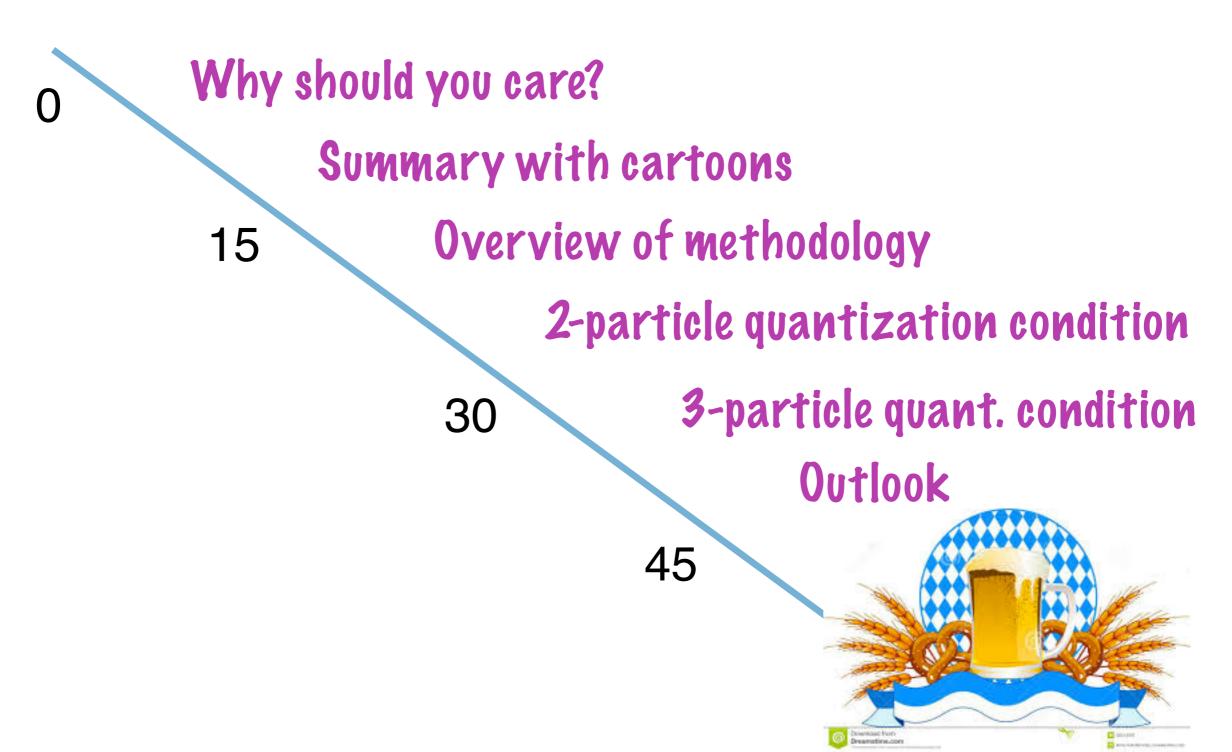
Overview

- This talk is more like a review
 - Aim to show where field stands and the major obstacles to progress
- Focus will be on theoretical issues (not simulations)
 - Though I will not go into many technical details
- The key theoretical issue is the impact of working in a finite spatial volume (always the case in simulations)
 - Discretization of space-time is not the issue, so can use continuum QFT
 - Use of Euclidean time in simulations is not (directly) the issue either

Outline



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What is the relation to "QCD FOR NEW PHYSICS AT THE PRECISION FRONTIER"?

"QCD FOR NEW PHYSICS AT THE PRECISION FRONTIER"?

- Weak decay and mixing amplitudes allow tests of the SM and thus indirect searches for BSM physics
- Many of these involve multiparticle final or intermediate states, e.g.
 - $K \rightarrow \pi \pi (\Delta I = \frac{1}{2} \text{ rule and } \epsilon' / \epsilon)$
 - $K_0 \overline{K_0}$ mixing (ΔM_K)
 - $\mathbf{B} \rightarrow \mathbf{K} \pi (+ \vec{l} \cdot \vec{l})$
 - K→πππ
 - D→ππ, KK, ηη, 4π,
 - $D_0 \overline{D_0}$ mixing
 -
- Tests require lattice QCD (LQCD) calculations of corresponding hadronic matrix elements
- These need both theoretical developments (finite-volume QFT) and advances in simulations

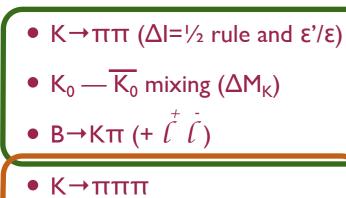
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 - B→Kπ (+ ℓ⁺ℓ[¯])
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Theory developed; fully controlled LQCD results in a few years [RBC/UKQCD, Meinel,...]

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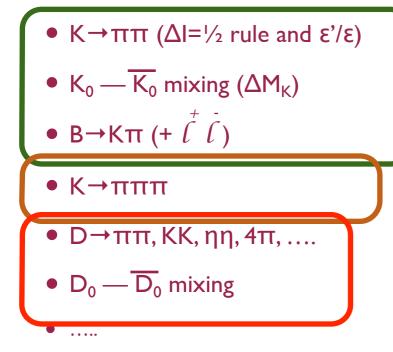
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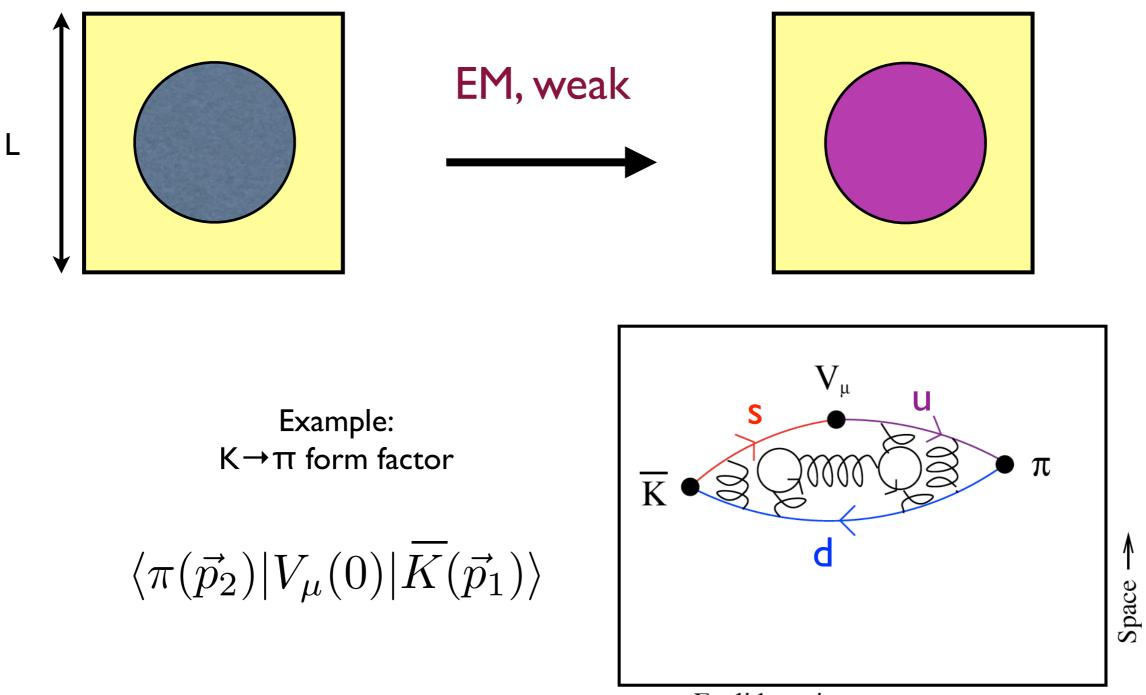
Theory remains to be developed

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Summary with cartoons

Well-controlled LQCD calculations

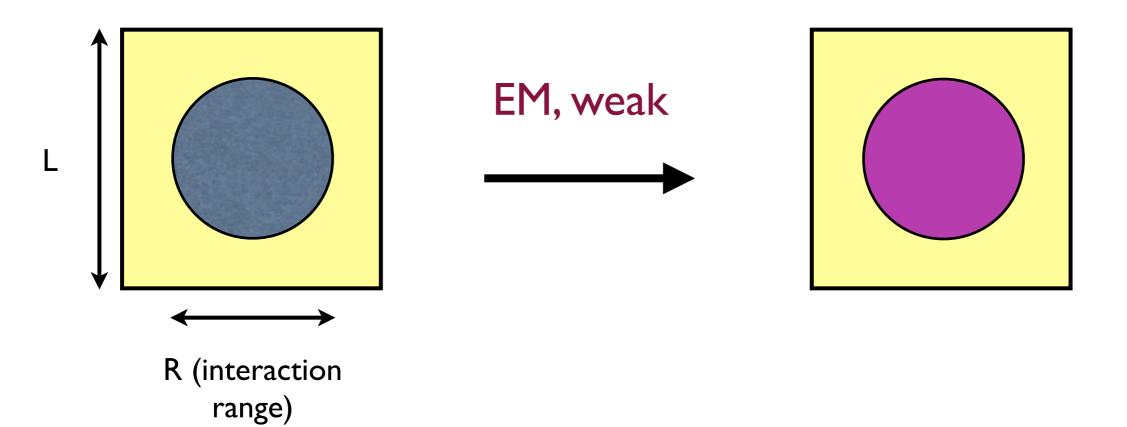
Discussed in Aida's talk; averages for many quantities presented by FLAG



Euclidean time ->

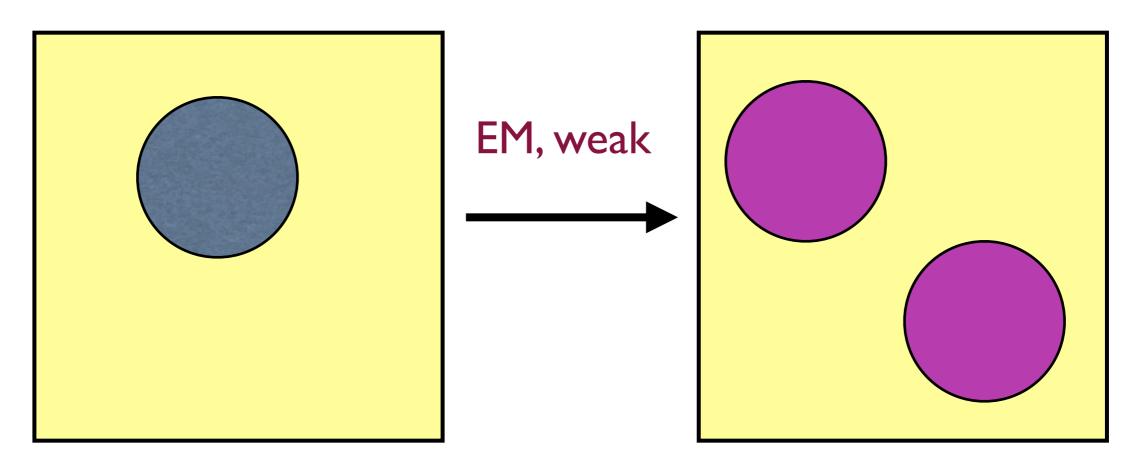
Well controlled LQCD calculations

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For large enough boxes (L>2R) dominant finite-volume effects for singleparticle states fall as $exp(-M_{\pi}L)$ [Lüscher] and can be made small

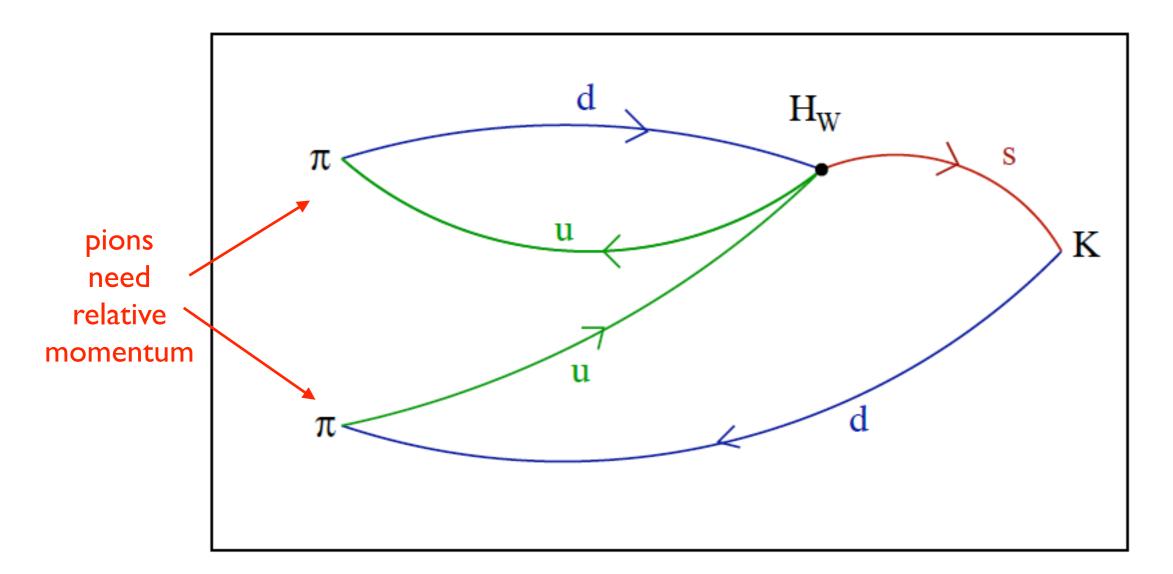
Present frontier (1)



e.g. $K \rightarrow \pi\pi$ (I=0 & 2) [RBC/UKQCD]

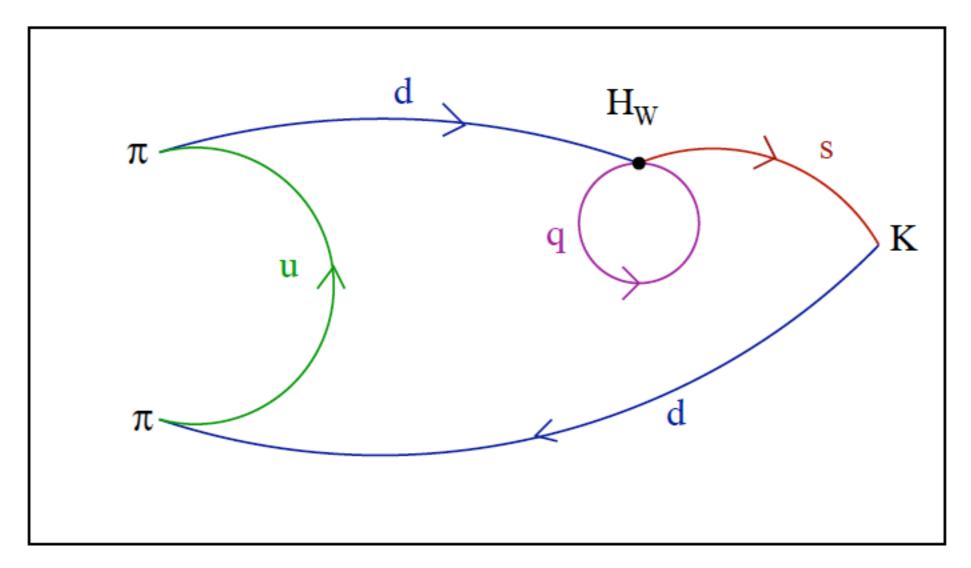
- Issues associated with 2 particles (I/Lⁿ finite-volume effects,...) are theoretically understood [Lüscher, Lellouch & Lüscher, ...]
- Numerical implementations expanding despite computational challenges

Computational challenges



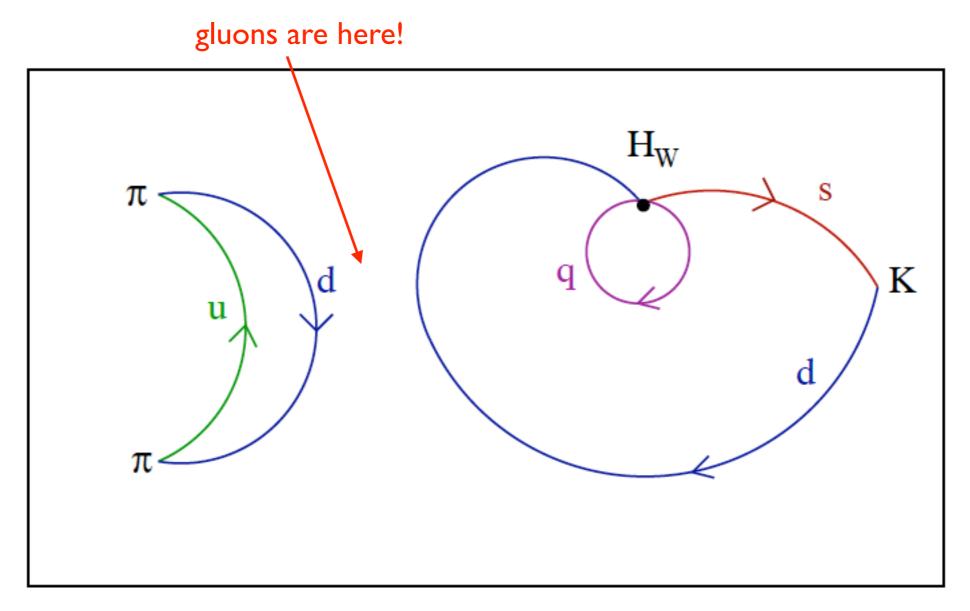
Four-point function

Computational challenges



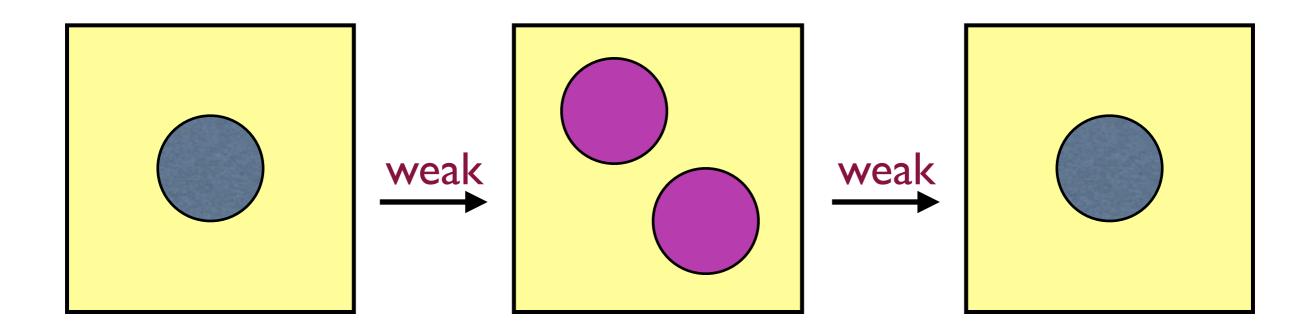
Partially quark-disconnected contractions

Computational challenges



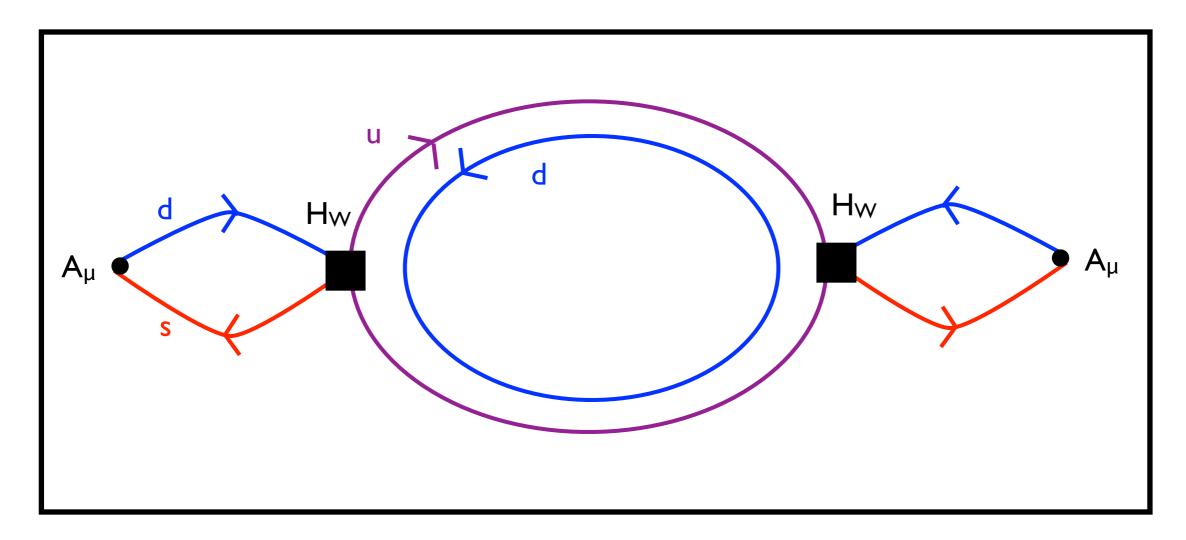
Fully quark-disconnected contractions

Present frontier (2) $\Delta M_{K}: K_{0} \rightarrow \pi \pi \text{ (virtual)} \rightarrow \overline{K}_{0} \text{ [RBC/UKQCD]}$



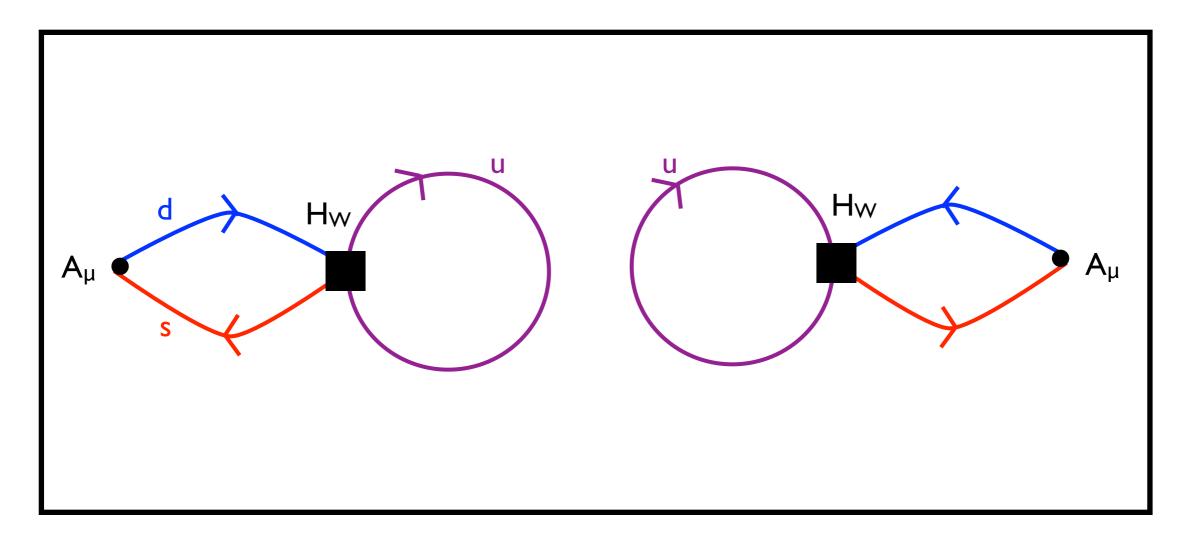
- Issues associated with intermediate two-particle states are theoretically understood [Christ, Feng, Martinelli, Sachrajda]
- Pilot numerical calculation [RBC/UKQCD]

Present frontier (2) $\Delta M_{K}: K_{0} \rightarrow \pi\pi \text{ (virtual)} \rightarrow \overline{K}_{0} \text{ [RBC/UKQCD]}$



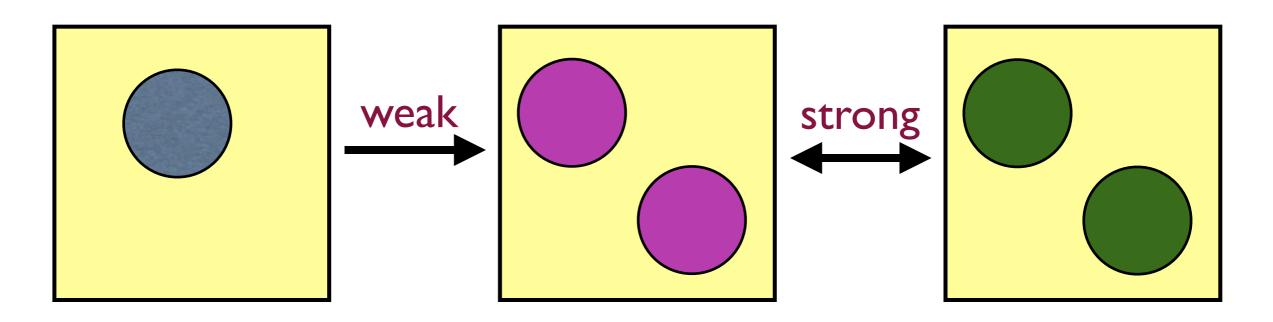
Four-point function involving two weak currents

Present frontier (2) $\Delta M_{K}: K_{0} \rightarrow \pi\pi \text{ (virtual)} \rightarrow \overline{K}_{0} \text{ [RBC/UKQCD]}$



Quark-disconnected contributions

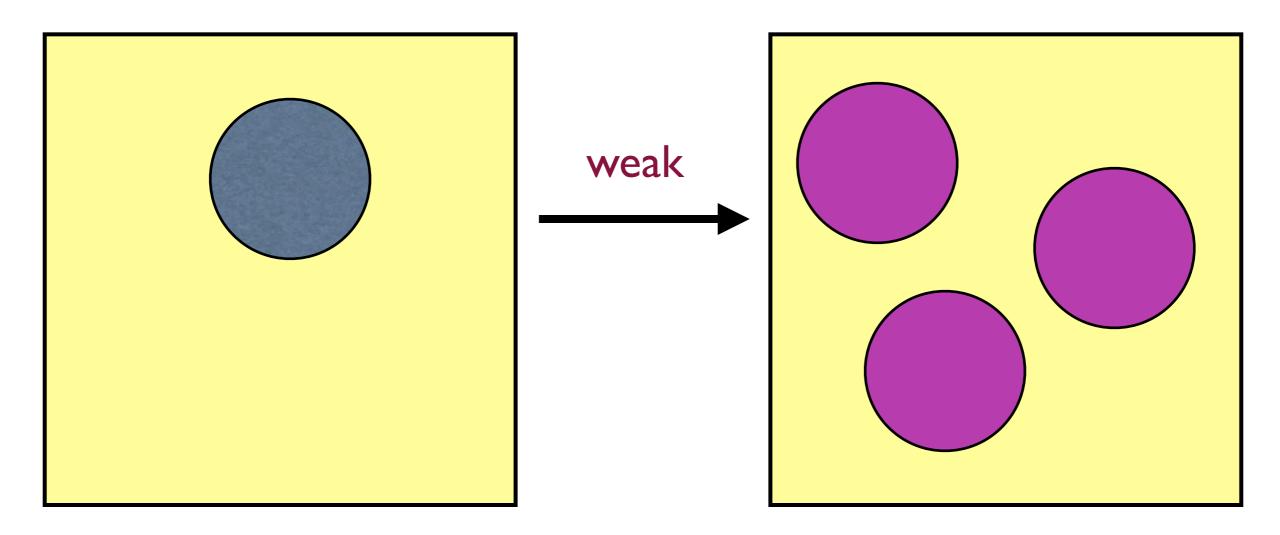
Present frontier (3)



e.g. $K_0 \rightarrow \pi_+ \pi_- \& \pi_0 \pi_0$ in presence of isospin breaking

- Theoretical challenge: finite-volume eigenstates are inevitably mixtures of final states
- Formalism for disentangling this mixing and obtaining correct (infinite volume) normalization and phases for amplitudes exists [Hansen & SS; Briceño, Hansen & Walker-Loud]

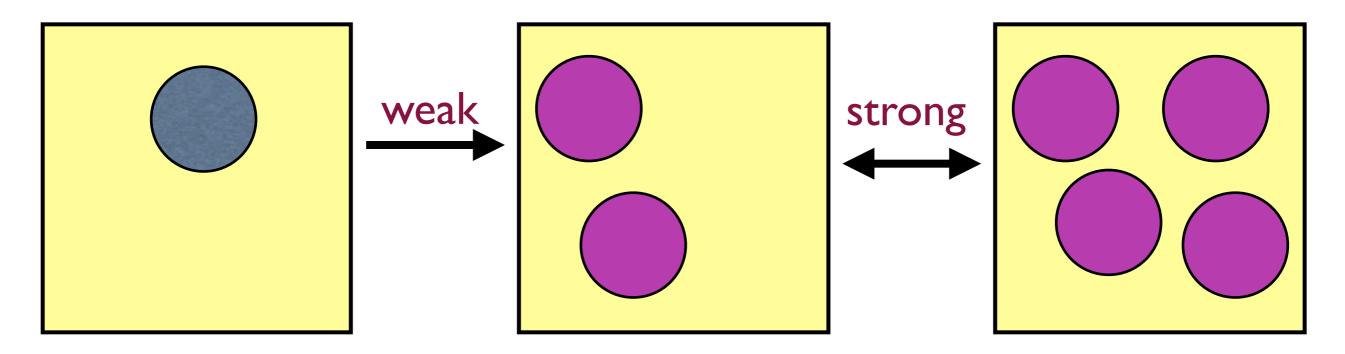
Pushing the frontier



e.g. $K_0 \rightarrow \pi \pi \pi$

- Theoretical challenge: removing I/Lⁿ finite-volume effects
- Partial progress (3 particle quantization condition) [Hansen & SS]

Beyond the frontier



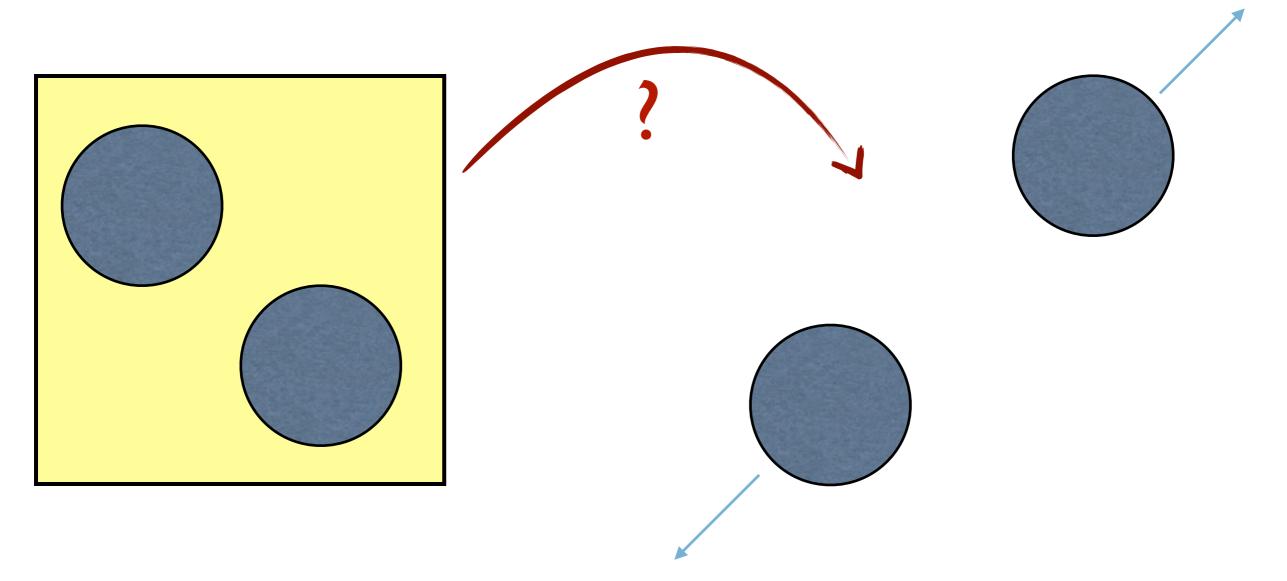
e.g. D→ππ & 4π & KK & ηη & 6π

- Finite-volume eigenstates at $E=M_D$ are inevitably mixtures of all open channels
- Need to separate these (to get individual "out" states)
- Similar issues arise in D—D mixing for virtual intermediate states
- Open theoretical problem
- Issues for simulations are also challenging (but less so?)

Overview of methodology

The fundamental issues

- Lattice QCD can calculate energy levels of multiparticle systems in a box and matrix elements involving these states
- How are these related to infinite-volume scattering amplitudes and decay amplitudes?



1st fundamental issue

- Lattice QCD car calculate energy levels of multiparticle systems in a box and matrix elements involving these states
- How are these related to infinite-volume scattering amplitudes and decay amplitudes?

$E_2(L)$ $E_1(L)$ $E_0(L)$	$i\mathcal{M}_{n \to m}$
Discrete energy	Scattering
spectrum	amplitudes

2nd fundamental issue

- Lattice QCD can calculate energy levels of multiparticle systems in a box and matrix elements involving these states
- How are these related to infinite-volume scattering amplitudes and decay amplitudes?

finite-volume state interpolated by two pion operator with $E_n = M_D$

 $L\langle n|\mathcal{H}_W|D\rangle_L$

 $_{\mathrm{out}}\langle \pi\pi|\mathcal{H}_W|D
angle$

desired infinite-volume matrix element including phase

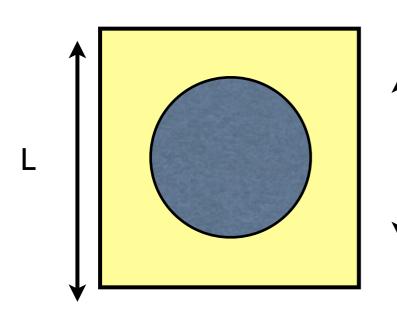
The fundamental issues

- Lattice QCD can calculate energy levels of multiparticle systems in a box and matrix elements involving these states
- How are these related to infinite-volume scattering amplitudes and decay amplitudes?

Must understand first issue before one can address the second

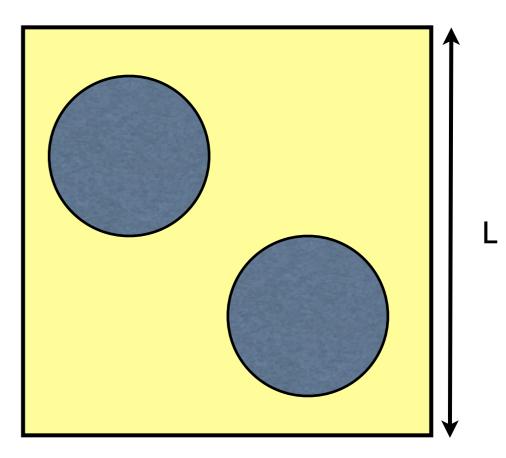
Two-particle quantization condition

When is spectrum related to scattering amplitudes?



R (interaction range)

Single (stable) particle with L>R Particle not "squeezed" Spectrum same as in infinite volume up to corrections proportional to $e^{-M_{\pi}L}$ [Lüscher]



L>2R

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

[Lüscher,...]

Single-channel 2-particle quantization condition [Lüscher 86 & 91; Rummukainen & Gottlieb 85; Kim, Sachrajda & SS 05; ...]

- Two particles (say pions) in cubic box of size L with PBC and total momentum P
- Below inelastic threshold (4 pions), the finite-volume spectrum E₁, E₂, ... is given by solutions to a secular equation in partial-wave (*l*,*m*) space (up to exponentially suppressed corrections)

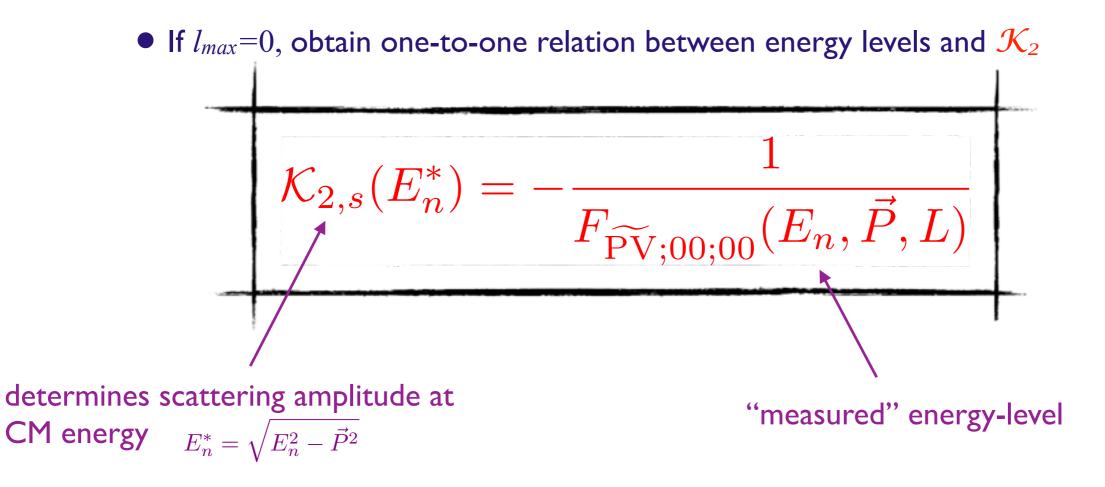
$$\det\left[(F_{\widetilde{\mathrm{PV}}})^{-1} + \mathcal{K}_2\right] = 0$$

- $\mathcal{K}_2 \sim \tan \delta/q$ is the K-matrix, which is diagonal in *l,m* space
- F_{PV} is a known kinematical zeta-function, depending on the box shape & E; It is an off-diagonal matrix in *l,m*, since the box violates rotation symmetry

Single-channel 2-particle quantization condition

$$\det\left[(F_{\widetilde{\mathrm{PV}}})^{-1} + \mathcal{K}_2\right] = 0$$

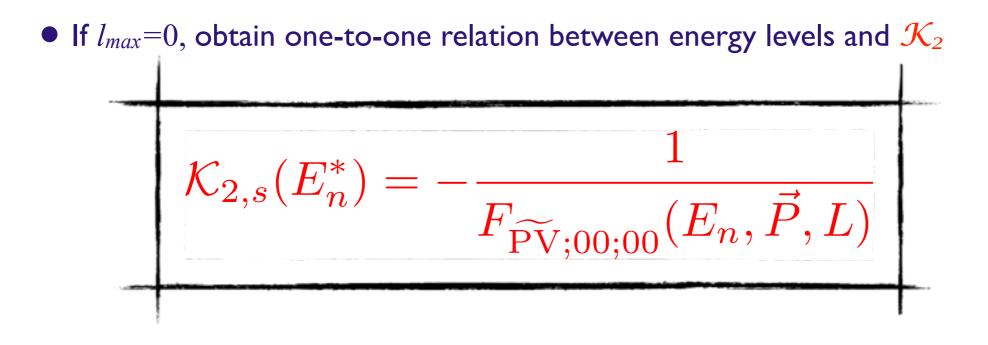
• Infinite dimensional determinant must be truncated to be practical; truncate by assuming that \mathcal{K}_2 vanishes above l_{max}



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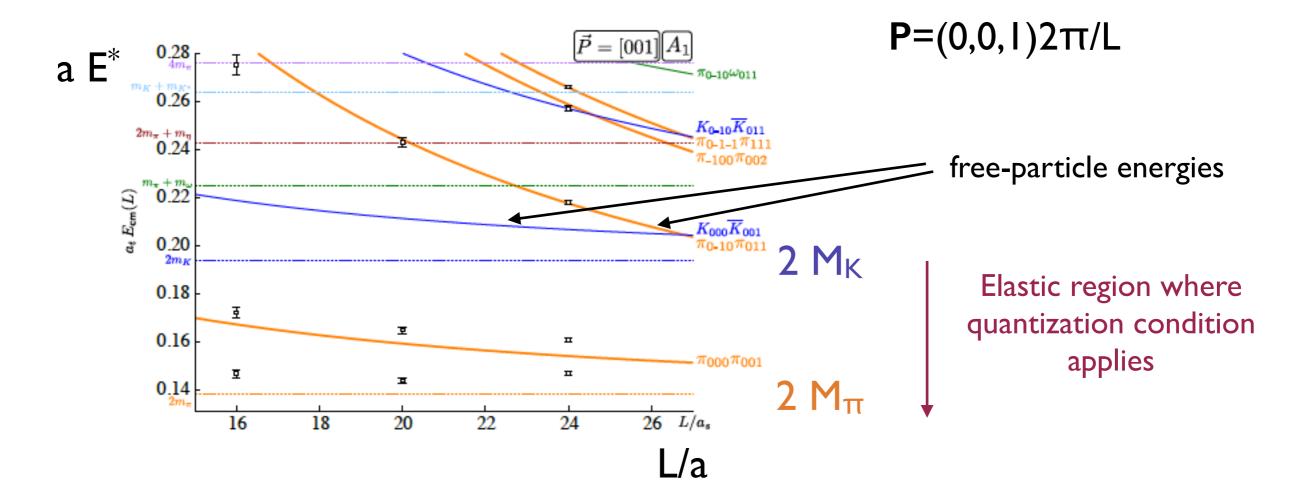
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Equivalent to: $\tan[\delta(q^*)] = -\tan[\phi^P(q^*)],$

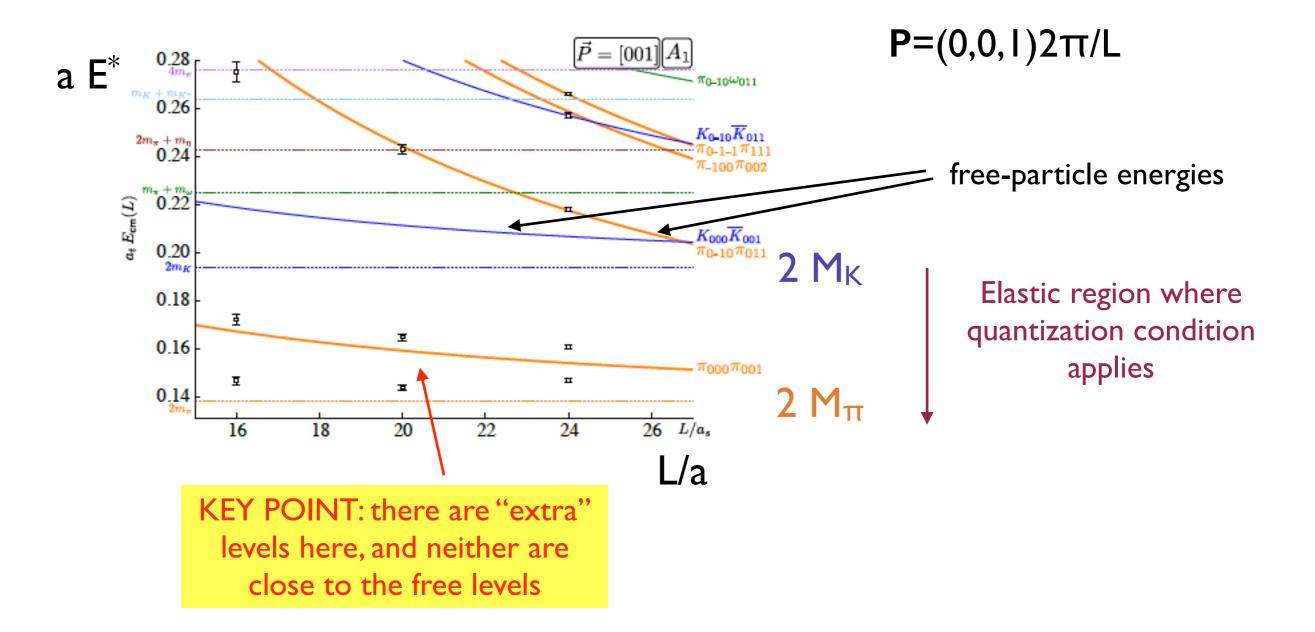
[Dudek, Edwards & Thomas, 1212.0830]

• Proof of principle calculation with $M_{\pi} \sim 400$ MeV, several P, many spectral levels

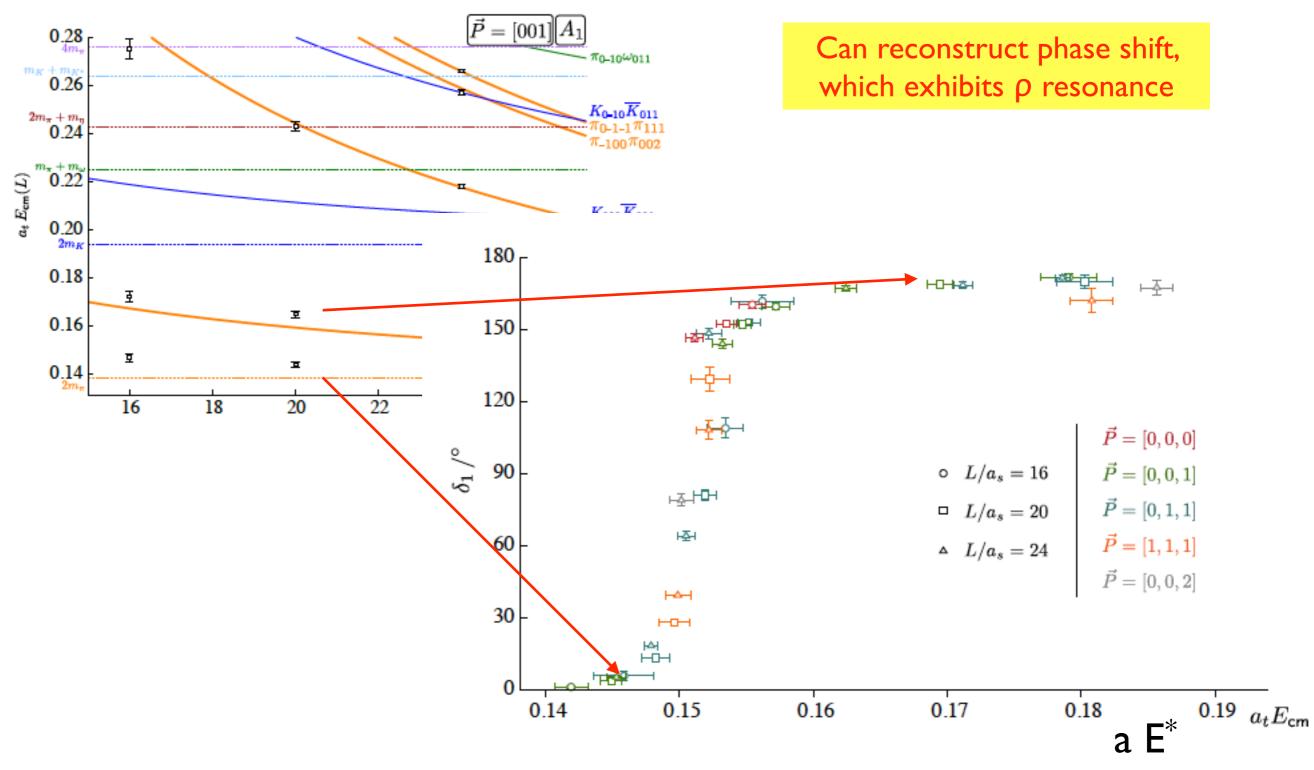


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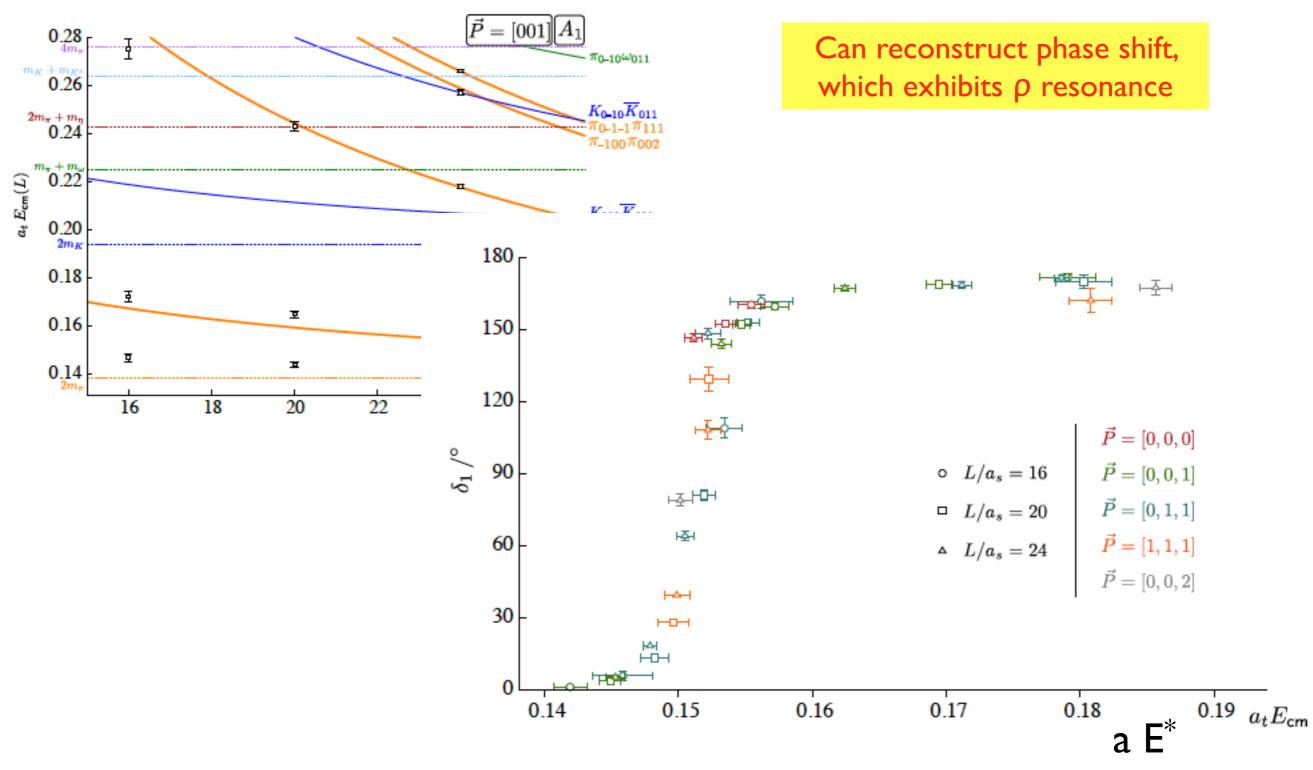
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Status for 2 particles

- Long understood in NRQM [Huang & Yang 57,]
- 1st
 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; ...]

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 - Relation between finite volume I→2 weak amplitude (e.g. K→ππ) 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. γ^{*}π→ρ→ππ, γ^{*}N→Δ→πN, γD→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;...]

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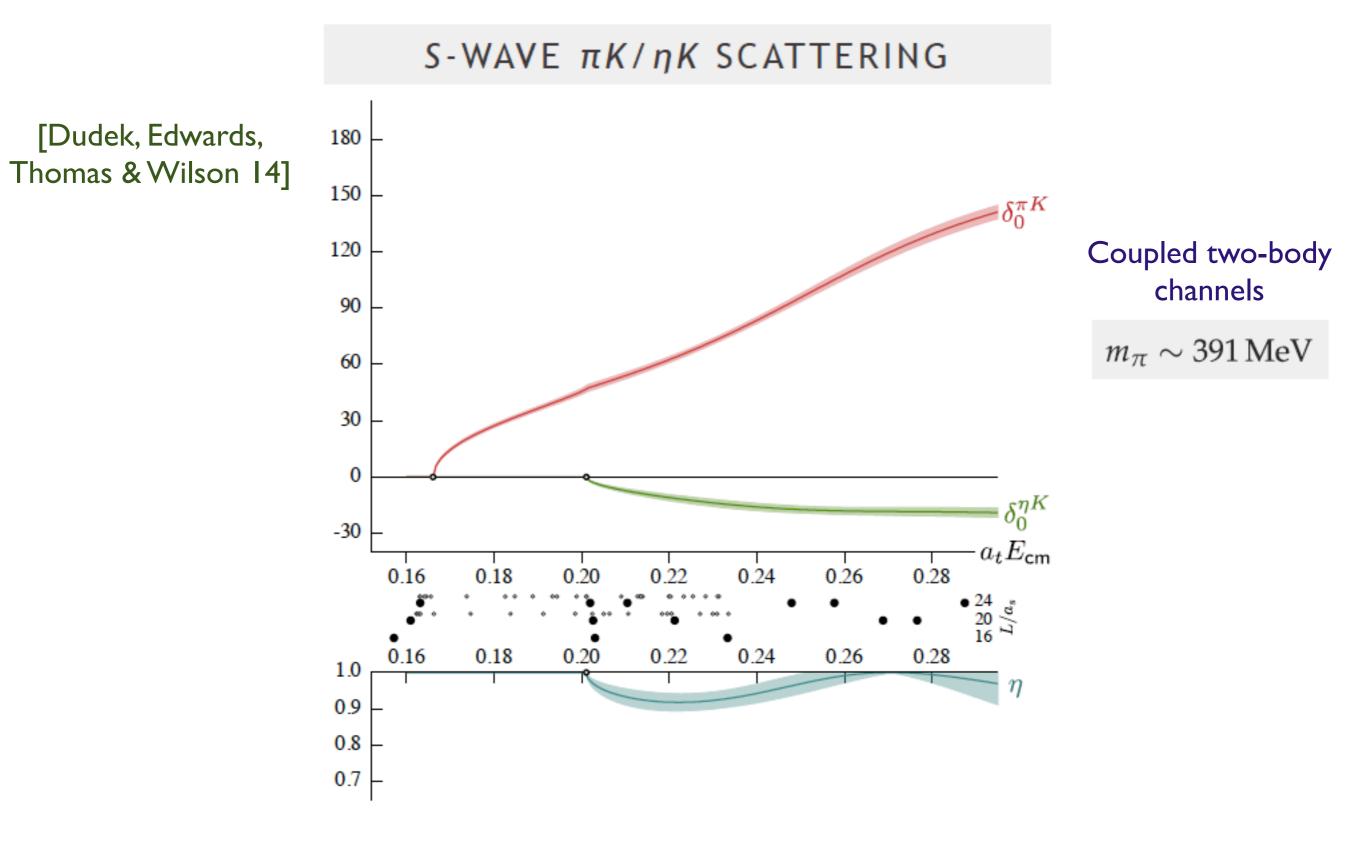
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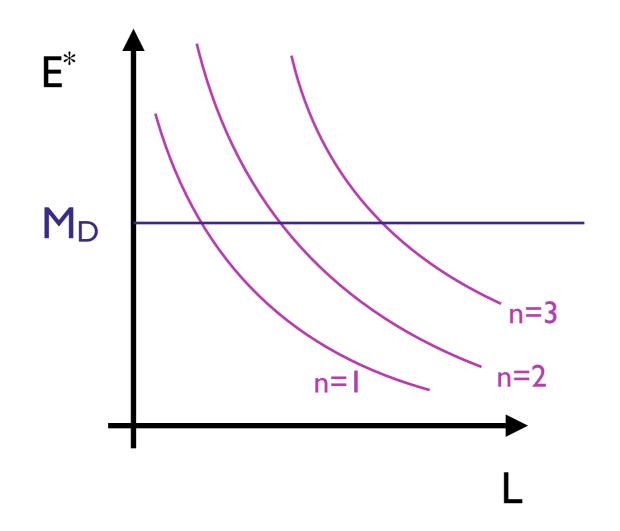
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 - Leading order QED effects on quantization condition determined; do NOT fit into general formalism [Beane & Savage 14]

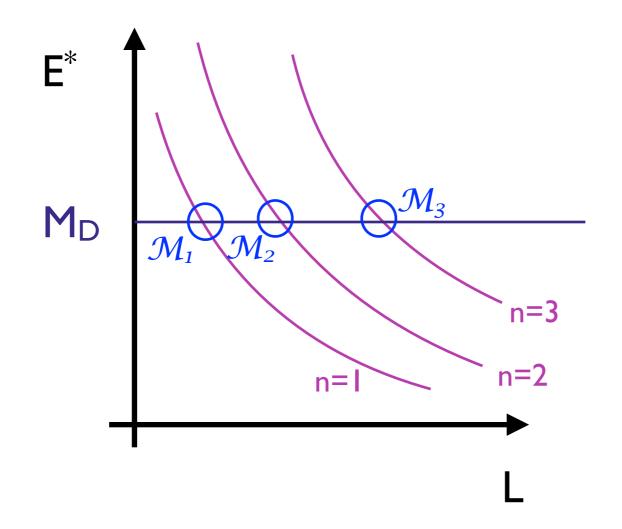
State of the art: multiple 2-particle channels



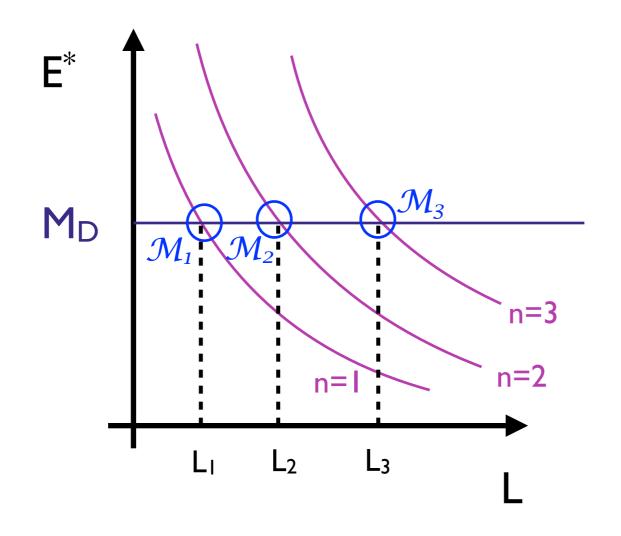
- Illustrate with an unphysical scenario:
 - Consider $D \rightarrow$ strange weak decays, and assume $D \rightarrow K\pi \& K\eta$ only
- Calculate amplitudes $\mathcal{M}_n = |A| = |A$
- Calculate values of L_n and slopes S_n of same three spectral lines at $E_n^*=M_D$



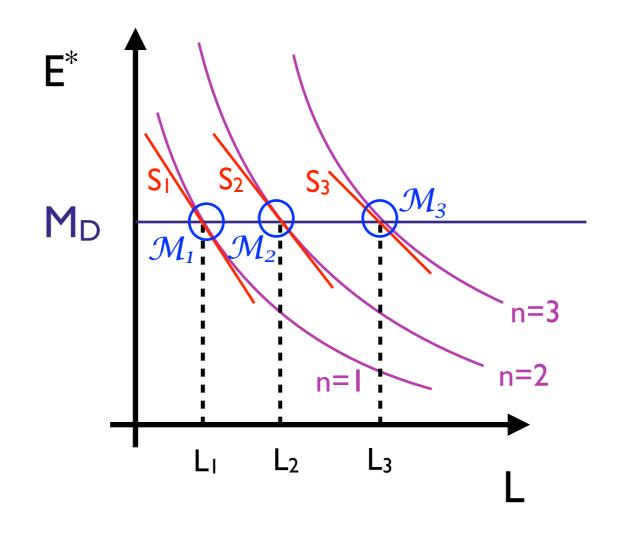
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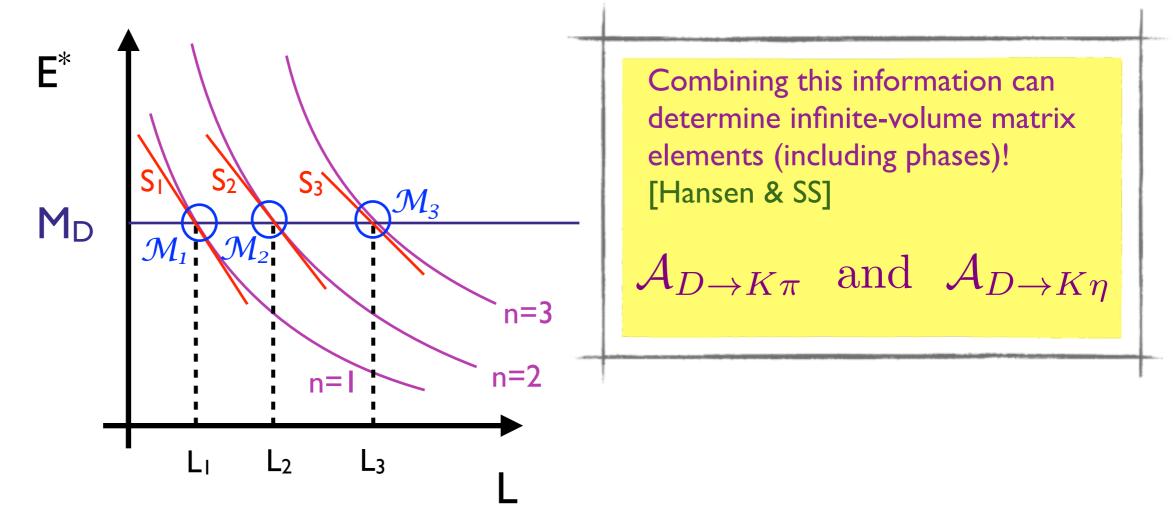
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Three-particle quantization condition

Applications of 3-particle formalism

• Studying resonances with three particle decay channels

 $\omega(782) \to \pi\pi\pi \qquad K^* \longrightarrow K\pi\pi \qquad N(1440) \to N\pi\pi$

 Calculating weak decay amplitudes/form factors involving 3 particles, e.g. K→πππ

Determining NNN interactions

- Input for effective field theory treatments of larger nuclei & nuclear matter
- Similarly, $\pi\pi\pi$, $\pi K\overline{K}$, ... interactions needed for study of pion/kaon condensation

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
- [HALQCD: Aoki *et al.* 13] use alternative method based on Bethe-Salpeter wavefunction: potentially more powerful but based on certain assumptions

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Theory considered for 3 particles

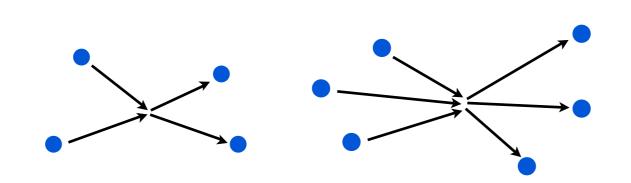
• Work in continuum (assume that LQCD can control discretization errors)

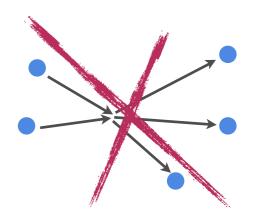
- Cubic box of size L with periodic BC, and infinite (Minkowski) time
 - Spatial loops are sums:

$$\frac{1}{L^3}\sum_{\vec{k}} \qquad \vec{k} = \frac{2\pi}{L}\vec{n}$$

L

- Consider identical particles with physical mass m, interacting <u>arbitrarily</u> except for a Z₂ (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





S. Sharpe, "Multiparticle processes" 09/28/15 INT workshop

3-particle quantization condition [Hansen & SS]

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

$$\det\left[F_3^{-1} + \mathcal{K}_{\mathrm{df},3}\right] = 0$$

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

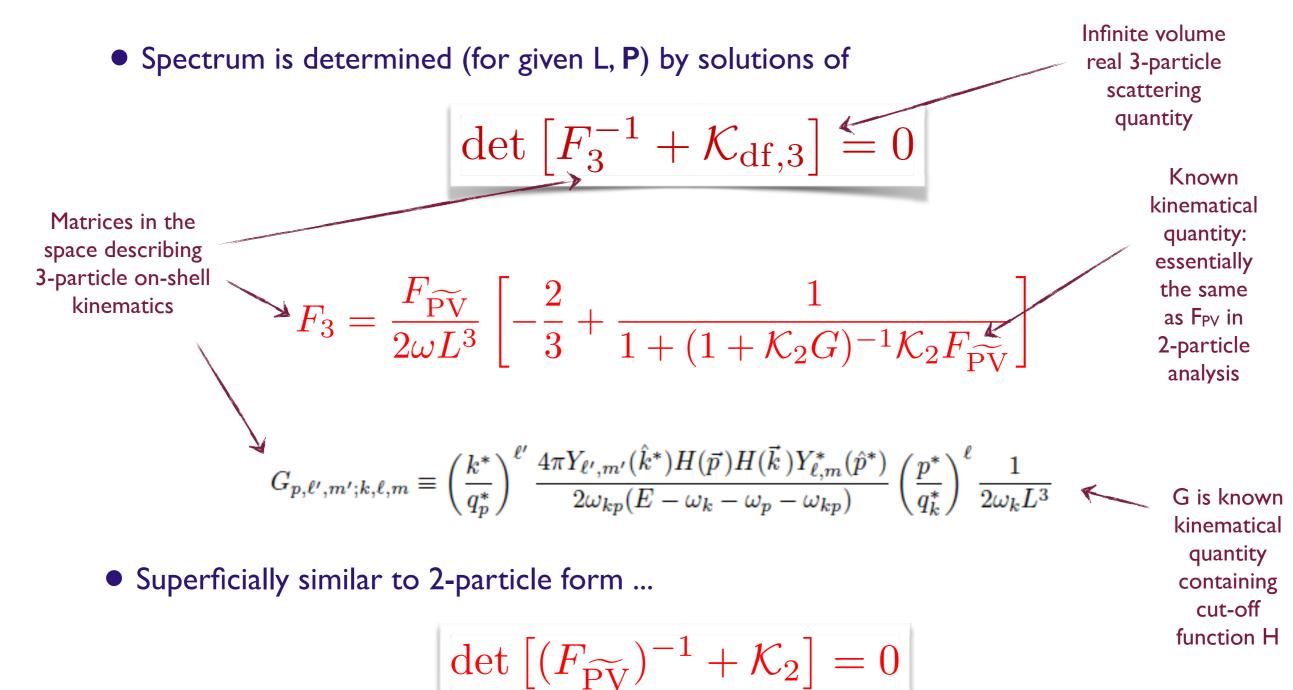
$$G_{p,\ell',m';k,\ell,m} \equiv \left(\frac{k^*}{q_p^*}\right)^{\ell'} \frac{4\pi Y_{\ell',m'}(\hat{k}^*)H(\vec{p}\,)H(\vec{k}\,)Y_{\ell,m}^*(\hat{p}^*)}{2\omega_{kp}(E-\omega_k-\omega_p-\omega_{kp})} \left(\frac{p^*}{q_k^*}\right)^{\ell} \frac{1}{2\omega_k L^3}$$

• Superficially similar to 2-particle form ...

$$\det\left[(F_{\widetilde{\mathrm{PV}}})^{-1} + \mathcal{K}_2\right] = 0$$

• ... but F₃ contains both kinematical, finite-volume quantities (F_{PV} & G) and the dynamical, infinite-volume quantity \mathcal{K}_2

3-particle quantization condition [Hansen & SS]



• ... but F₃ contains both kinematical, finite-volume quantities (F_{PV} & G) and the dynamical, infinite-volume quantity \mathcal{K}_2

Final result for 3 particles

$$\det \left[F_3^{-1} + \mathcal{K}_{df,3} \right] = 0$$

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

• All quantities are (infinite-dimensional) matrices, e.g. (F₃)_{klm;pl'm'}, with indices

[finite volume "spectator" momentum: $k=2\pi n/L$] x [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~m [provided by H(k)] Final result for 3 particles

$$\det \left[F_3^{-1} + \mathcal{K}_{df,3} \right] = 0$$

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- Important limitation: our present derivation requires that all two-particle subchannels lie below resonance poles 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

Truncation in 3 particle case

$$\det \left[F_3^{-1} + \mathcal{K}_{df,3} \right] = 0$$

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

- 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)
- I is truncated if both \mathcal{K}_2 and $\mathcal{K}_{df, 3}$ vanish for $I > I_{max}$
- Yields determinant condition truncated to $[N(2l_{max}+I)]^2$ block

Truncation in 3 particle case

$$\Delta_{L,P}(E) = \det \left[F_3^{-1} + \mathcal{K}_{df,3} \right] = 0$$
$$F_3 = \frac{F_{\widetilde{PV}}}{2\omega L^3} \left[-\frac{2}{3} + \frac{1}{1 + (1 + \mathcal{K}_2 G)^{-1} \mathcal{K}_2 F_{\widetilde{PV}}} \right]$$

- 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 $\mathcal{K}_{df,3}$ depends only on E^{*} (and thus is indep. of k, l, m)
- Also assume \mathcal{K}_2 only non-zero for s-wave ($\Rightarrow I_{max}=0$) and known
- Truncated [N x N] problem simplifies: $\mathcal{K}_{df,3}$ has only 1 non-zero eigenvalue, and problem collapses to a single equation:

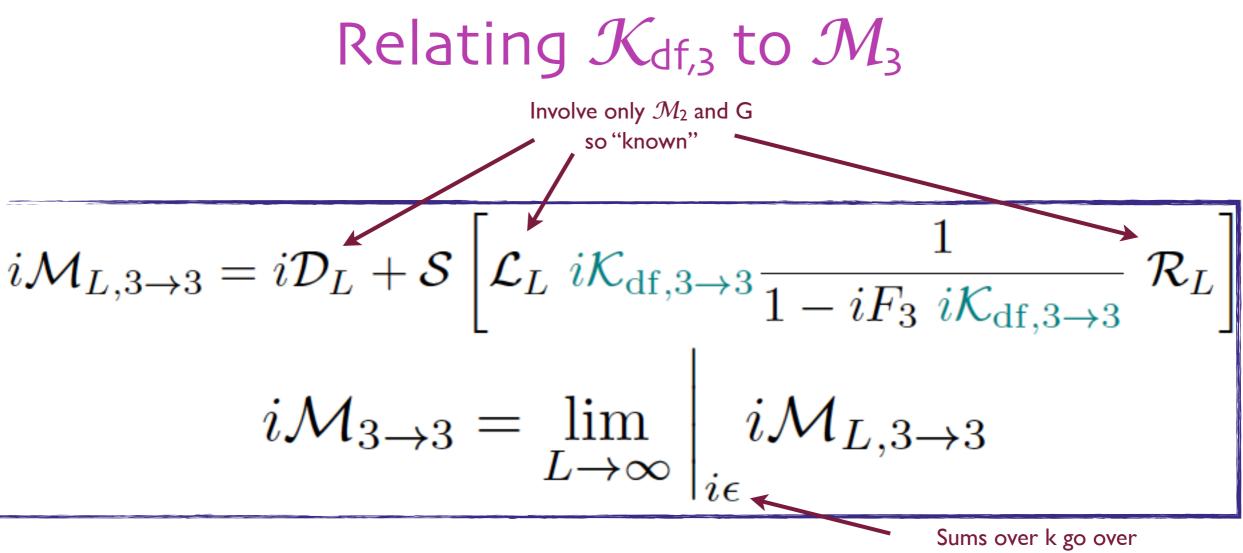
$$1 + F_3^{\text{iso}} \mathcal{K}_{\text{df},3}^{\text{iso}}(E^*) = 0$$

Known in terms of two particle scattering amplitude

$$F_3^{\rm iso} \equiv \sum_{\vec{k},\vec{p}} \frac{1}{2\omega_k L^3} \left[F_{\widetilde{\rm PV}}^s \left(-\frac{2}{3} + \frac{1}{1 + [1 + \mathcal{K}_2^s G^s]^{-1} \mathcal{K}_2^s F_{\widetilde{\rm PV}}^s} \right) \right]_{k,p}$$

Relating $\mathcal{K}_{df,3}$ to \mathcal{M}_3

- Three particle quantization condition depends on $\mathcal{K}_{df,3}$ rather than the three particle scattering amplitude \mathcal{M}_3
- $\mathcal{K}_{df,3}$ 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
 - It was forced on us by the analysis, and is some sort of local vertex
- \bullet To complete the quantization condition we must relate $\mathcal{K}_{df,3}$ to \mathcal{M}_3



to integrals with it pole prescription

- Result is an integral equation giving \mathcal{M}_3 in terms of $\mathcal{K}_{df,3}$
- Requires knowing \mathcal{M}_2 (including continued below threshold)
- Completes formalism—shows that finite volume spectrum is given by infinite-volume scattering amplitudes

Summary & Outlook

Outlook: many challenges remain!

- Tremendous progress over last decade (theory & simulations)
 - Two-particle cases theoretically understood & simulations underway
 - Key examples: $K \rightarrow \pi\pi$ [RBC/UKQCD], $\gamma\pi \rightarrow \rho \rightarrow \pi\pi$ [JLAB]
- Frontier is 3 particles: need to 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 $I \rightarrow 3$ decay amplitudes (e.g. for $K \rightarrow \pi \pi \pi$)
 - Include $1 \rightarrow 2, 2 \rightarrow 3, \dots$ vertices
- Develop models of amplitudes so that new results can be implemented in simulations
- Onwards to 4 or more particles?!?

Thank you! Questions?

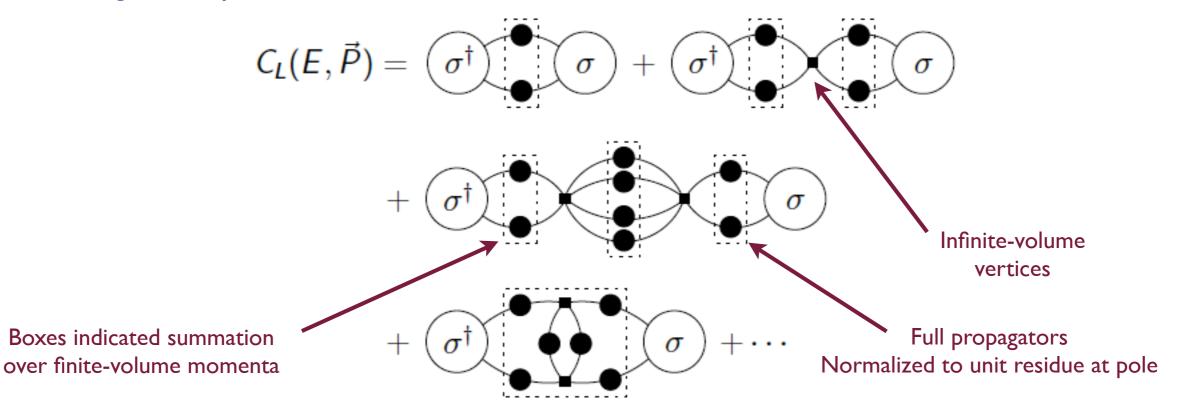
Backup slides: the details!

Set-up & main ideas

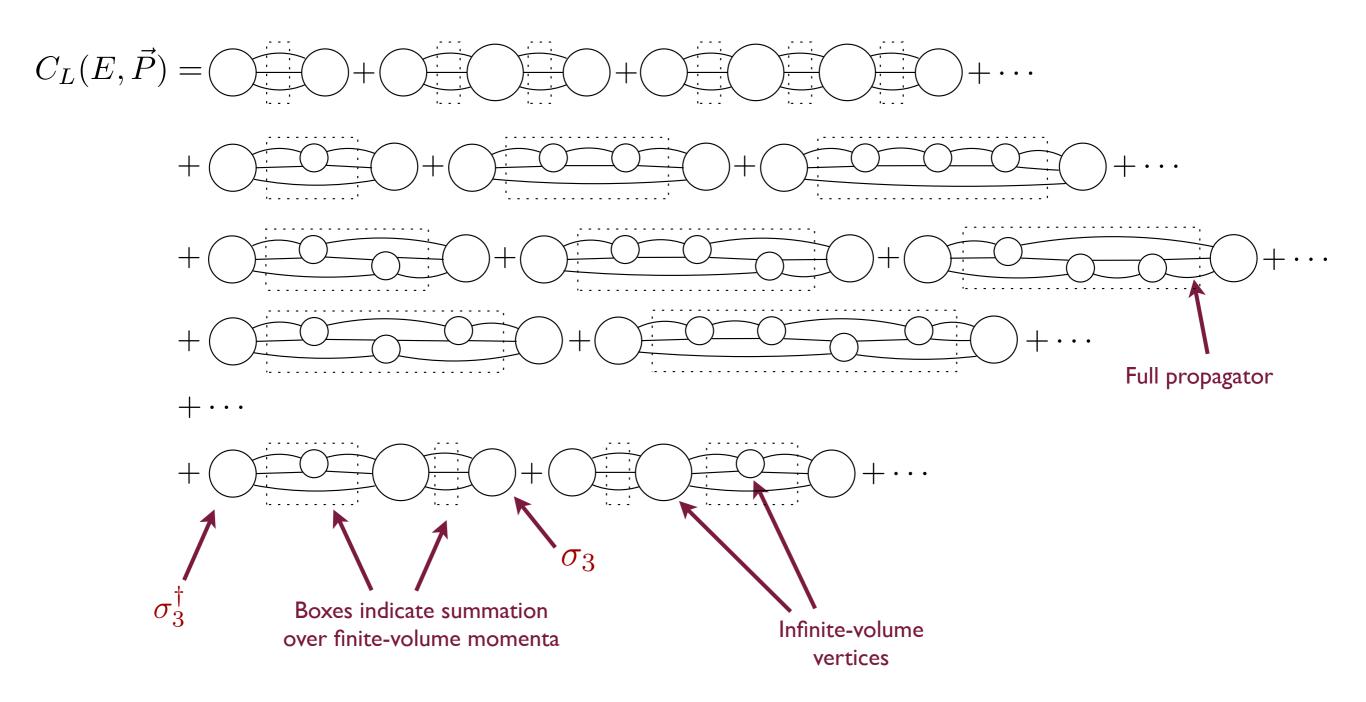
Methodology

• Calculate (for some P=2TTn_P/L) $C_{L}(E, \vec{P}) \equiv \int_{L} d^{4}x \ e^{-i\vec{P}\cdot\vec{x}+iEt} \langle \Omega | T\sigma(x)\sigma^{\dagger}(0) | \Omega \rangle_{L}$ 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
- E.g. for 2 particles:



3-particle correlator



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

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

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

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

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

• Use "sum=integral + [sum-integral]" if integrand has pole, with [Kim,Sachrajda,SS 05]

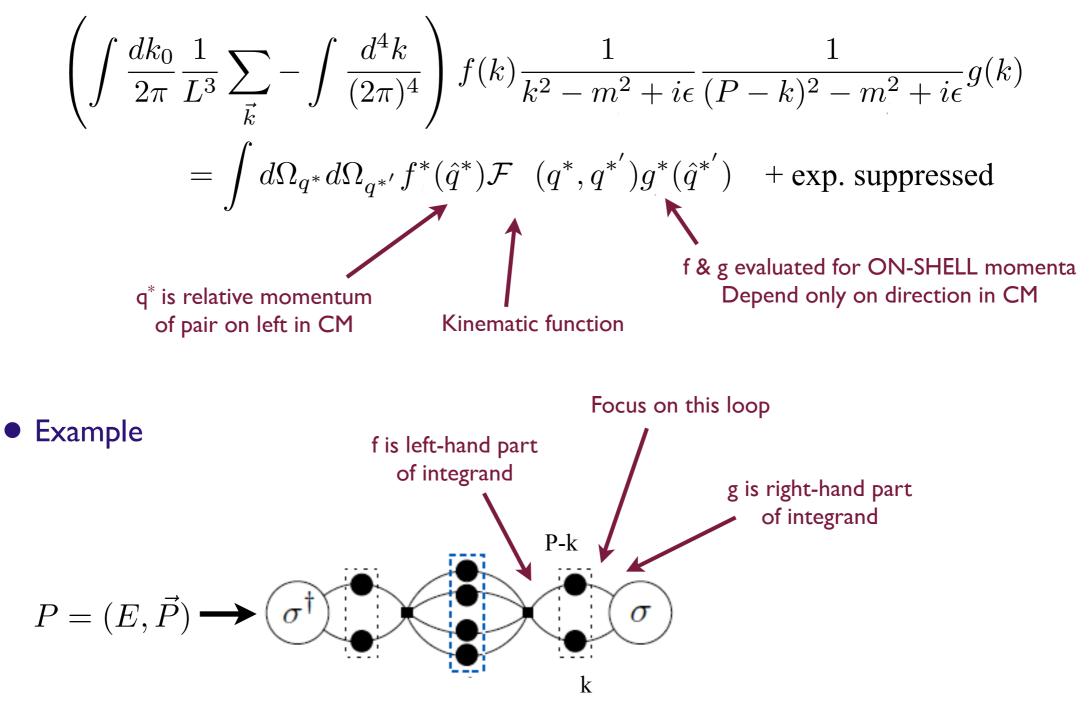
$$\begin{pmatrix} \int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^4k}{(2\pi)^4} \end{pmatrix} f(k) \frac{1}{k^2 - m^2 + i\epsilon} \frac{1}{(P - k)^2 - m^2 + i\epsilon} g(k)$$

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

$$f \& \text{g evaluated for ON-SHELL momenta}$$

$$\text{Depend only on direction in CM}$$

• Use "sum=integral + [sum-integral]" if integrand has pole, with [Kim,Sachrajda,SS 05]



• Use "sum=integral + [sum-integral]" where integrand has pole, with [KSS]

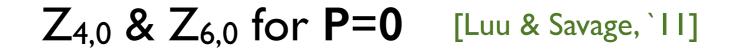
$$\left(\int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{d^4k}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2 + i\epsilon} \frac{1}{(P-k)^2 - m^2 + i\epsilon} g(k)$$
$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F} \ (q^*, q^{*'}) g^*(\hat{q}^{*'})$$

• Decomposed into spherical harmonics, $\mathcal F$ becomes

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

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

Kinematic functions



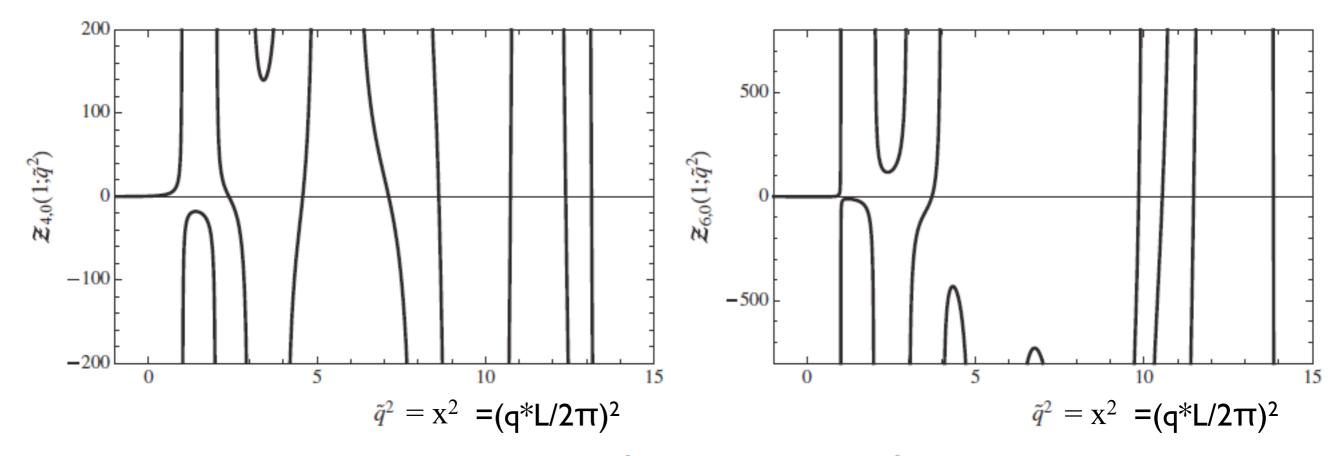
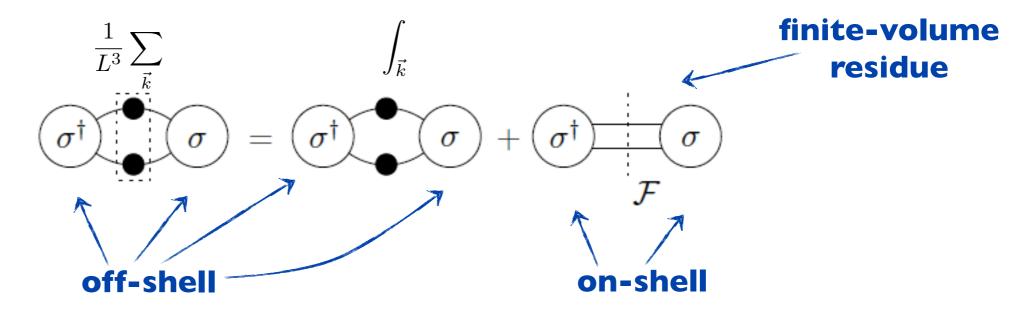


FIG. 29. The functions $Z_{4,0}(1; \tilde{q}^2)$ (left panel) and $Z_{6,0}(1; \tilde{q}^2)$ (right panel).

• Use "sum=integral + [sum-integral]" where integrand has pole, with [KSS]

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

• Diagrammatically



Variant of key step 2

• For generalization to 3 particles use (modified) PV prescription instead of iε

$$\left(\int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} - \int \frac{\widetilde{PV}}{(2\pi)^4} \right) f(k) \frac{1}{k^2 - m^2} + \underbrace{\swarrow}_{(P-k)^2 - m^2} + \underbrace{\swarrow}_{(P-k)^2 - m^2} g(k)$$
$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F}_{\widetilde{PV}}(q^*, q^{*'}) g^*(\hat{q}^{*'})$$

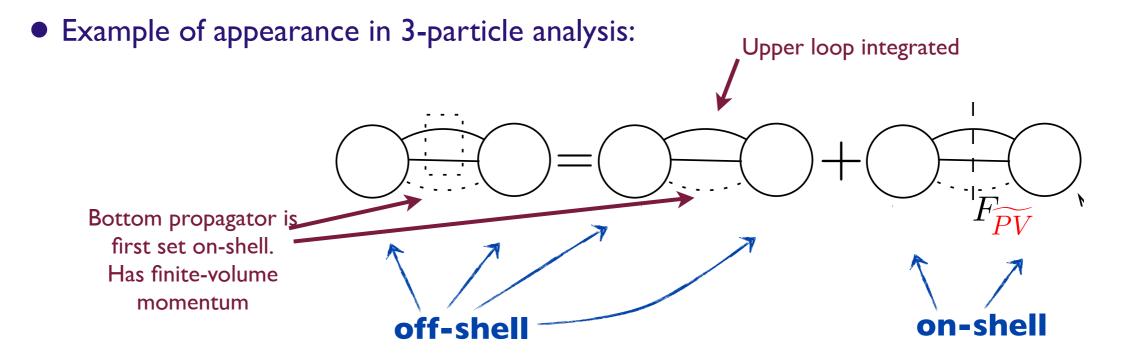
• Key properties of FPV (discussed below): real and no unitary cusp at threshold

Variant of key step 2

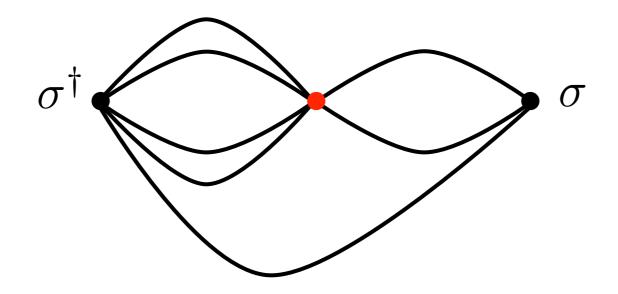
• For generalization to 3 particles use (modified) PV prescription instead of iε

$$\left(\int \frac{dk_0}{2\pi} \frac{1}{L^3} \sum_{\vec{k}} -\int \frac{\widetilde{PV}}{(2\pi)^4} d^4k \right) f(k) \frac{1}{k^2 - m^2} + \mathbf{K} \frac{1}{(P-k)^2 - m^2} + \mathbf{K} g(k)$$
$$= \int d\Omega_{q^*} d\Omega_{q^{*'}} f^*(\hat{q}^*) \mathcal{F}_{\widetilde{PV}}(q^*, q^{*'}) g^*(\hat{q}^{*'})$$

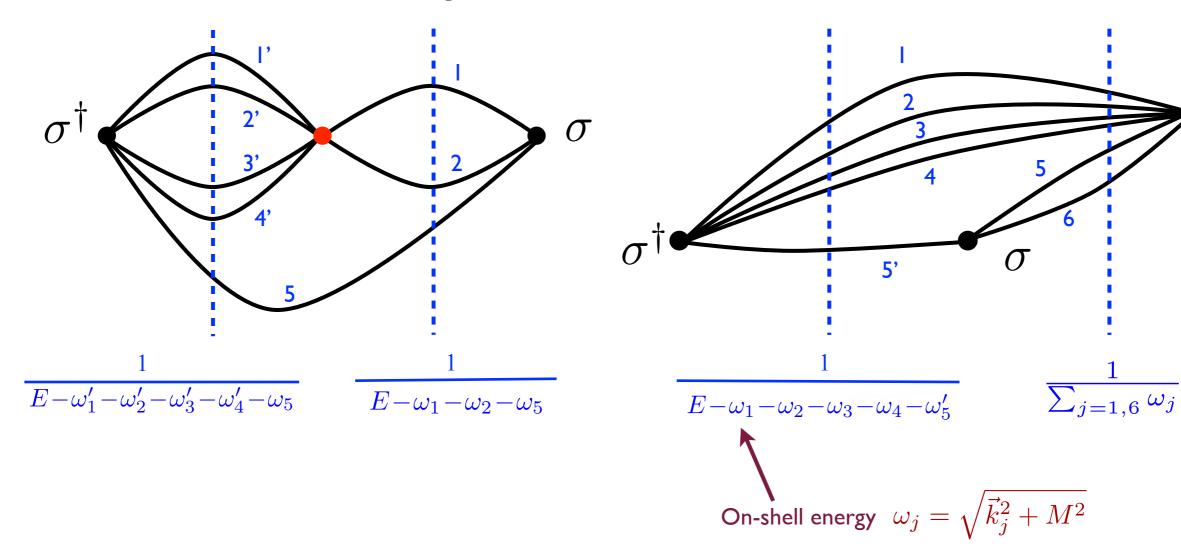
• Key properties of FPV (discussed below): real and no unitary cusp at threshold



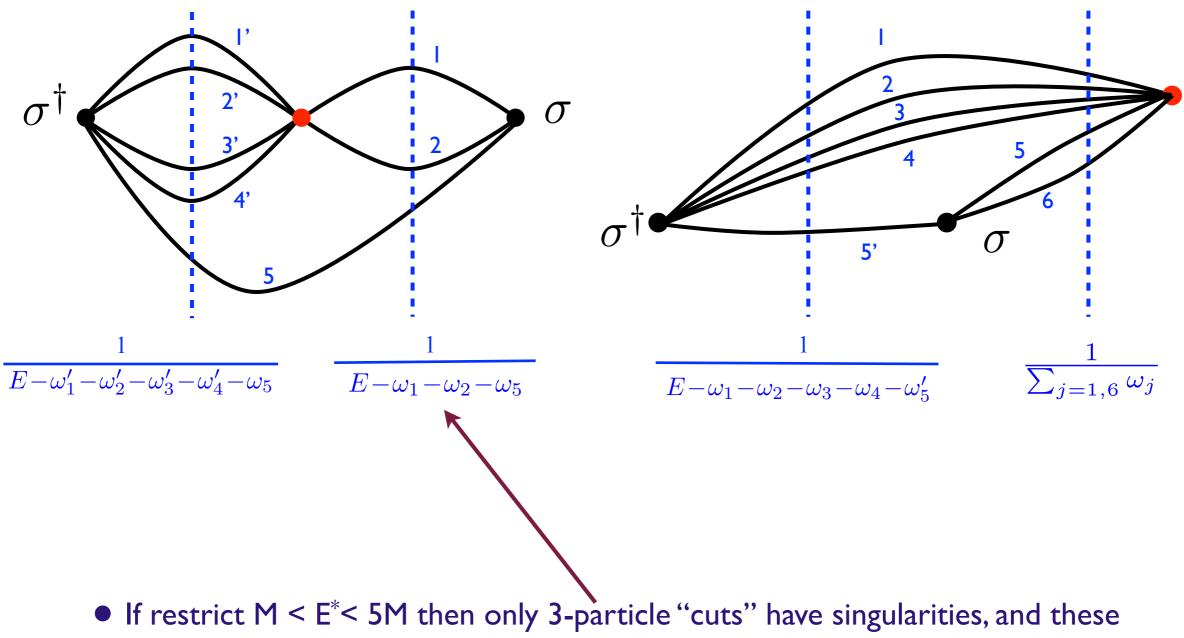
- Identify potential singularities: can use time-ordered PT (i.e. do k₀ integrals)
- Example



• 2 out of 6 time orderings:



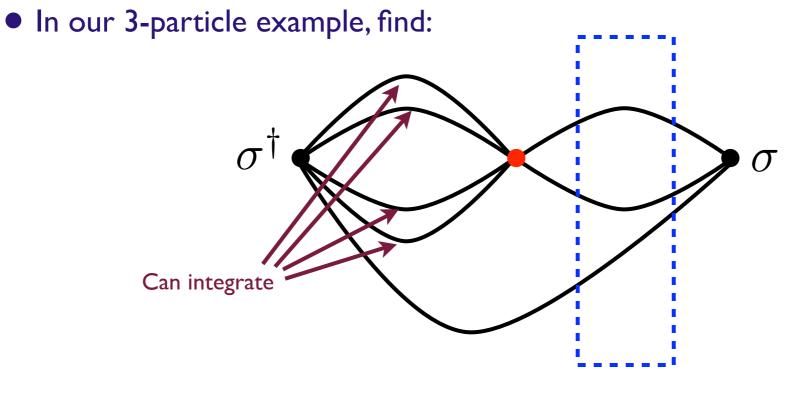
• 2 out of 6 time orderings:



occur only when all three particles to go on-shell

Combining key steps 1-3

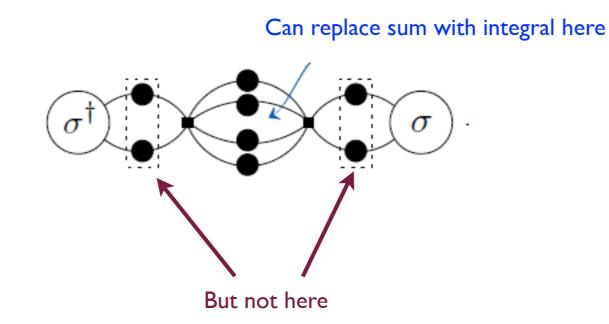
• For each diagram, determine which momenta must be summed, and which can be integrated



Must sum momenta passing through box

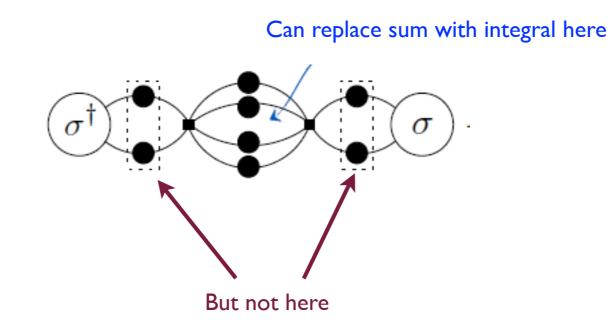
Combining key steps 1-3

- For each diagram, determine which momenta must be summed, and which can be integrated
- In our 2-particle example, find:



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:



• Then repeatedly use sum=integral + "sum-integral" to simplify

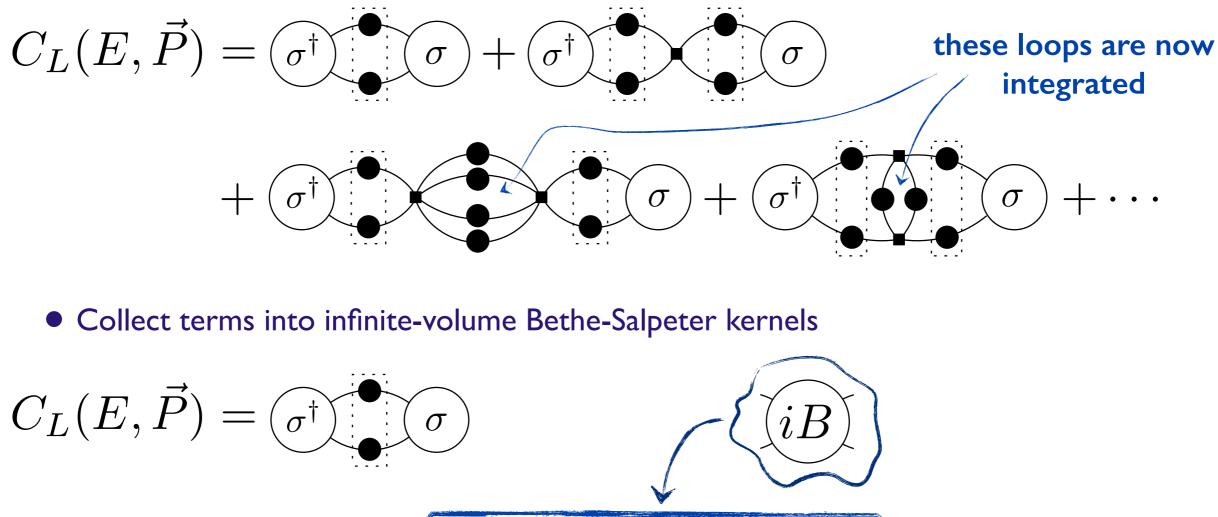
Key issues 4-6

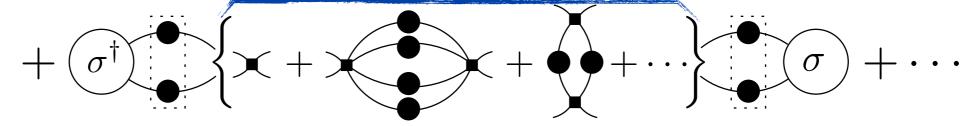
- Dealing with cusps, avoiding divergences in 3-particle scattering amplitude, and dealing with breaking of particle interchange symmetry
- Discuss later!

2-particle quantization condition

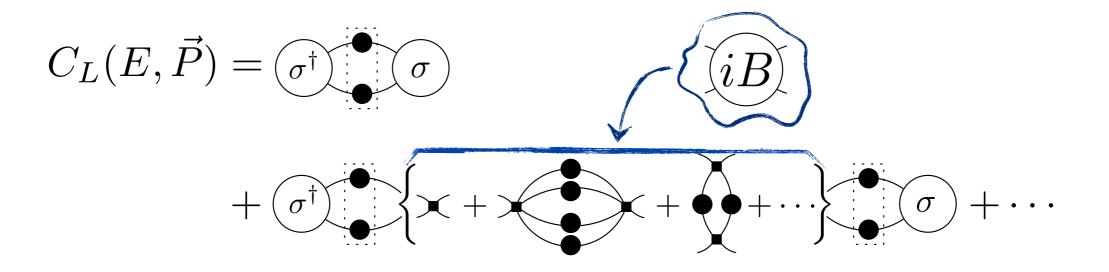
Following method of [Kim, Sachrajda & SS 05]

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

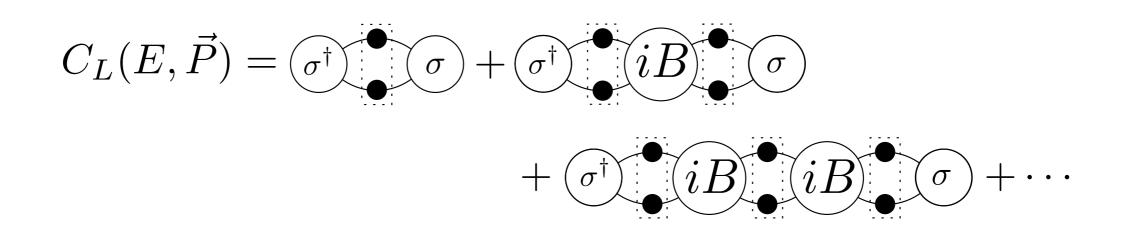




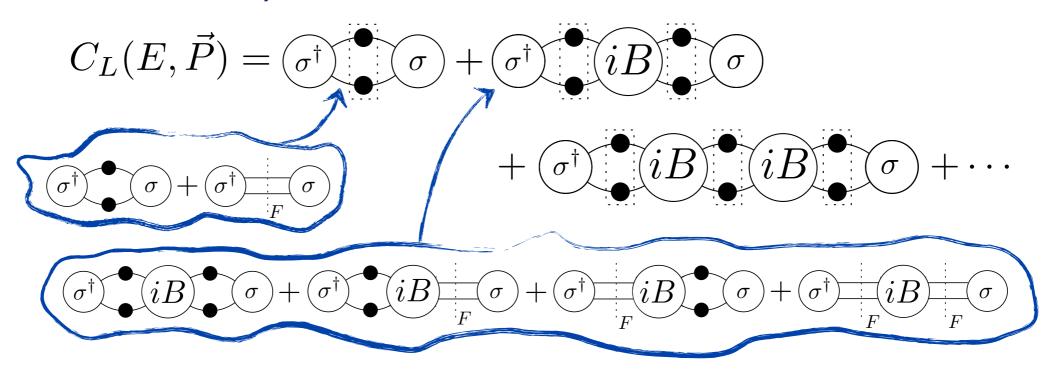
- Apply previous analysis to 2-particle correlator
- Collect terms into infinite-volume Bethe-Salpeter kernels



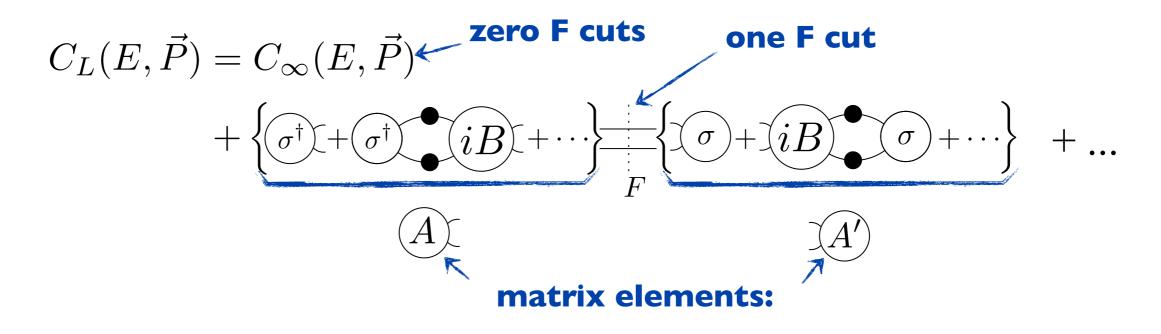
• Leading to



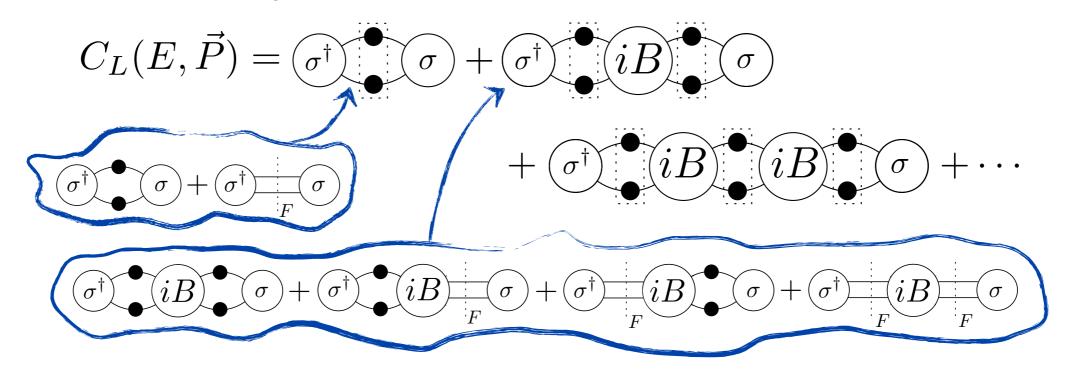
• Next use sum identity



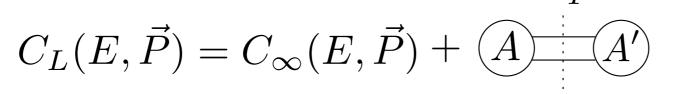
• And regroup according to number of "F cuts"

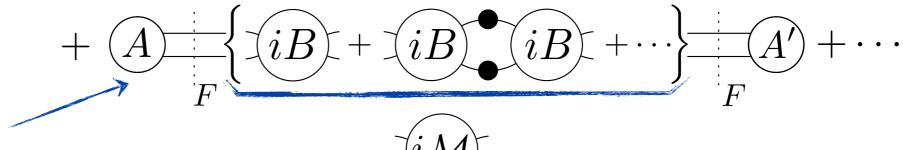


• Next use sum identity



• And keep regrouping according to number of "F cuts"

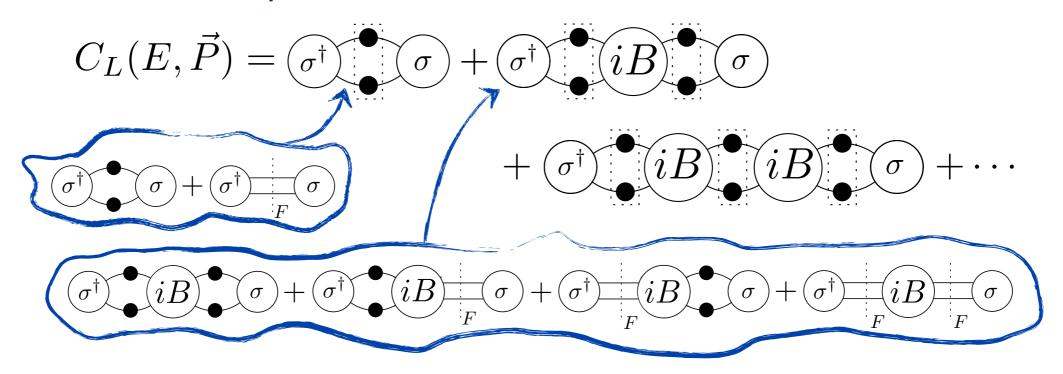




two F cuts

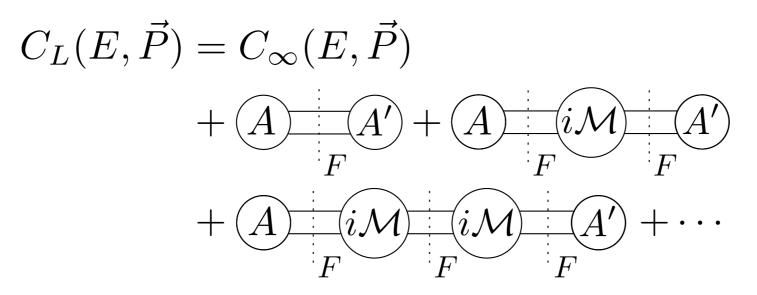
the infinite-volume, on-shell 2→2 scattering amplitude

• Next use sum identity



• Alternate form if use PV-tilde prescription: $C_{L}(E, \vec{P}) = C_{\infty}^{\widetilde{PV}}(E, \vec{P}) + (A_{\overline{PV}}) + (A_{\overline{PV$





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

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



$$C_{L}(E, \vec{P}) = C_{\infty}(E, \vec{P})$$

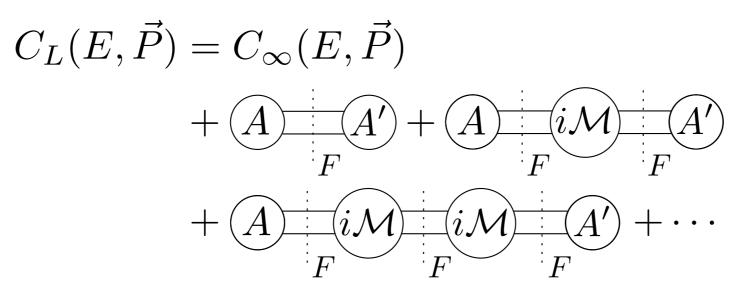
$$+ (A) + (A)$$

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

•
$$C_L(E, \vec{P}) = C_{\infty}(E, \vec{P}) + A'iF \frac{1}{1 - i\mathcal{M}_{2 \to 2}iF} A$$
 no poles,
only cuts matrices in l,m space

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

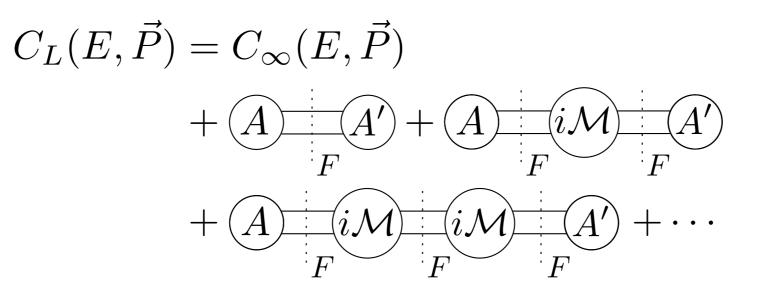




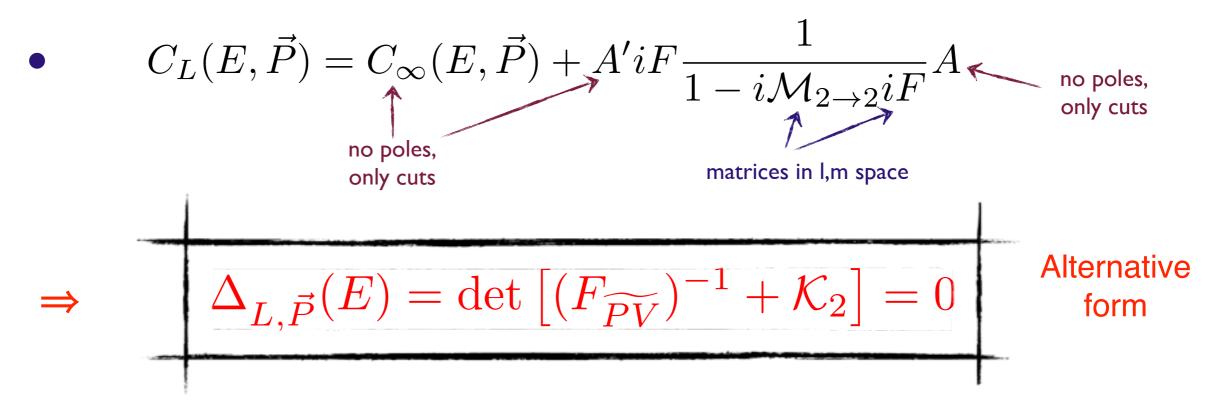
•
$$C_L(E, \vec{P}) = C_{\infty}(E, \vec{P}) + \sum_{n=0}^{\infty} A' i F[i\mathcal{M}_{2\to 2}iF]^n A$$

•
$$C_L(E, \vec{P}) = C_{\infty}(E, \vec{P}) + A'iF \frac{1}{1 - i\mathcal{M}_{2 \to 2}iF} A$$
 no poles,
only cuts matrices in l,m space
 $\Delta_{L, \vec{P}}(E) = \det \left[(iF)^{-1} - i\mathcal{M}_{2 \to 2} \right] = 0$



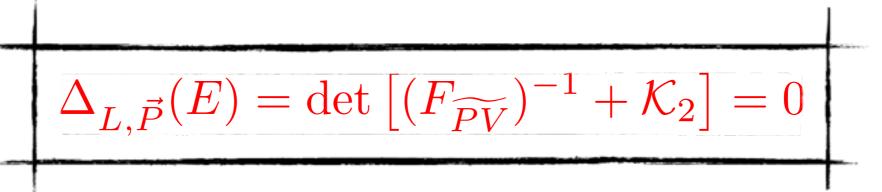


•
$$C_L(E, \vec{P}) = C_{\infty}(E, \vec{P}) + \sum_{n=0}^{\infty} A' i F[i\mathcal{M}_{2\to 2}iF]^n A$$



2-particle quantization condition

• At fixed L & P, the finite-volume spectrum E₁, E₂, ... is given by solutions to



- \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 I_{max}

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

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

S. Sharpe, "Multiparticle processes" 09/28/15 INT workshop

-1

3-particle quantization condition

Following [Hansen & SS 14]

Recall Final result

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

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

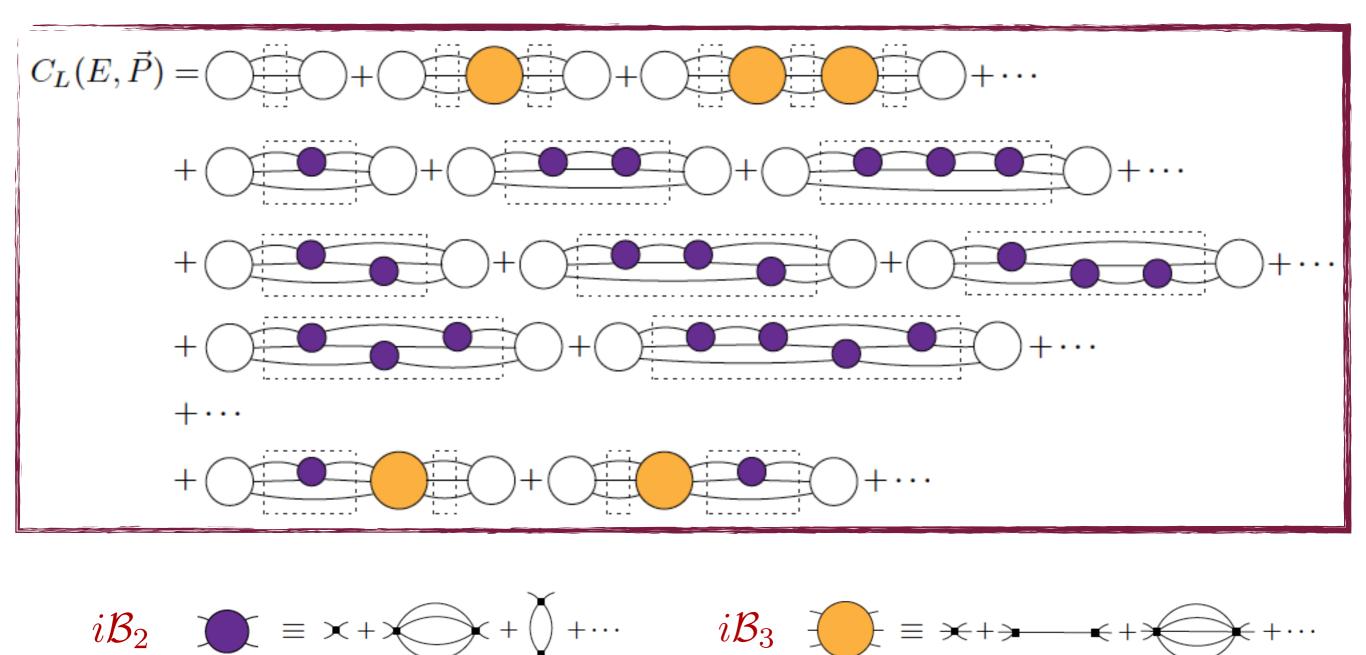
. .

- 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

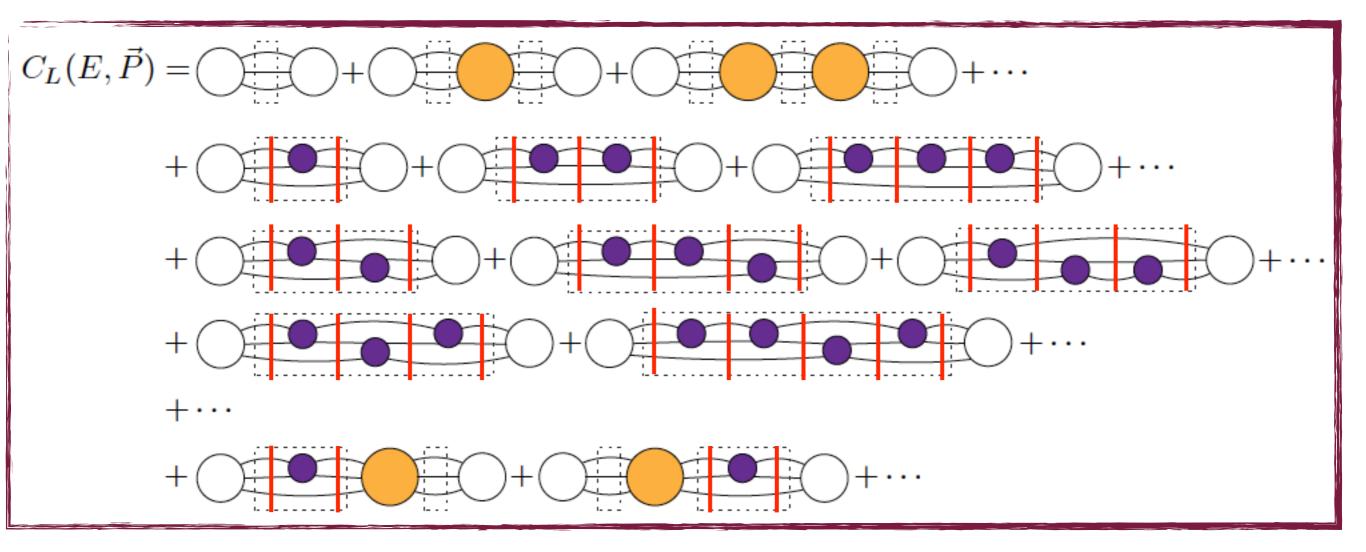
• Can sum subdiagrams without 3-particle cuts into Bethe-Salpeter kernels

 \Rightarrow Skeleton expansion in terms of Bethe-Salpeter kernels

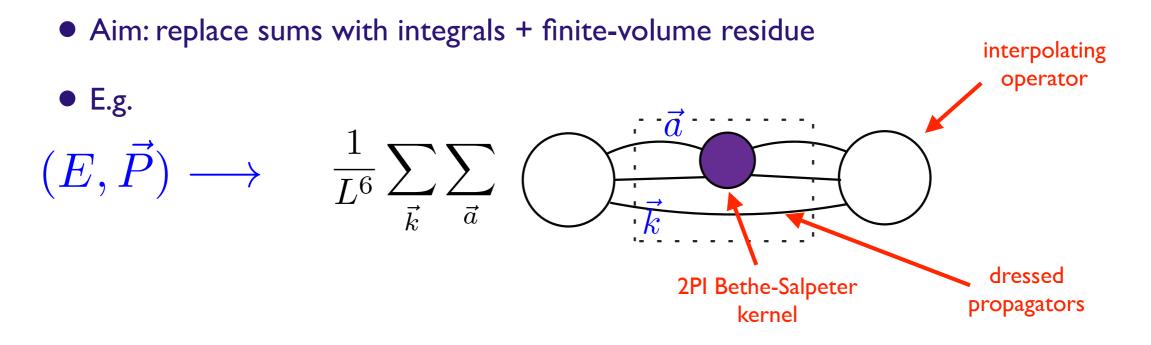


Key issue 4: dealing with cusps

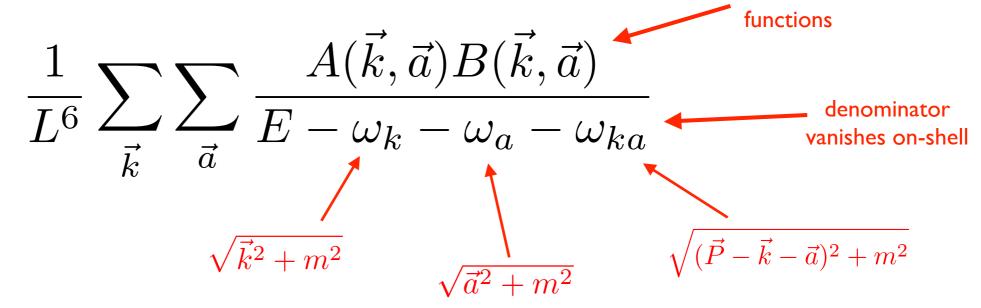
- Want to replace sums with integrals + F-cuts as in 2-particle analysis
- Straightforward implementation fails when have 3 particle intermediate states adjacent to 2→2 kernels



Cusp analysis (1)



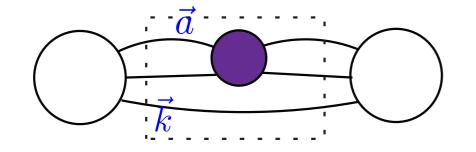
- Can replace sums with integrals for smooth, non-singular parts of summand
- Singular part of left-hand 3-particle intermediate state



S. Sharpe, "Multiparticle processes" 09/28/15 INT workshop

smooth

Cusp analysis (2)



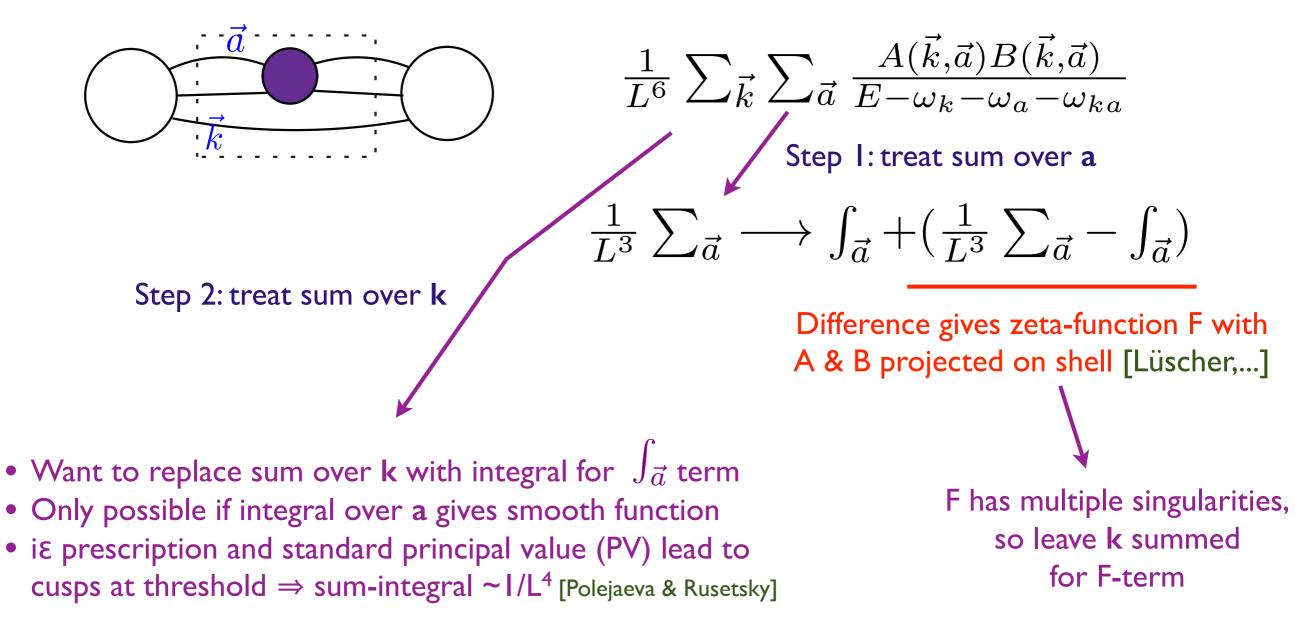
$$\frac{1}{L^{6}} \sum_{\vec{k}} \sum_{\vec{a}} \frac{A(\vec{k}, \vec{a}) B(\vec{k}, \vec{a})}{E - \omega_{k} - \omega_{a} - \omega_{ka}}$$
Step I: treat sum over a

$$\frac{1}{L^3} \sum_{\vec{a}} \longrightarrow \int_{\vec{a}} + \left(\frac{1}{L^3} \sum_{\vec{a}} - \int_{\vec{a}}\right)$$

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

F has multiple singularities, so leave k summed for F-term

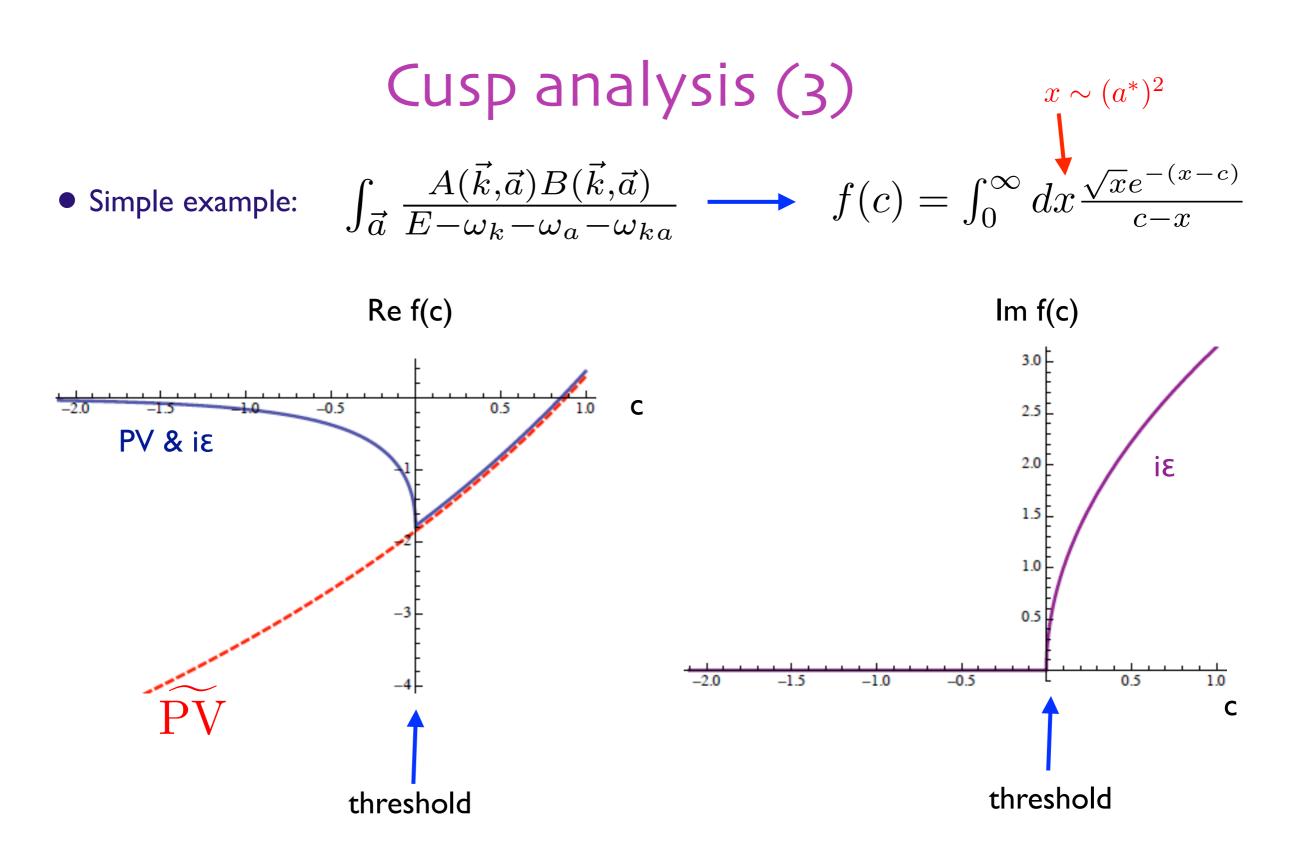
Cusp analysis (2)



- Requires use of modified $\widetilde{PV}\xspace$ prescription

Result:

$$\frac{1}{L^6} \sum_{\vec{k}} \sum_{\vec{a}} = \int_{\vec{k}} \int_{\vec{a}} + \sum_{\vec{k}}$$
"F term"

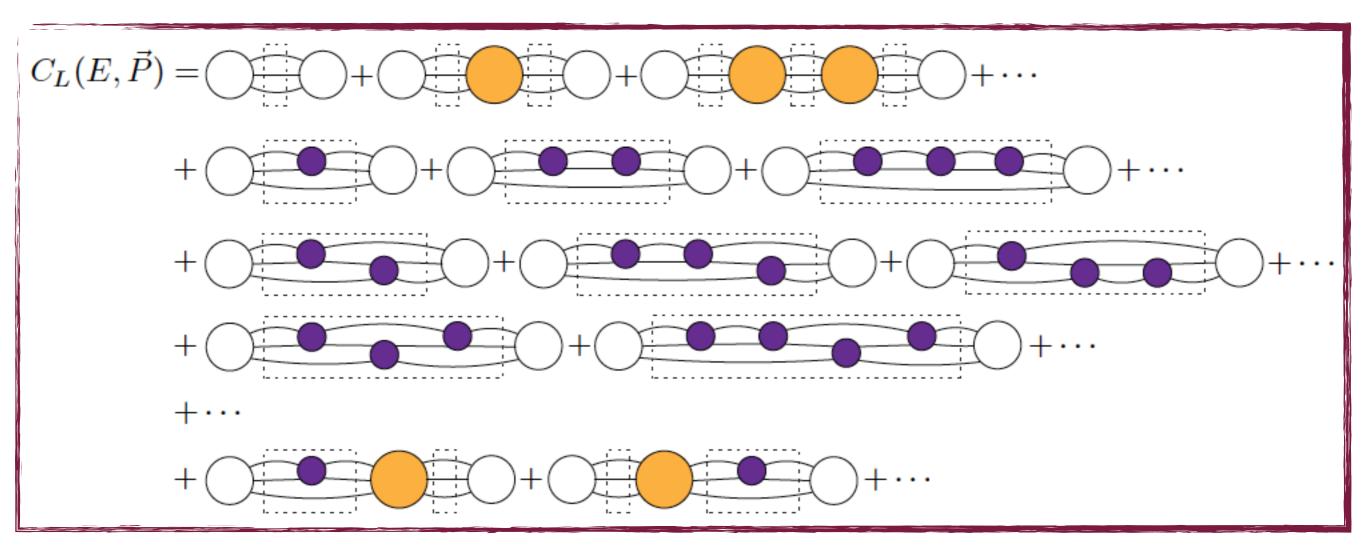


• Far below threshold, \overline{PV} smoothly turns back into PV

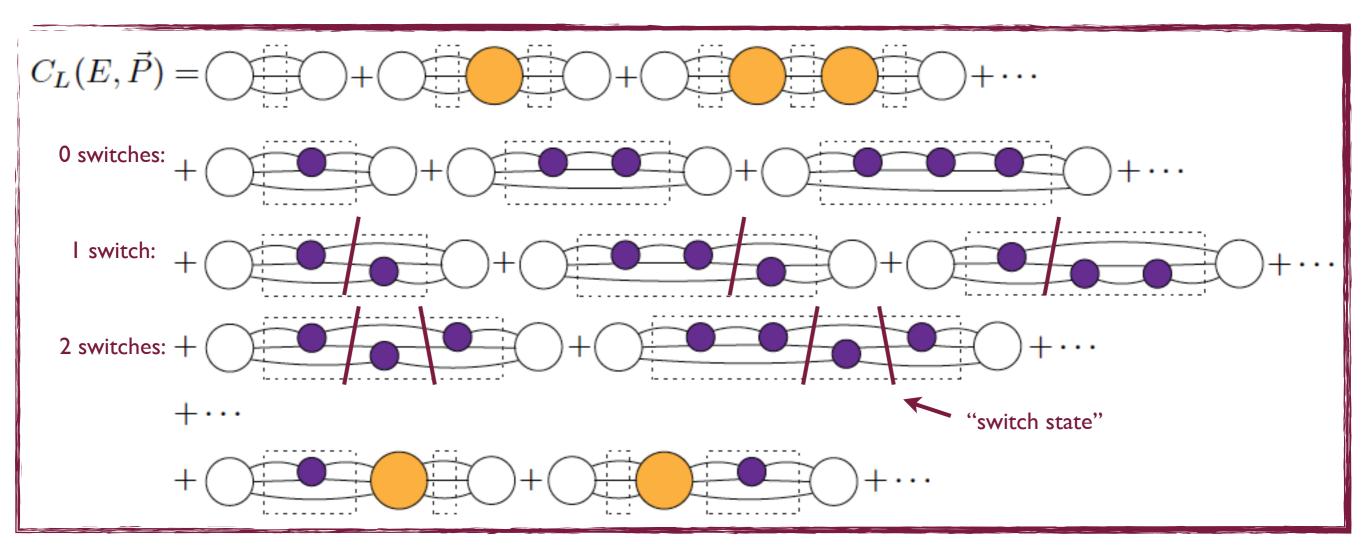
Cusp analysis (4)

- \bullet Bottom line: must use \widetilde{PV} prescription for all loops
- This is why K-matrix \mathcal{K}_2 appears in 2-particle summations
- \mathcal{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 \mathcal{M}_2^{ℓ}

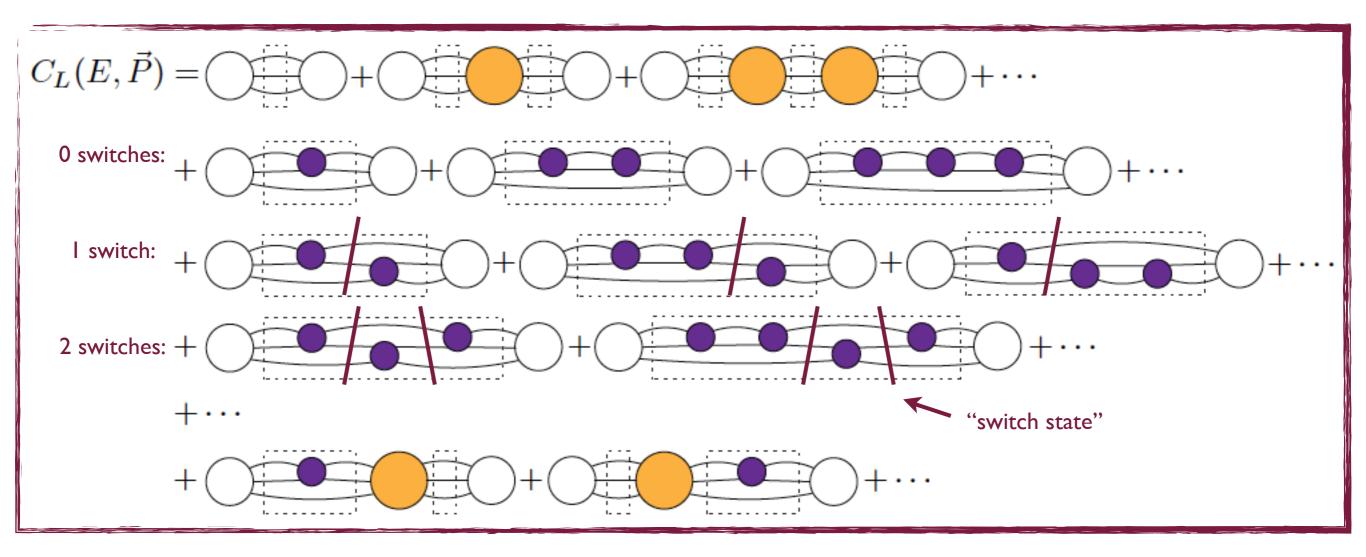
Key issue 5: dealing with "switches"



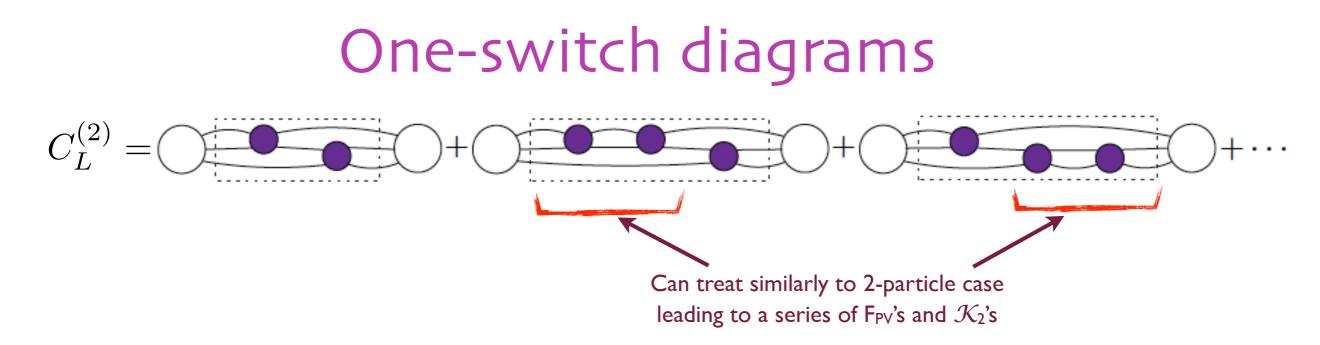
Key issue 5: dealing with "switches"



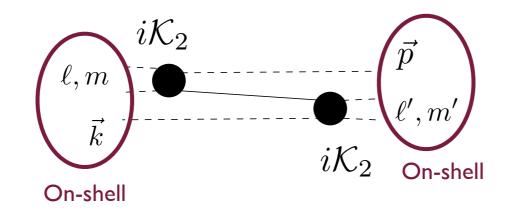
Key issue 5: dealing with "switches"



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

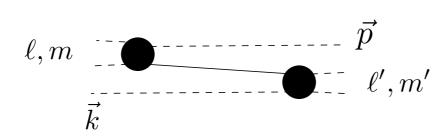


• End up with L-dependent part of $C^{(2)}$ having at its core:

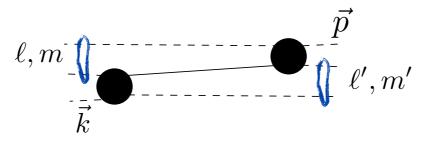


• This is our first contribution to the infinite-volume 3 particle scattering amplitude

One-switch problem



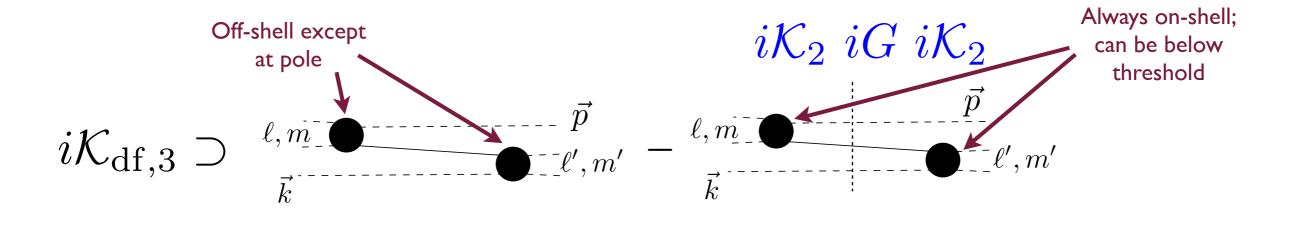
- Amplitude is singular for some choices of k, p in physical regime
 - Propagator goes on shell if top two (and thus bottom two) scatter elastically
- Not a problem per se, but leads to difficulties when amplitude is symmetrized
 - Occurs when include three-switch contributions



- Singularity implies that decomposition in $Y_{l,m}$ 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]

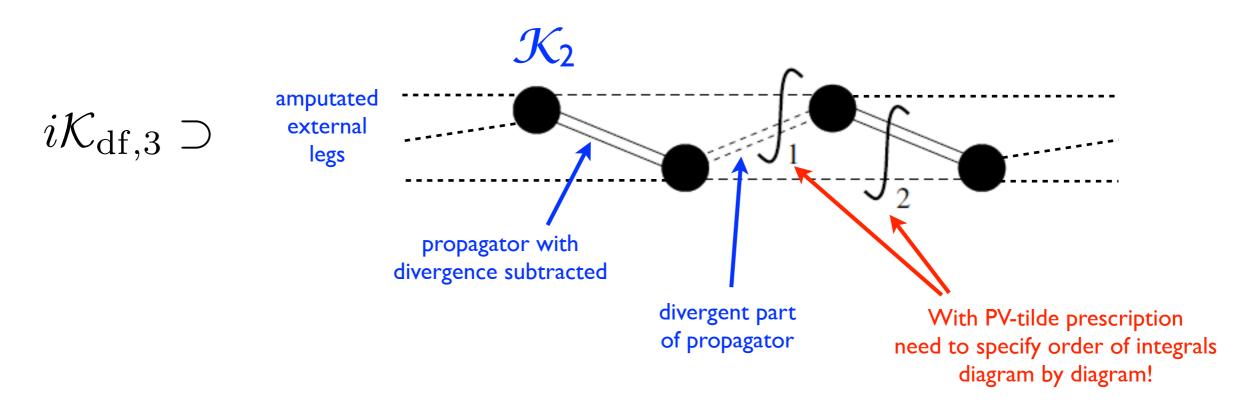


$$G_{p,\ell',m';k,\ell,m} \equiv \left(\frac{k^*}{q_p^*}\right)^{\ell'} \frac{4\pi Y_{\ell',m'}(\hat{k}^*)H(\vec{p}\,)H(\vec{k}\,)Y_{\ell,m}^*(\hat{p}^*)}{2\omega_{kp}(E-\omega_k-\omega_p-\omega_{kp})} \left(\frac{p^*}{q_k^*}\right)^{\ell} \frac{1}{2\omega_k L^3}$$

- Key point: $\mathcal{K}_{df,3}$ 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

Key issue 6: symmetry breaking

- $\bullet \mbox{ Using } PV$ prescription breaks particle interchange symmetry
 - Top two particles treated differently from spectator
 - Leads to very complicated definition for $\mathcal{K}_{df,3}$, e.g.



• Can extend definition of $\mathcal{K}_{df,3}$ to all orders, in such a way that it is symmetric under interchange of external particles

Key issue 6: symmetry breaking

- Final definition of $\mathcal{K}_{df,3}$ is, crudely speaking:
 - Sum all Feynman diagrams contributing to \mathcal{M}_3
 - Use $\widetilde{\mathrm{PV}}$ 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
- $\mathcal{K}_{df,3}$ is an UGLY infinite-volume quantity related to scattering
- At the time of our initial paper, we did not know the relation between $\mathcal{K}_{df,3}$ and \mathcal{M}_3 & \mathcal{M}_2 , although we had reasons to think that such a relationship exists
- Now we know the relationship

Infinite volume relation between $\mathcal{K}_{df,3}$ & \mathcal{M}_3

[Hansen & SS 15, in preparation]

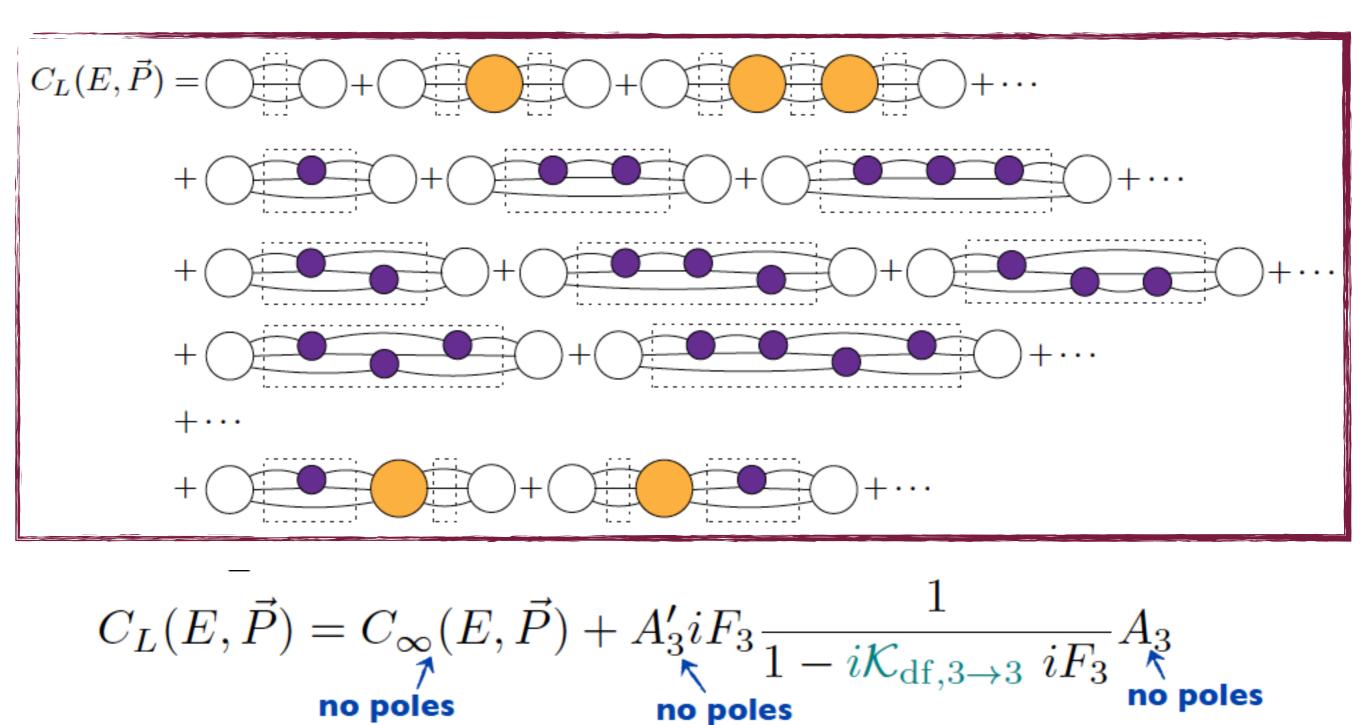
The issue

- Three particle quantization condition depends on $\mathcal{K}_{df,3}$ rather than the three particle scattering amplitude \mathcal{M}_3
- $\mathcal{K}_{df,3}$ 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
- \bullet To complete the quantization condition we must relate $\mathcal{K}_{df,3}$ to \mathcal{M}_3

The method

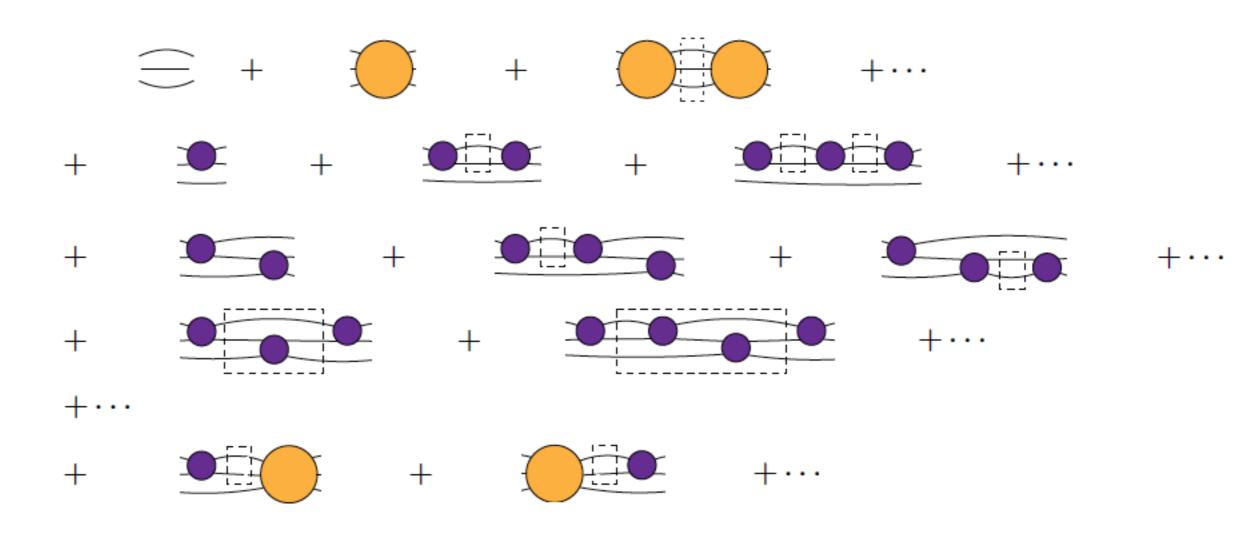
- Define a "finite volume scattering amplitude" $\mathcal{M}_{L,3}$ which goes over to \mathcal{M}_3 in an (appropriately taken) $L \rightarrow \infty$ limit
- Relate $\mathcal{M}_{L,3}$ to $\mathcal{K}_{df,3}$ at finite volume—which turns out to require a small generalization of the methods used to derive the quantization condition
- Take $L \rightarrow \infty$, obtaining nested integral equations

Modifying CL to obtain $\mathcal{M}_{\mathrm{L,3}}$



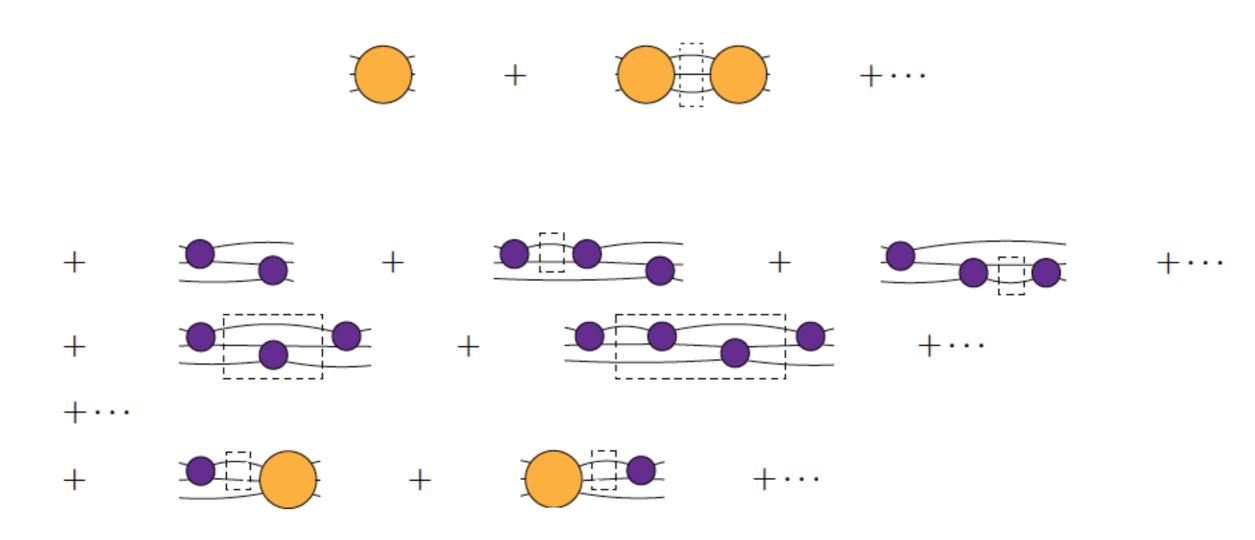
S. Sharpe, "Multiparticle processes" 09/28/15 INT workshop

Modifying CL to obtain $\mathcal{M}_{L,3}$



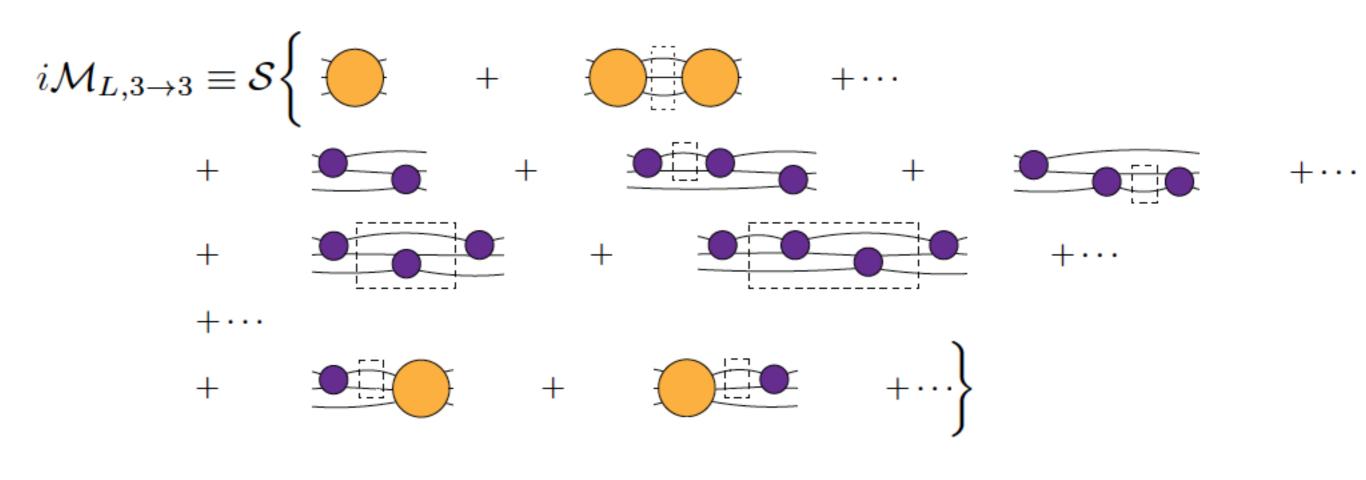
Step I: "amputate"

Modifying CL to obtain $\mathcal{M}_{L,3}$



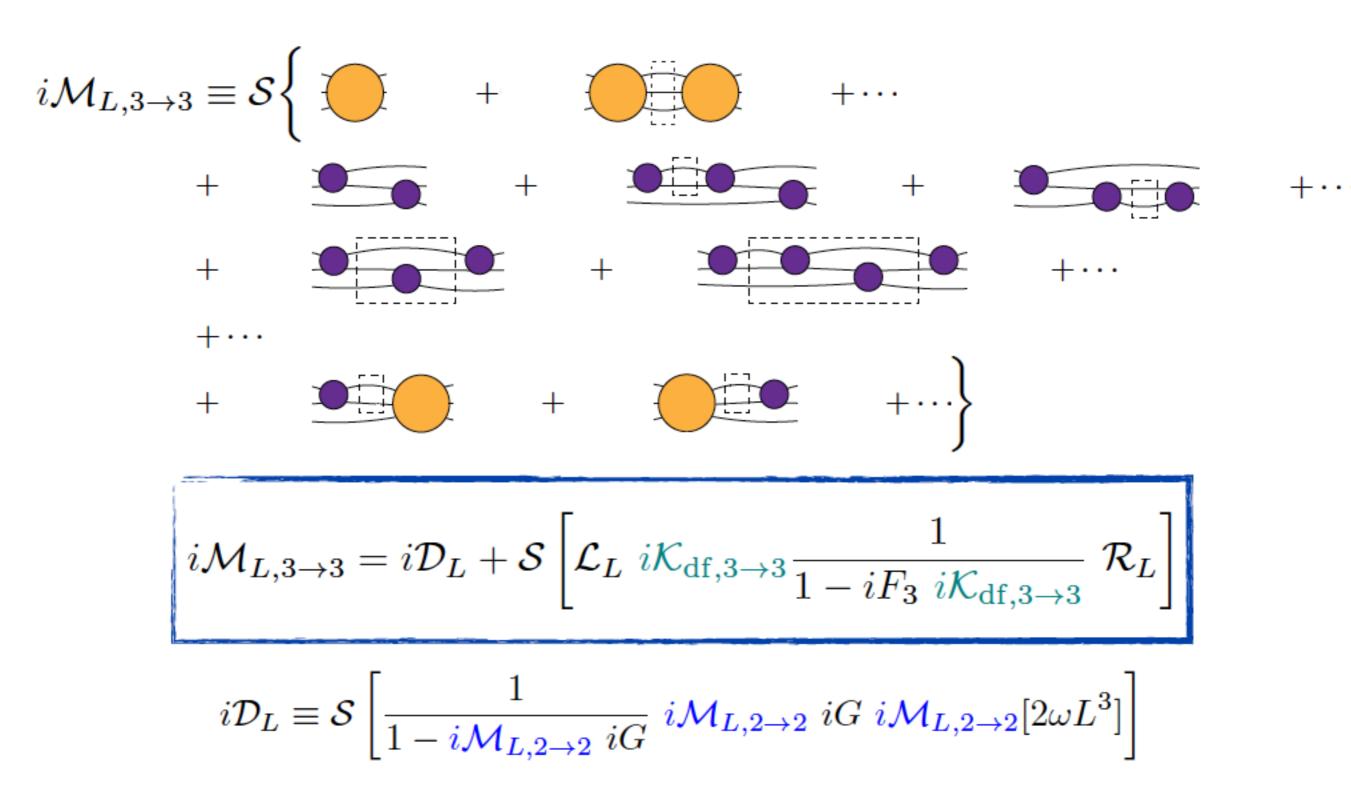
Step 2: Drop disconnected diagrams

Modifying CL to obtain $\mathcal{M}_{\mathrm{L,3}}$



Step 3: Symmetrize

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



S. Sharpe, "Multiparticle processes" 09/28/15 INT workshop

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

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

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

- \mathcal{L}_L and \mathcal{R}_L depend only on $\mathcal{M}_{L,2}$, G and F_{PV}
- $\mathcal{M}_{L,2}$ is "finite volume two particle scattering amplitude"

$$i\mathcal{M}_{L,2\to2} \equiv i\mathcal{K}_{2\to2} \frac{1}{1 - iF_{\widetilde{PV}}i\mathcal{K}_{2\to2}}$$

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

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

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

• Key point: the same (ugly) $\mathcal{K}_{df,3}$ appears in $\mathcal{M}_{L,3}$ as in C_L

$$C_L(E,\vec{P}) = C_{\infty}(E,\vec{P}) + A'_3 i F_3 \frac{1}{1 - i \mathcal{K}_{df,3\to 3} i F_3} A_3$$

• Can use $\mathcal{M}_{L,3}$ to derive quantization condition

Final step: taking $L \rightarrow \infty$

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

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

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

• All equations involve matrices with indices k, l, m

Spectator momentum $\mathbf{k} = 2 \mathbf{n} \pi / \mathbf{L}$ Summed over \mathbf{n}

Already in infinite volume variables

Final step: taking $L \rightarrow \infty$

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

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

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

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

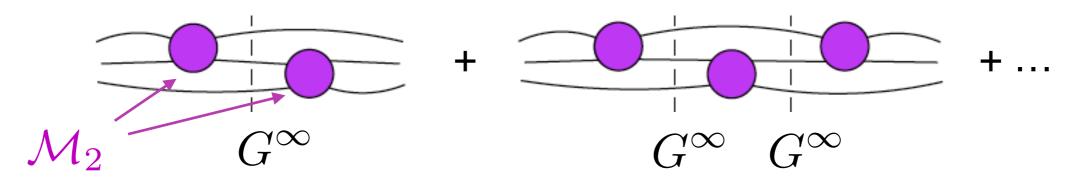
$$i\mathcal{M}_{3\to3} = \lim_{L\to\infty} \left| i\mathcal{M}_{L,3\to3} \right|_{i\epsilon}$$

Final result: nested integral equations (1) Obtain $L \rightarrow \infty$ limit of \mathcal{D}_L

$$i\mathcal{D}^{(u,u)}(\vec{p},\vec{k}) = i\mathcal{M}_2(\vec{p})iG^\infty(\vec{p},\vec{k})i\mathcal{M}_2(\vec{k}) + \int_s \frac{1}{2\omega_s}i\mathcal{M}_2(\vec{p})iG^\infty(\vec{p},\vec{s})i\mathcal{D}^{(u,u)}(\vec{s},\vec{k})$$

$$G^{\infty}_{\ell'm';\ell m}(\vec{p},\vec{k}) \equiv \left(\frac{k^{*}}{q_{p}^{*}}\right)^{\ell'} \frac{4\pi Y_{\ell'm'}(\hat{k}^{*})H(\vec{p})H(\vec{k})Y^{*}_{\ell m}(\hat{p}^{*})}{2\omega_{kp}(E-\omega_{k}-\omega_{p}-\omega_{kp}+i\epsilon)} \left(\frac{p^{*}}{q_{k}^{*}}\right)^{\ell}$$

- Quantities are still matrices in *l,m* space
- Presence of cut-off function means that integrals have finite range
- $\mathcal{D}^{(u,u)}$ sums geometric series which gives physical divergences in \mathcal{M}_3



Final result: nested integral equations (2) Sum geometric series involving $\mathcal{K}_{df,3}$

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

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

- $\rho(\mathbf{k})$ 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.

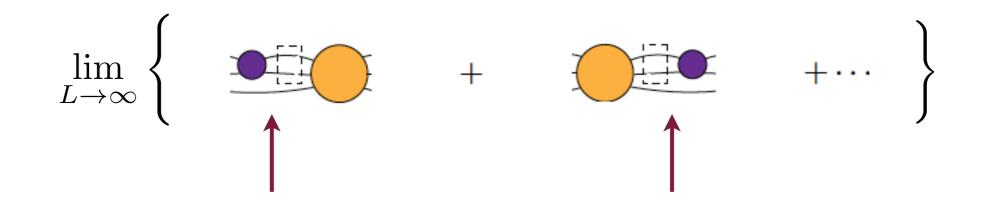
$$i\mathcal{K}_{\mathrm{df},3\to3}\frac{1}{1-iF_3\ i\mathcal{K}_{\mathrm{df},3\to3}}$$

Final result: nested integral equations

(3) Add in effects of external $2 \rightarrow 2$ scattering:

$$\underbrace{\mathcal{M}_{3}(\vec{p},\vec{k}) - \mathcal{S}\left\{\mathcal{D}^{(u,u)}(\vec{p},\vec{k})\right\}}_{\mathcal{M}_{df,3}} = -\mathcal{S}\left\{\int_{s}\int_{r}\mathcal{L}^{(u,u)}(\vec{p},\vec{s})\mathcal{T}(\vec{s},\vec{r})\mathcal{R}^{(u,u)}(\vec{r},\vec{k})\right\}$$

• Sums geometric series on "outside" of $\mathcal{K}_{df,3}$'s



• Can also invert and determine $\mathcal{K}_{df,3}$ given \mathcal{M}_3 and \mathcal{M}_2