Extracting 3-particle scattering amplitudes from the finite-volume spectrum

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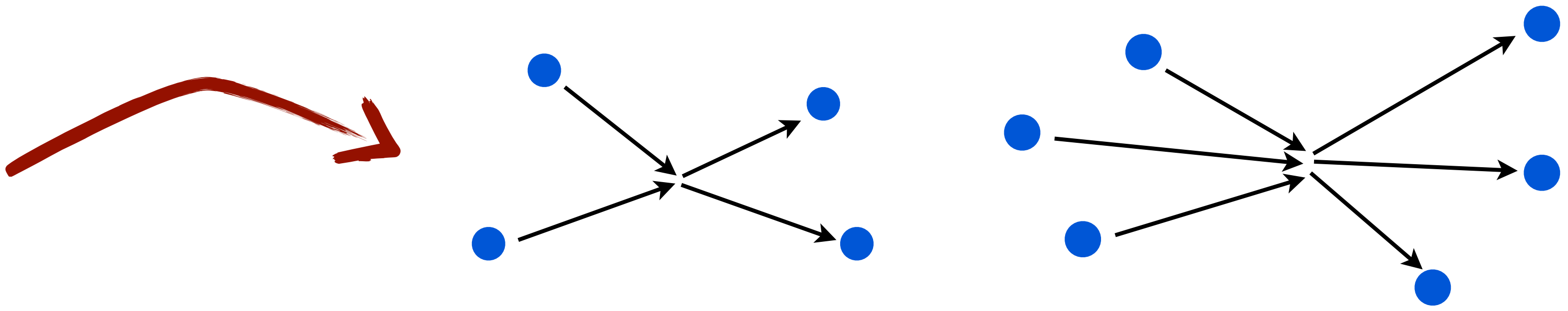
M. Hansen & S. Sharpe, arXiv:1408.5933 (PRD in press) + work in progress

The fundamental issue

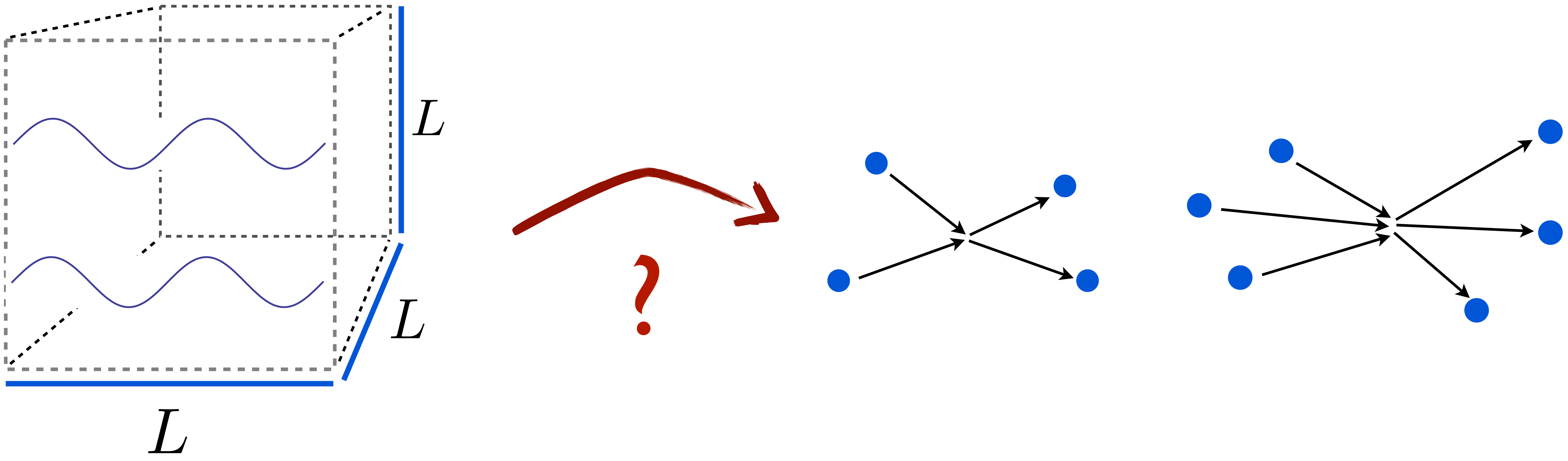
- Lattice simulations are done in finite volumes
- Experiments are not



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?



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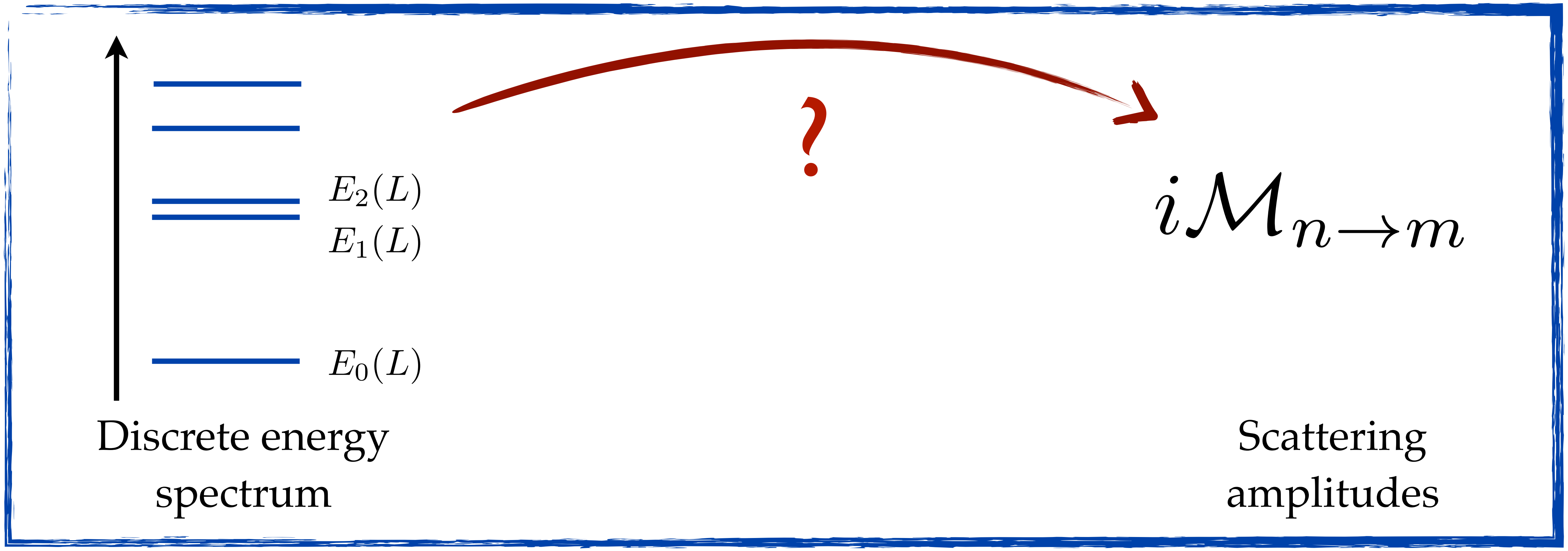


$E_2(L)$

$E_1(L)$

$E_0(L)$

?

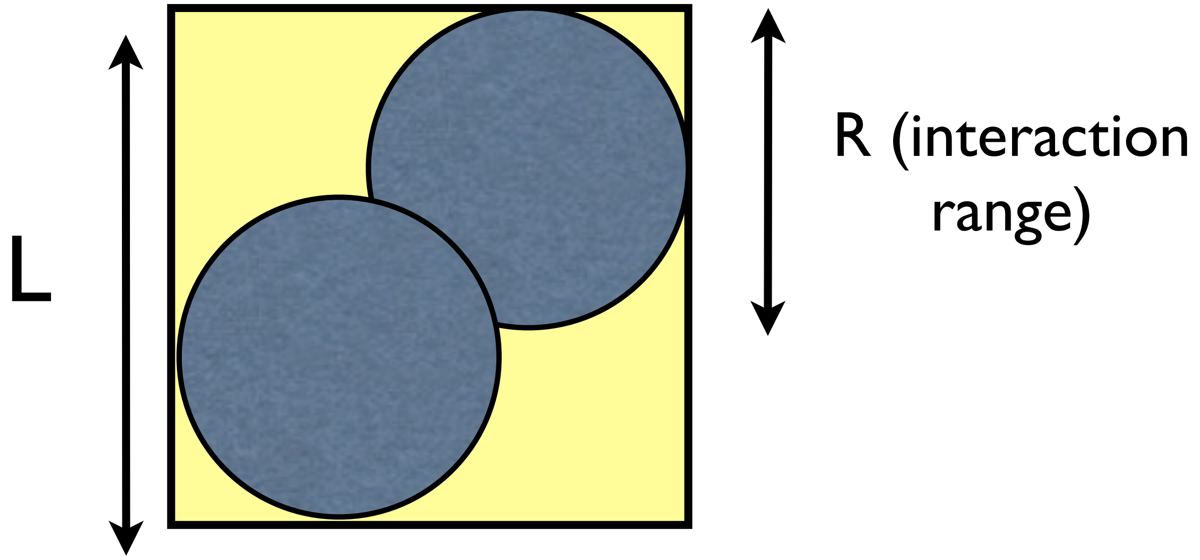
$i\mathcal{M}_{n\to m}$

Discrete energy spectrum

Scattering amplitudes

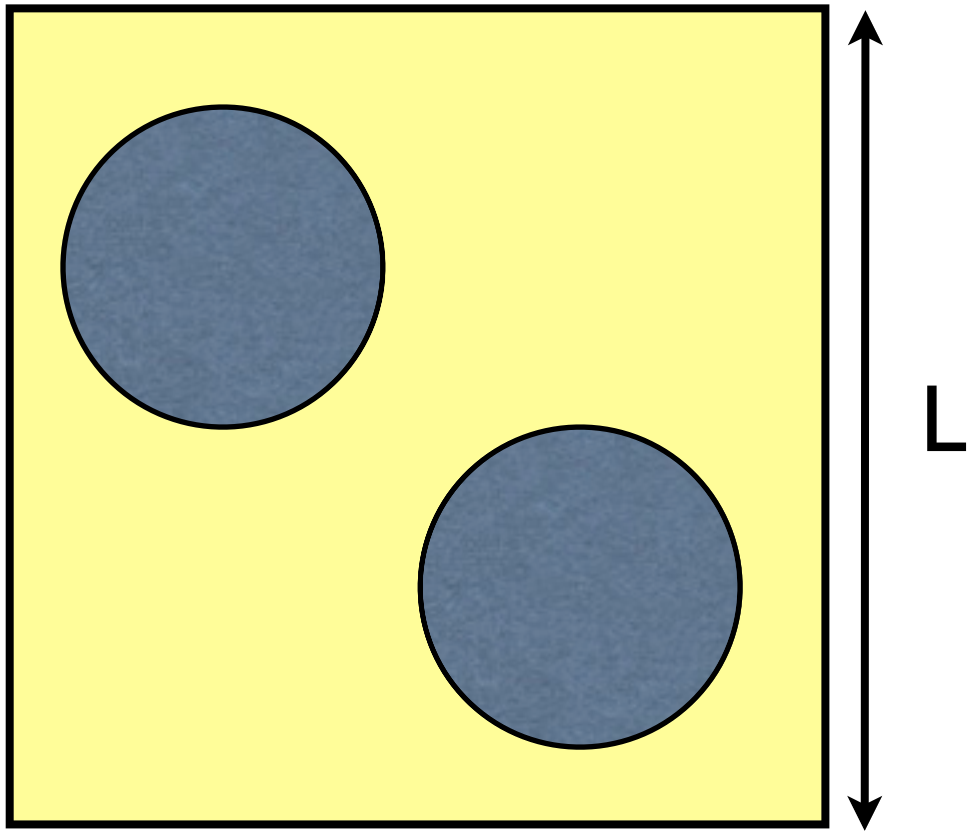
When is spectrum related to scattering amplitudes?

✗



L<2R
No "outside" region.
Spectrum NOT related to scatt. amps.
Depends on finite-density properties

✔

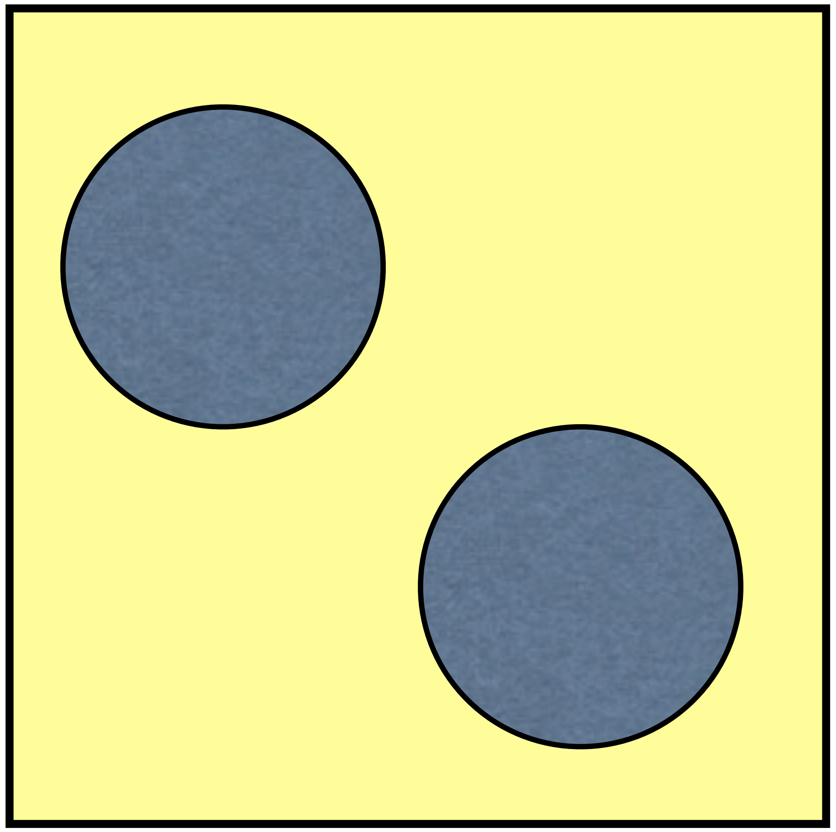


L>2R
There is an "outside" region.
Spectrum IS related to scatt. amps.
up to corrections proportional to
$e^{-M_\pi L}$

[Lüscher]

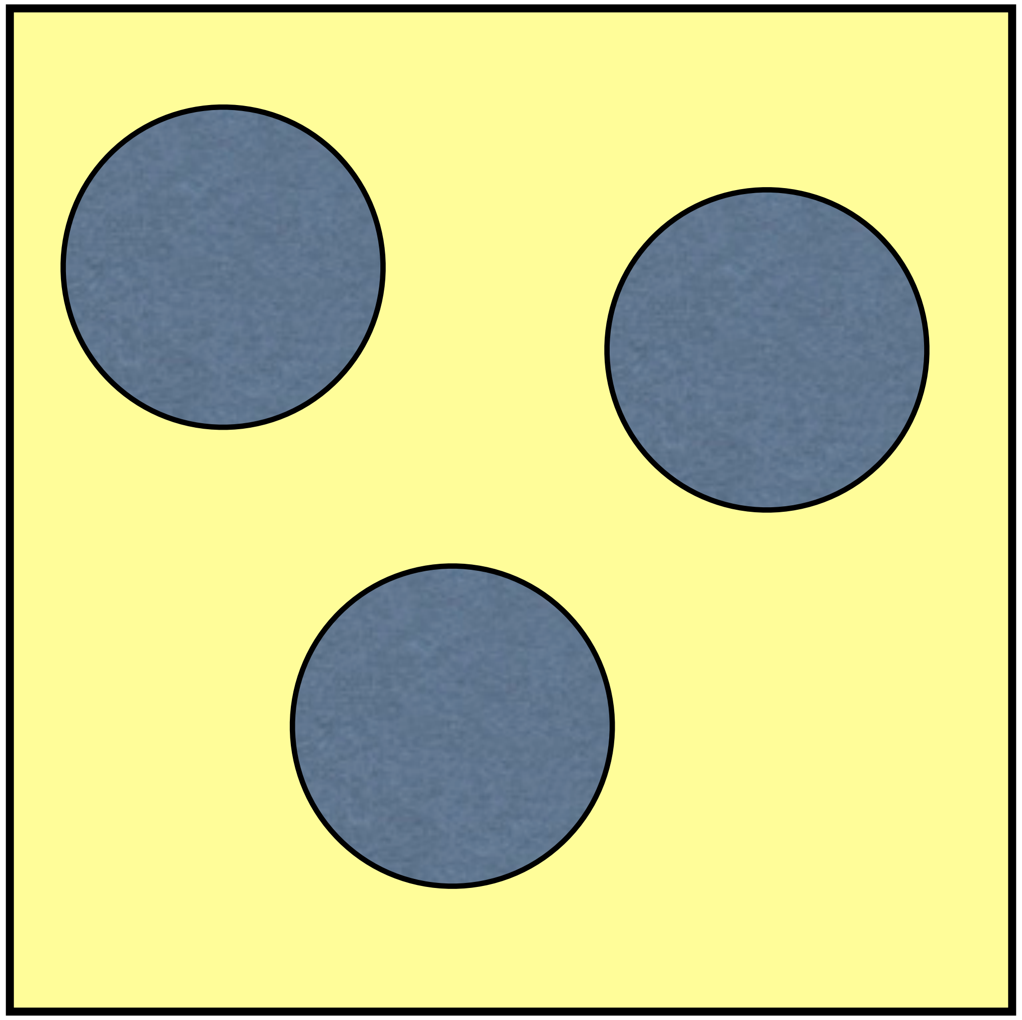
Problems considered today

L>2R



Previously solved;
solution used by simulations;
will sketch as warm-up problem

L>3R (?)



Will present new solution;
practical applicability under investigation

Outline

- Background & motivation
- Set-up and main ideas
- 2-particle quantization condition
- 3-particle quantization condition
- Utility of result: truncation
- Important check: threshold expansion
- Conclusions and outlook

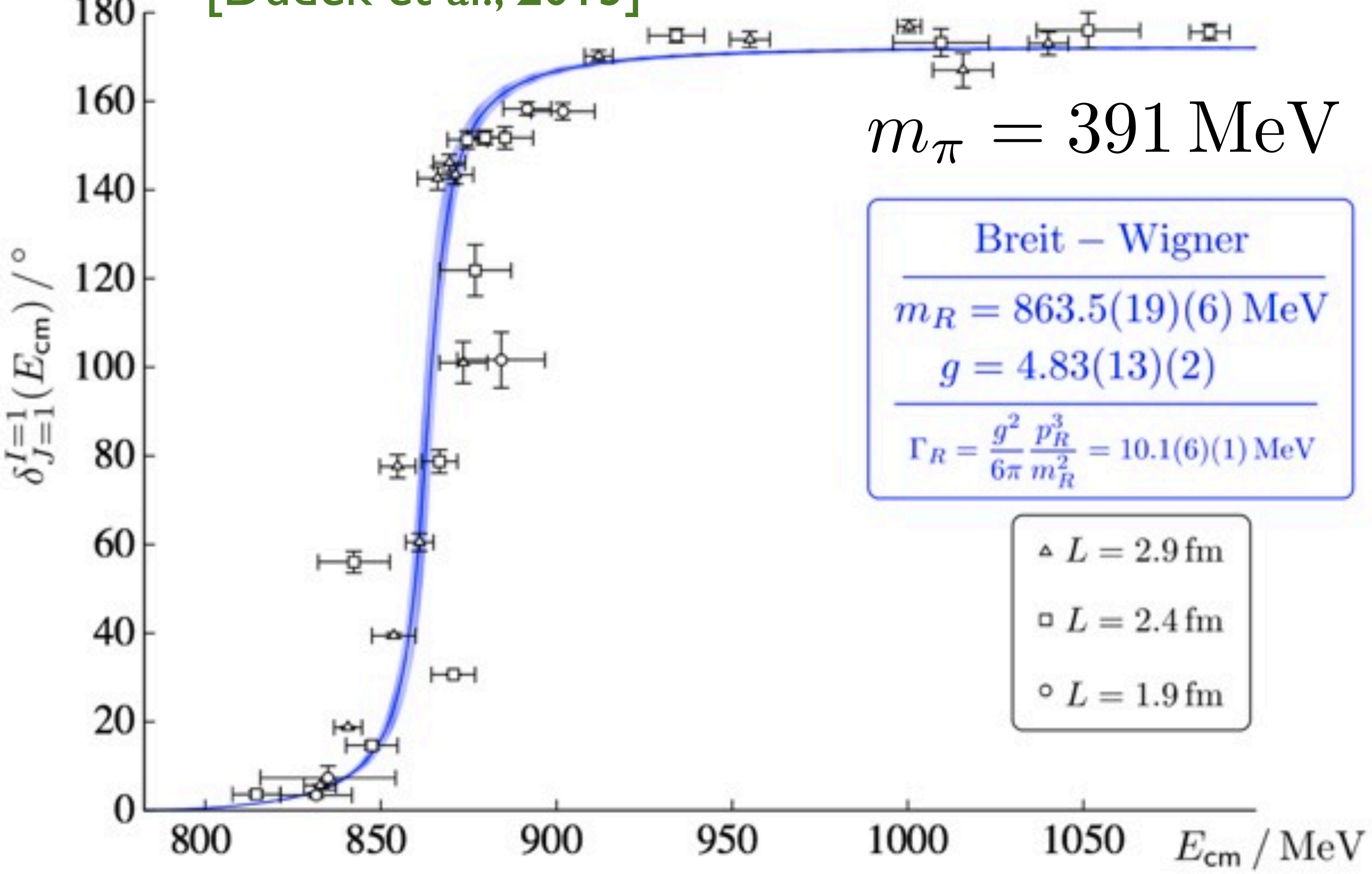
Background & motivation

2-particle resonances

- To predict & study the properties of hadrons using lattice QCD, we need to be able to study resonances
  - Resonances are not asymptotic states; show up in behavior of phase-shift
  - Luscher's method allows determination of 2→2 phase shifts in elastic regime

[Dudek et al., 2013]

ππ
phase
shift



$m_\pi = 391\,\text{MeV}$

Decay amplitudes

- Also want to calculate weak decay amplitudes, e.g. K→ππ
  - Lattice QCD can calculate $\langle K|H_W|\pi\pi\rangle_L$, but to use this requires determining the composition of the finite volume ππ state (which contains several partial waves with different normalizations). Solved by [Lellouch & Lüscher]
  - [RBC/UKQCD] obtained K→ππ (I=2) amplitude with physical kinematics
  - For I=0, pilot study completed, with results consistent with ΔI=1/2 rule
  - In ~3-5 years, we should be able to determine Standard Model prediction for direct CP violation in K→ππ, and compare to experimental result (ε'/ε)

Why 3 particles?

- Resonances with 3-particle decays

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

- 3-body interactions

$$\pi\pi\pi \longrightarrow \pi\pi\pi \qquad NNN \to NNN$$

- Weak decays to 3 (or more) particles

$$K \longrightarrow \pi\pi\pi \qquad D \longrightarrow \pi\pi \qquad D \longrightarrow K\overline{K}$$

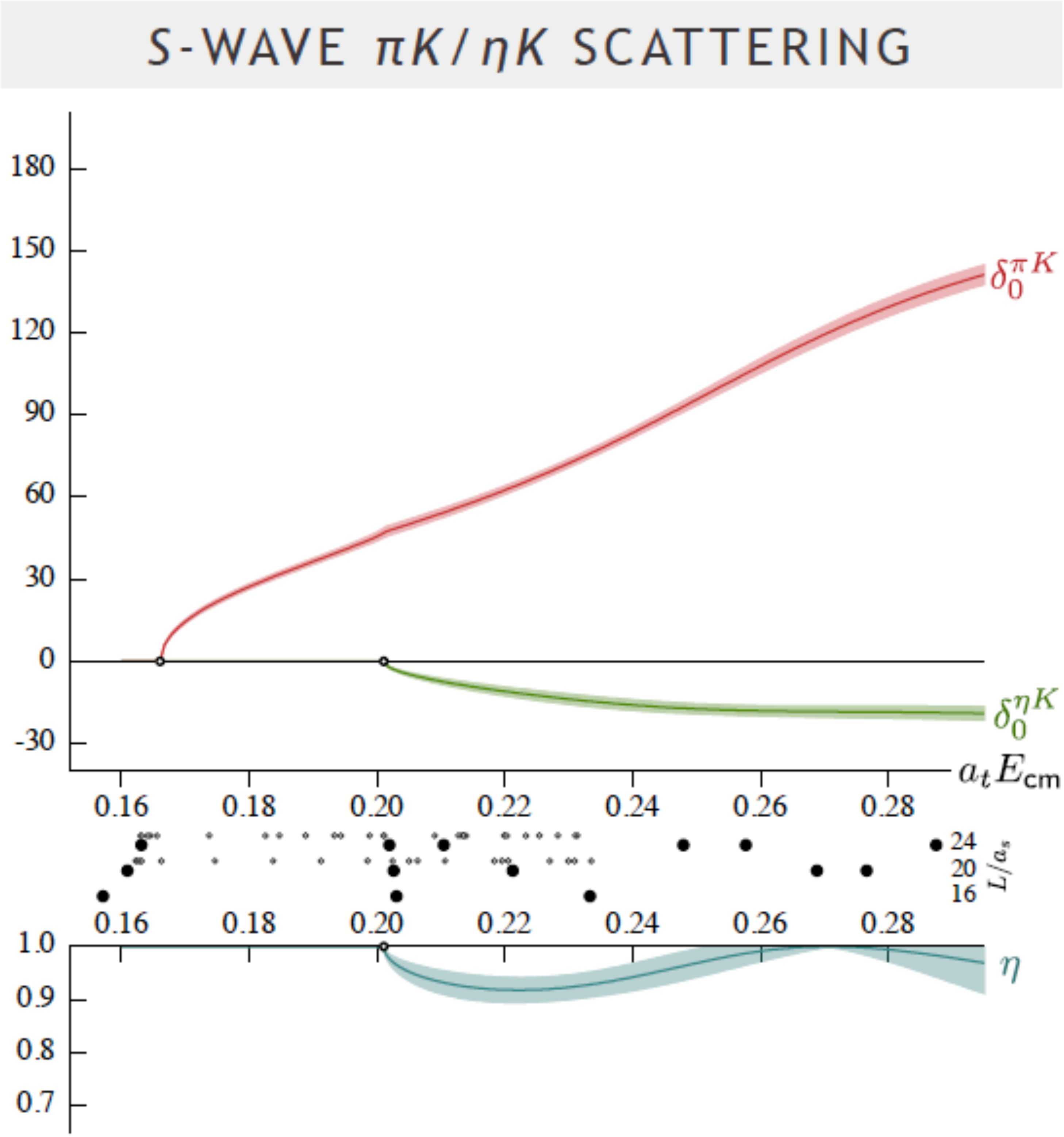
(coupled to $\pi\pi\pi\pi$)

Theoretical status for 2 particles

- Underlying idea is simple in 1-d: $e^{2i\delta(k)} = e^{-ikL}$
- Generalizations to 3-d in QM [Huang & Yang 57, ...]
- [Lüscher 86 & 91] derived quantization formula for energies below inelastic threshold (and for **P**=**0**) by converting QFT problem to one in NRQM
- [Rummukainen & Gottlieb 85] generalized to general **P** (using rel. QM)
- [Lellouch & Lüscher 00] generalized to weak decay amplitudes
- [Kim, Sachrajda & SS 05] gave alternate derivation directly in QFT allowing generalization of LL formula to general **P** (see also [Christ, Kim & Yamazaki 05])
- [Hansen & SS 12, Briceno & Davoudi 12, ...] generalized the quantization (and LL formula) to the case of any number of two particle channels (e.g. ππ, KK, ηη)
    - Used in recent work of [Dudek, Edwards, Thomas and Wilson, 14]
- [Briceno, Hansen & Walker-Loud 14] generalized to calculation of general 1→2 form factors (e.g. γπ→ππ)

State of the art

[Dudek, Edwards, Thomas & Wilson 14]



Coupled two-body channels

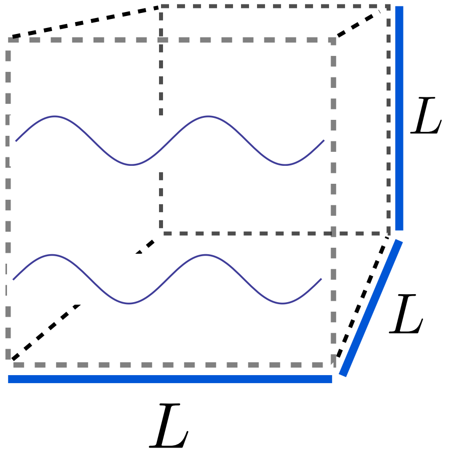
$m_\pi \sim 391\,\mathrm{MeV}$

Theoretical status for 3 particles

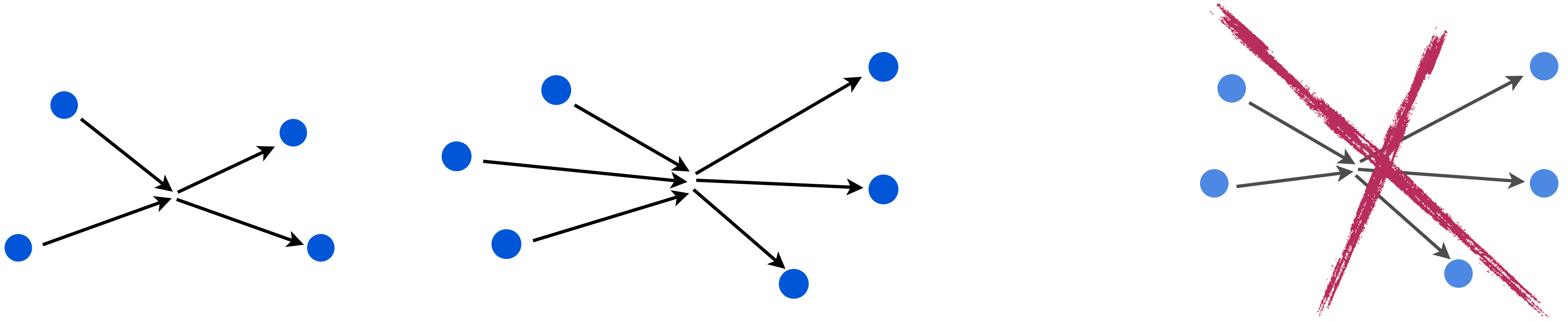
- [Beane, Detmold & Savage `07 and Tan `08] derived threshold expansion for n particles in NRQM, and argued it applied also in QFT
- [Polejaeva & Rusetsky ’12] Showed in NREFT that spectrum determined by infinite-volume scattering amplitudes, using integral equation
- [Briceno & Davoudi `12] Used a dimer 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
- Our aim: work in general, relativistic QFT and determine an algebraic relation between spectrum and scattering amplitudes

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 *arbitrarily* except for a Z_2 (G-parity-like) symmetry
  - Only vertices are 2→2, 2→4, 3→3, 3→1, 3→5, 5→7, etc.
  - Even & odd particle-number sectors decouple



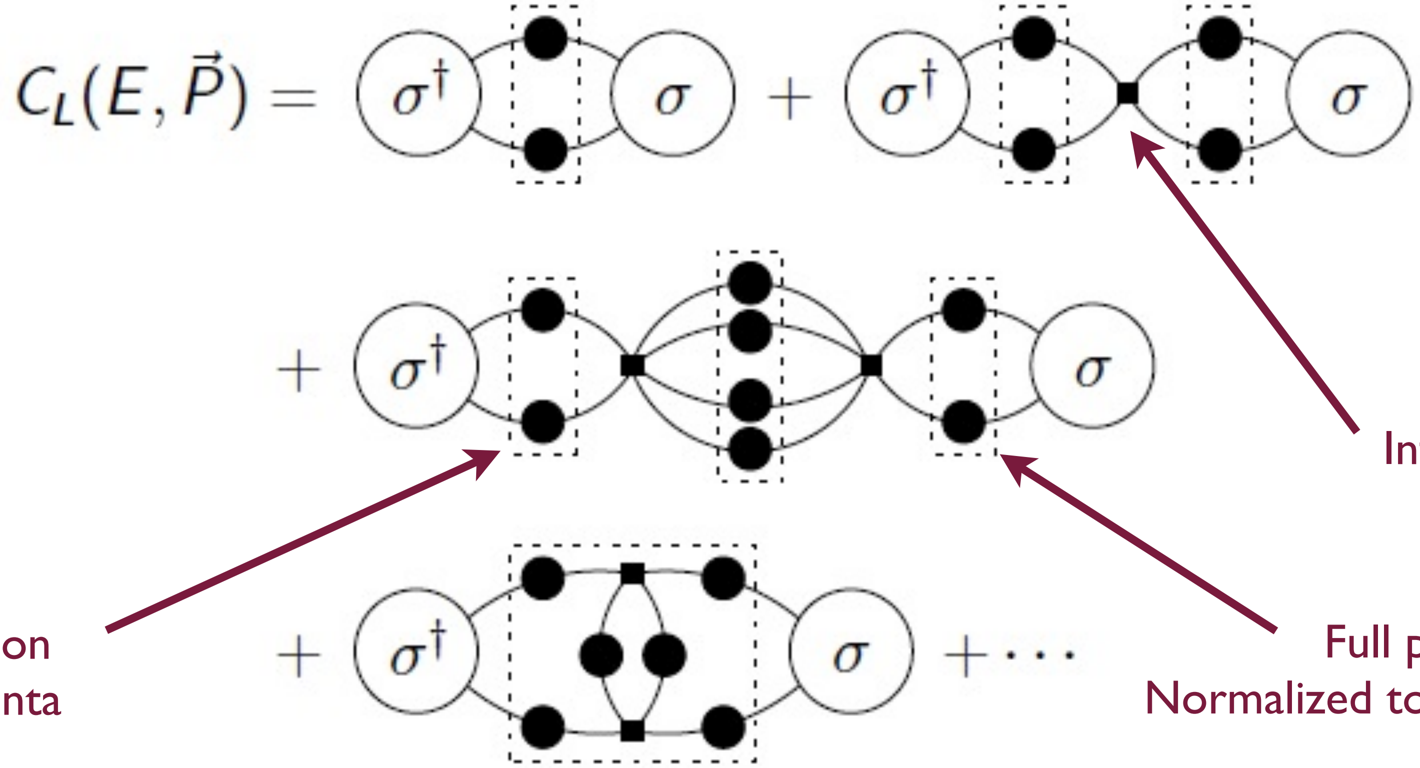
Methodology

- Calculate (for some **P**=2π**n_P**/L)

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

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

- 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:

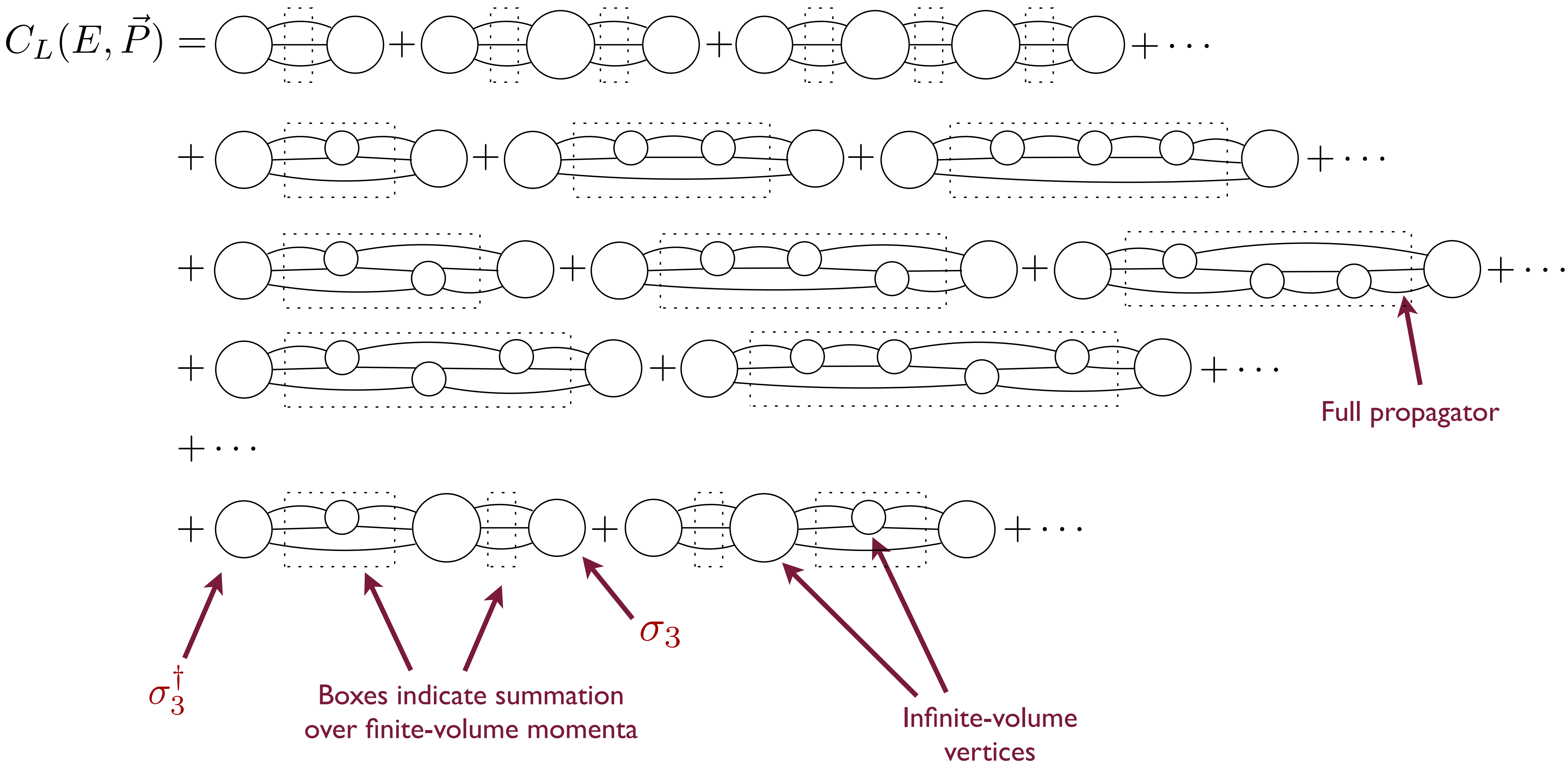


Infinite-volume vertices

Boxes indicated summation over finite-volume momenta

Full propagators
Normalized to unit residue at pole

3-particle correlator



Full propagator

$\sigma_3^\dagger$

Boxes indicate summation over finite-volume momenta

σ_3

Infinite-volume vertices

Key step 1

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

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

Key step 1

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

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

Key step 2

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

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

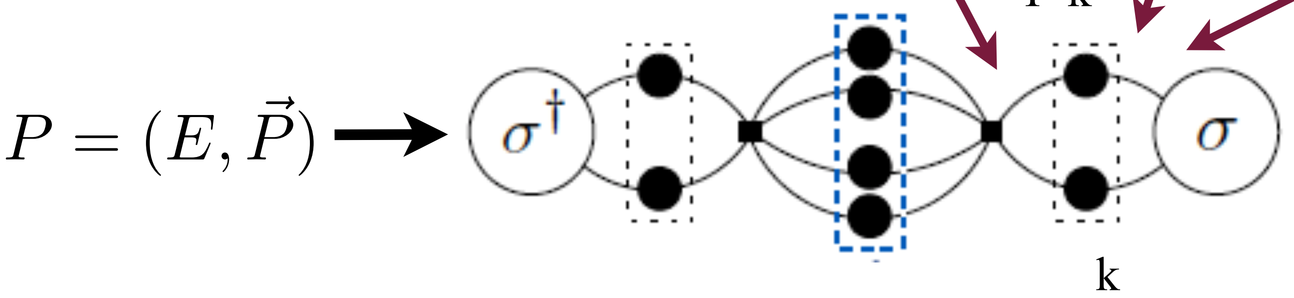
$$= \int d\Omega_{q^*} d\Omega_{q^{*\prime}}\, f^*(\hat{q}^*)\mathcal{F}\ \ (q^*, q^{*'})g^*(\hat{q}^{*'}) \quad + \text{exp. suppressed}$$

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

Kinematic function

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

- Example



f is left-hand part of integrand

Focus on this loop

g is right-hand part of integrand

Key step 2

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

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

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

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

$$F_{\ \ell_1,m_1;\ell_2,m_2} \equiv \quad \eta\left[\frac{\mathrm{Re}q^*}{8\pi E^*}\delta_{\ell_1\ell_2}\delta_{m_1m_2} + \right.$$
$$\left. \frac{i}{2\pi EL}\sum_{\ell,m} x^{-\ell}\,\mathcal{Z}^P_{\ell m}[1;x^2]\int d\Omega Y^*_{\ell_1,m_1}Y^*_{\ell,m}Y_{\ell_2,m_2}\right]$$

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

Kinematic functions

$Z_{4,0}$ & $Z_{6,0}$ for **P=0** [Luu & Savage, `11]

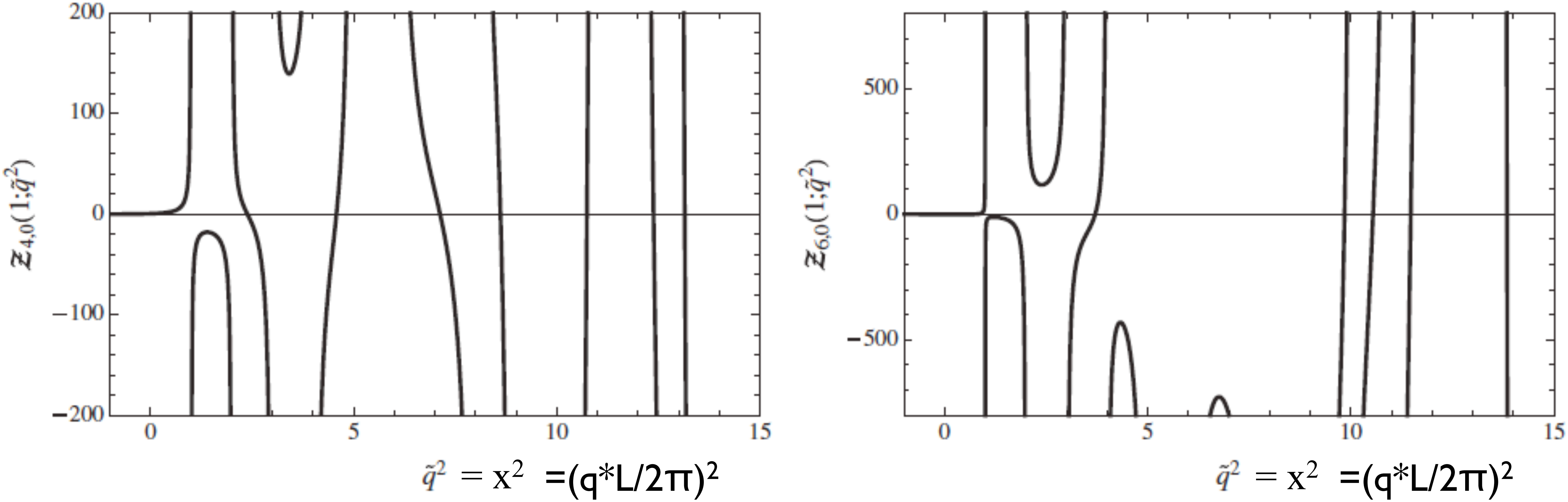


FIG. 29. The functions $Z_{4,0}(1;\tilde{q}^2)$ (left panel) and $Z_{6,0}(1;\tilde{q}^2)$ (right panel).

Key step 2

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

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

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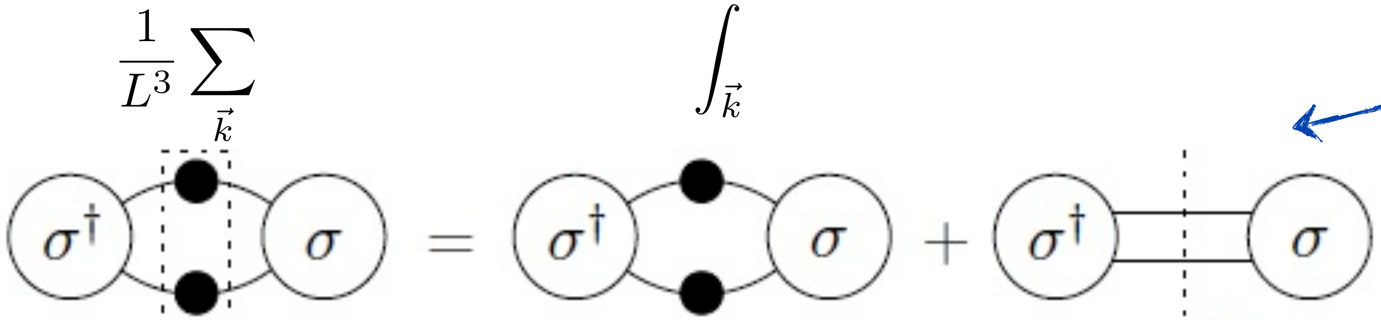
- Diagrammatically



finite-volume residue

off-shell

on-shell

Variant of key step 2

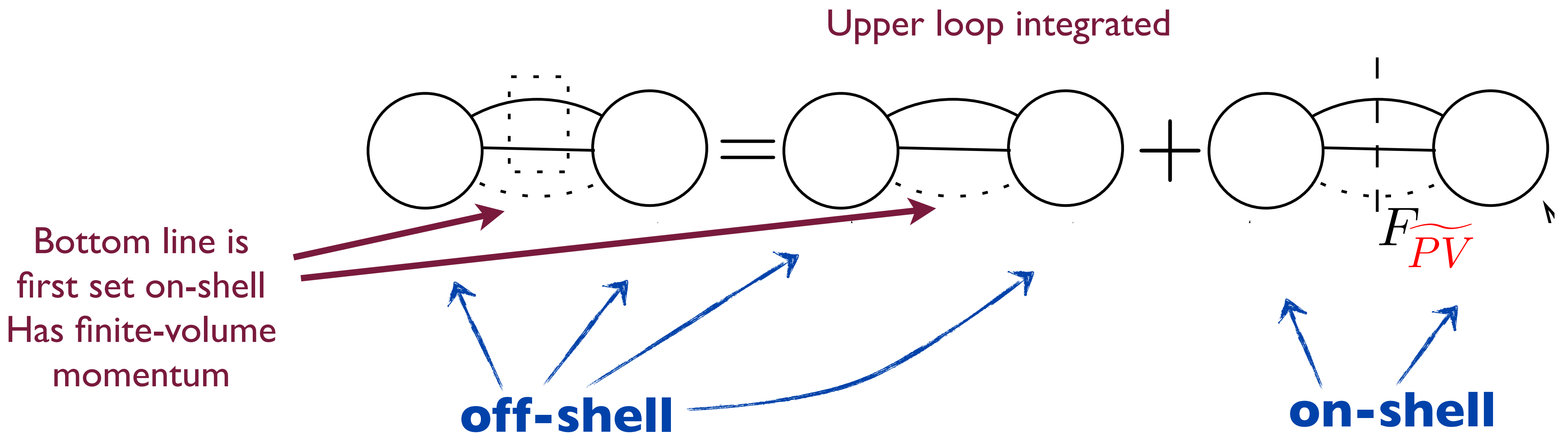
- For generalization to 3 particles use (modified) PV prescription instead of iε

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

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

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

- Example of appearance in 3-particle analysis:



Upper loop integrated

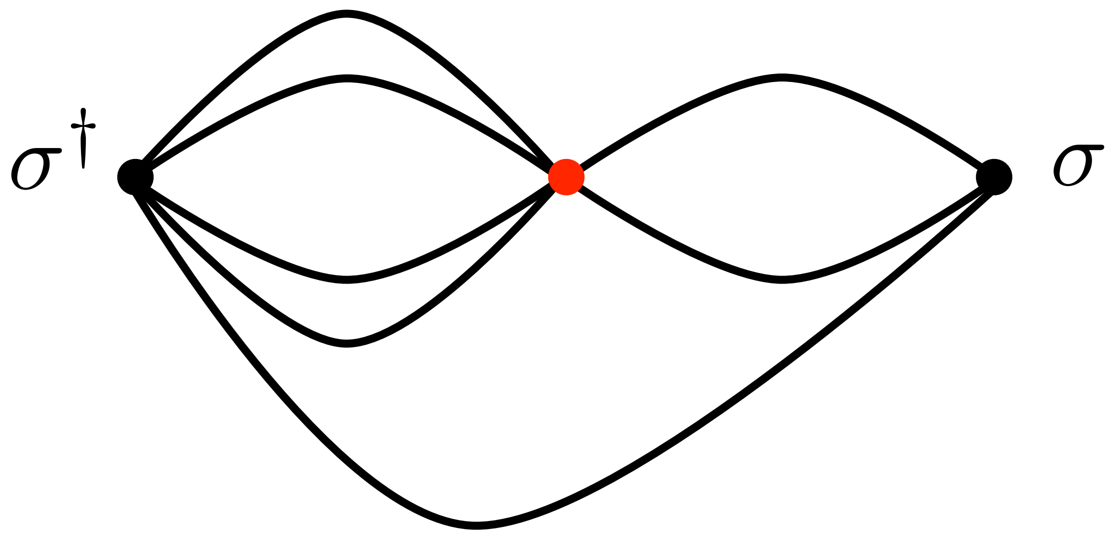
Bottom line is first set on-shell Has finite-volume momentum

off-shell

on-shell

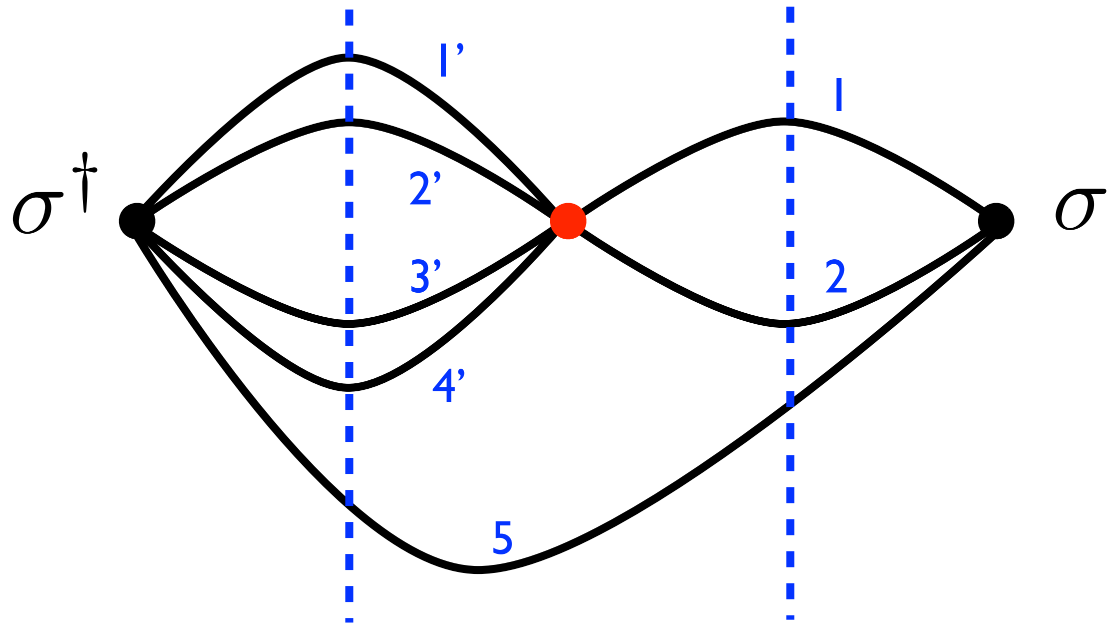
Key step 3

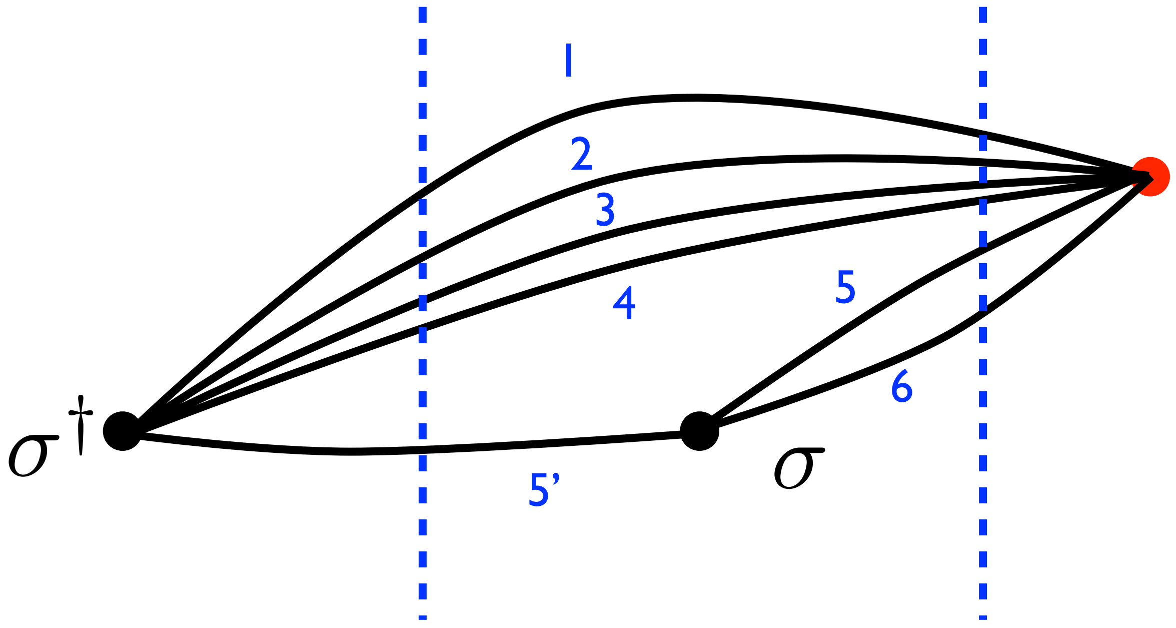
- Identify potential singularities: can use time-ordered PT (i.e. do k_0 integrals)
- Example



Key step 3

- 2 out of 6 time orderings:



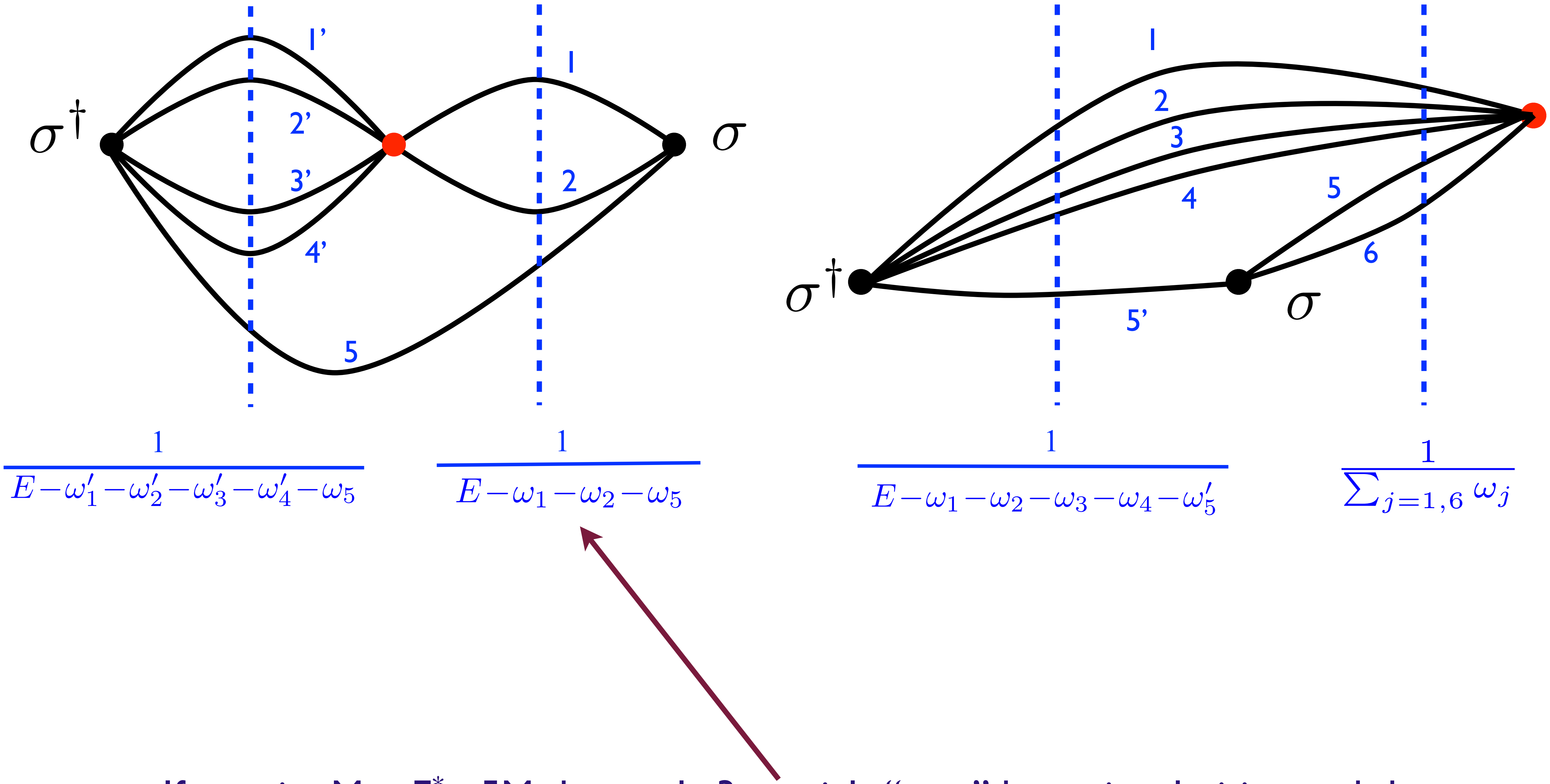


$$\frac{1}{E-\omega_1'-\omega_2'-\omega_3'-\omega_4'-\omega_5} \qquad \frac{1}{E-\omega_1-\omega_2-\omega_5} \qquad \frac{1}{E-\omega_1-\omega_2-\omega_3-\omega_4-\omega_5'} \qquad \frac{1}{\sum_{j=1,6}\omega_j}$$

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

Key step 3

- 2 out of 6 time orderings:

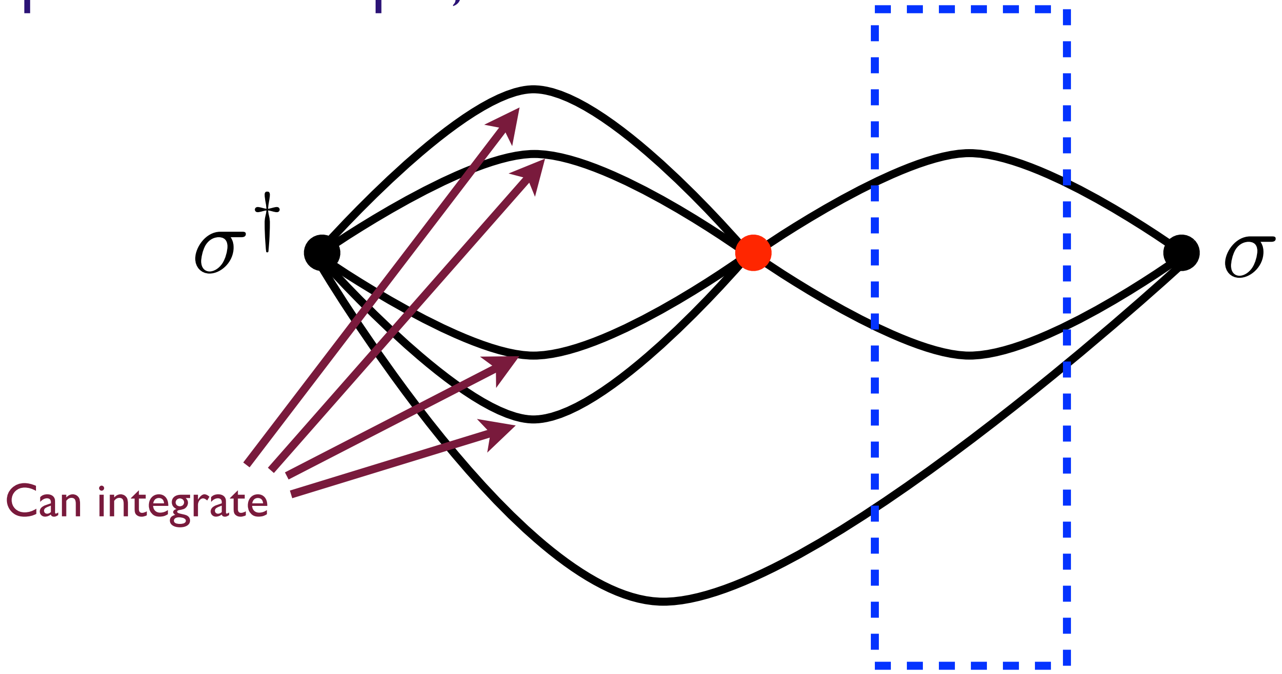


$$\frac{1}{E-\omega_1'-\omega_2'-\omega_3'-\omega_4'-\omega_5} \quad \frac{1}{E-\omega_1-\omega_2-\omega_5} \quad \frac{1}{E-\omega_1-\omega_2-\omega_3-\omega_4-\omega_5'} \quad \frac{1}{\sum_{j=1,6}\omega_j}$$

- 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:

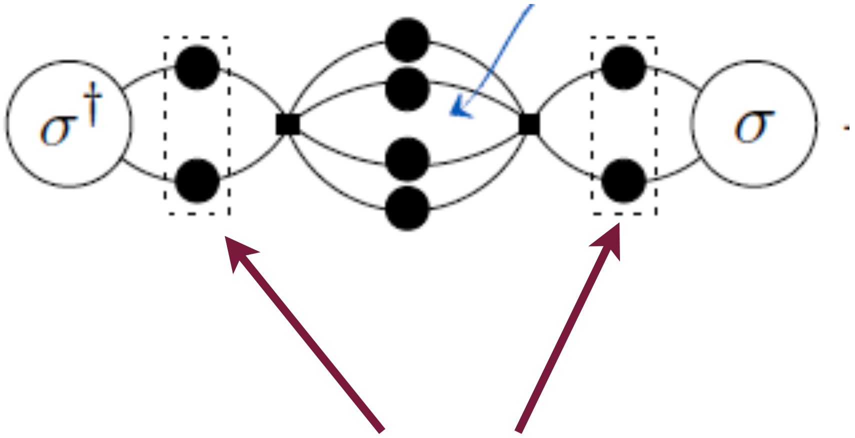


Must sum momenta passing through box

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:

Can replace sum with integral here



But not here

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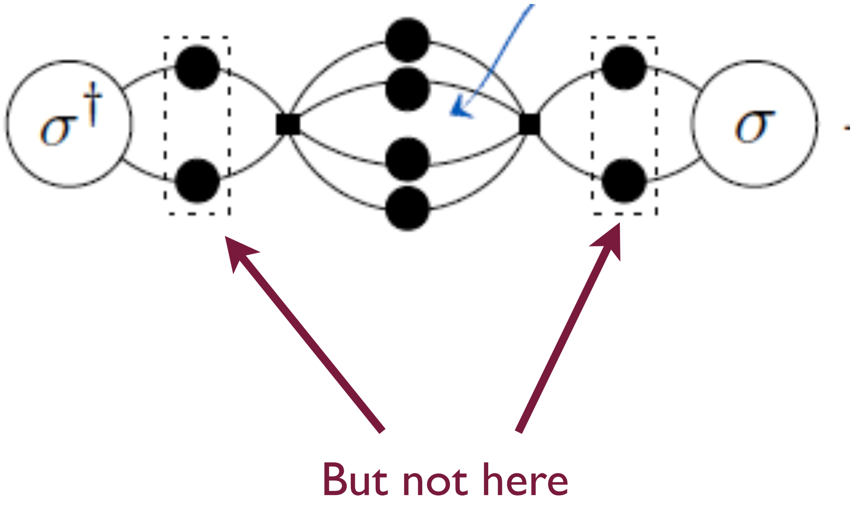


Can replace sum with integral here

But not here

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

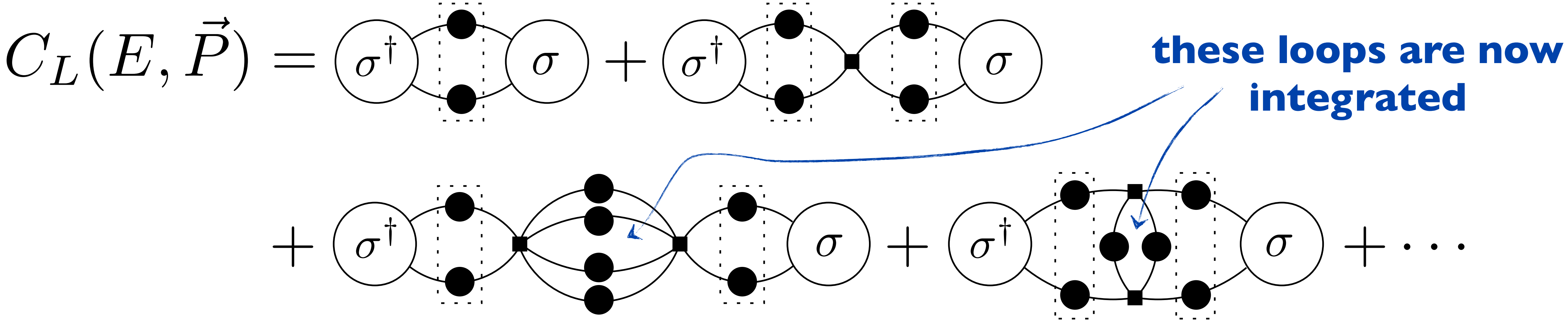
Key issues 4-6

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

2-particle quantization condition

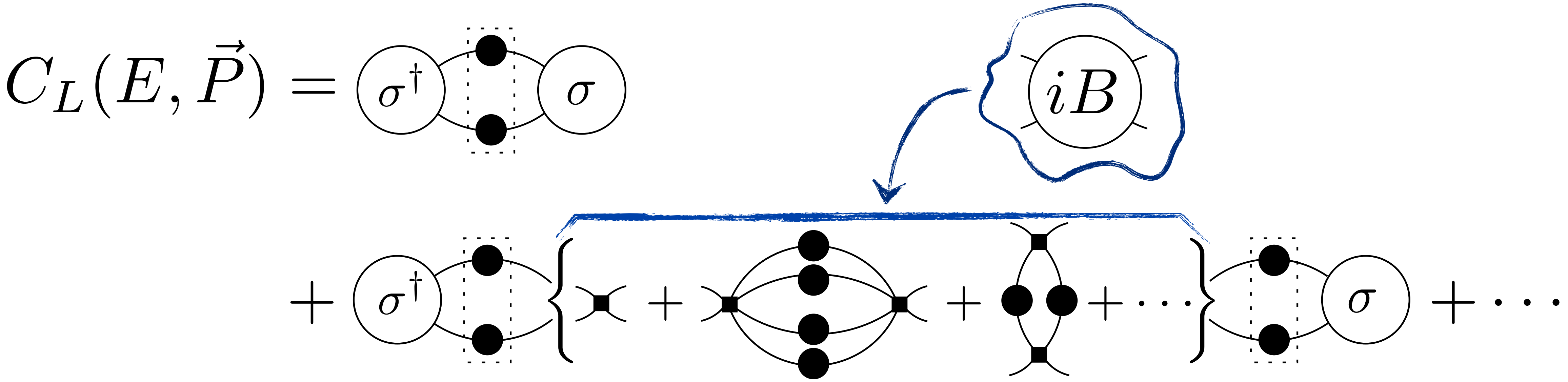
Following method of [Kim, Sachrajda & SS 05]

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



these loops are now integrated

- Collect terms into infinite-volume Bethe-Salpeter kernels



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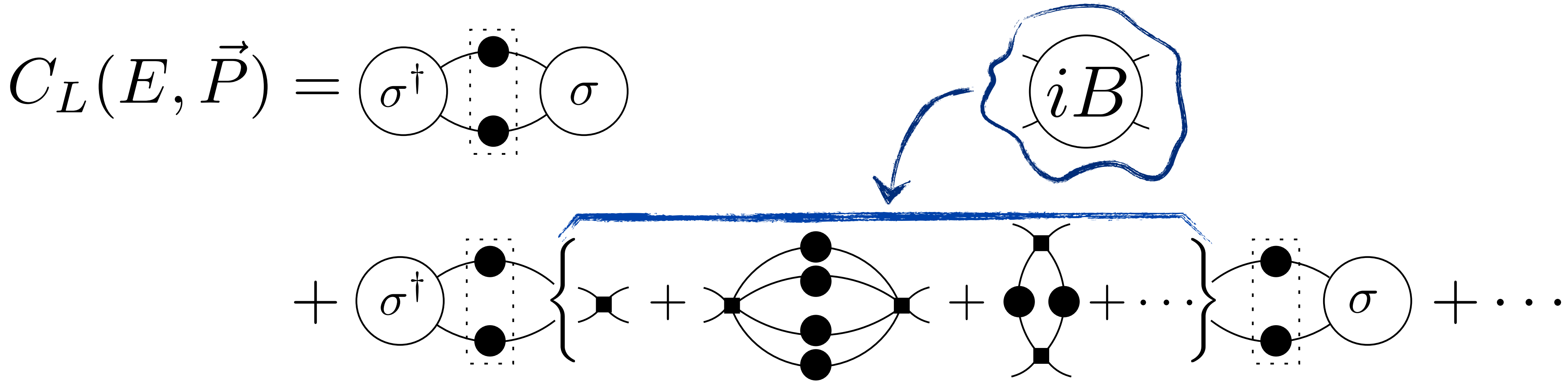
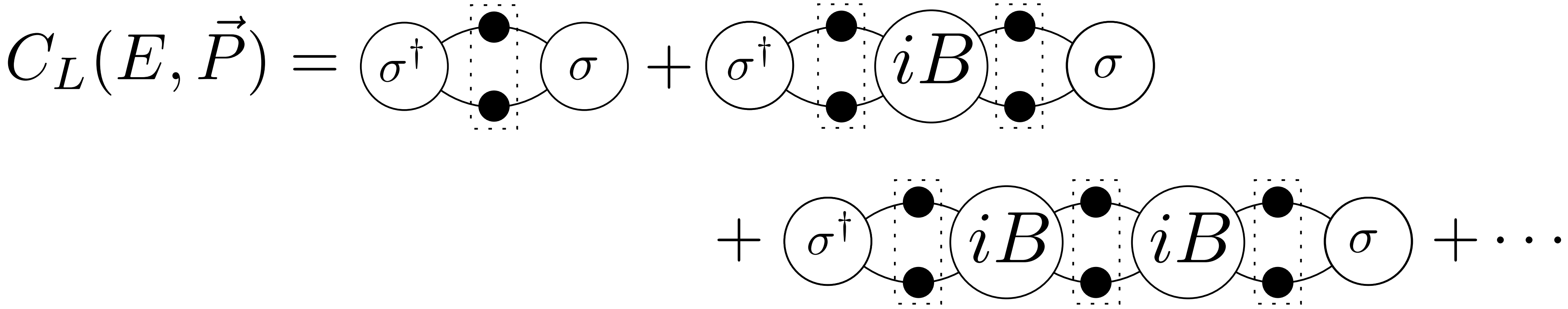
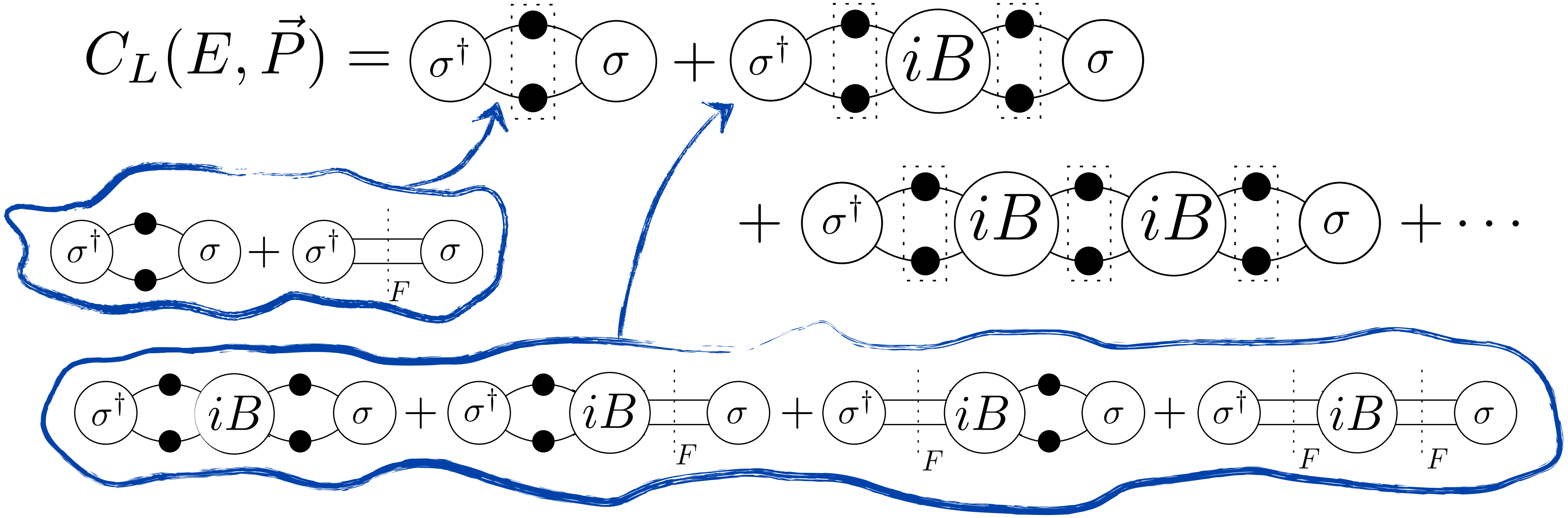


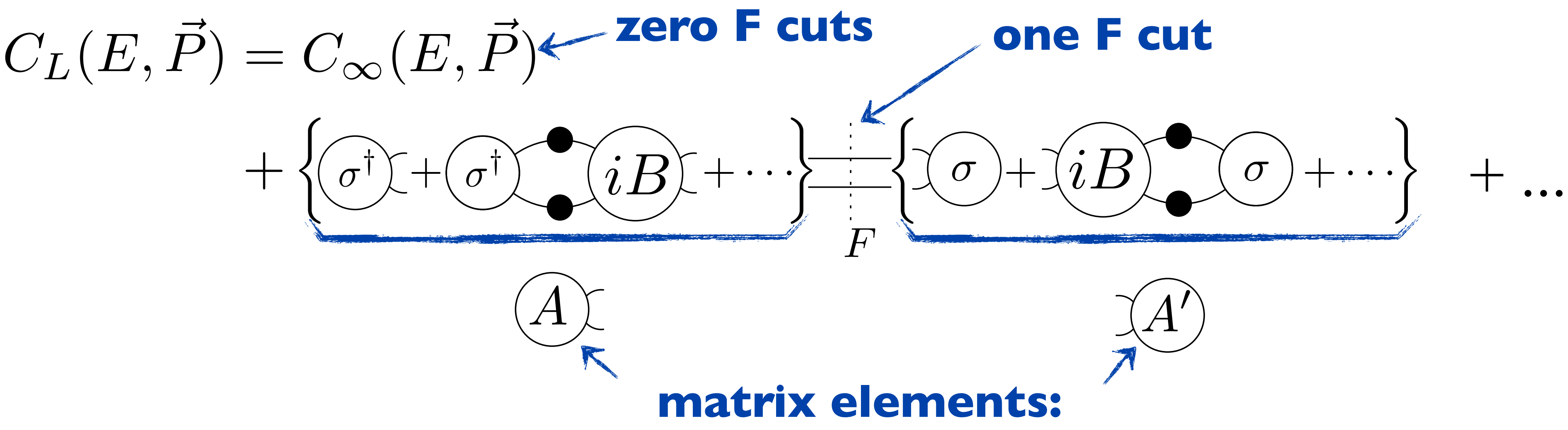
- Leading to



- Next use sum identity



- And regroup according to number of “F cuts”



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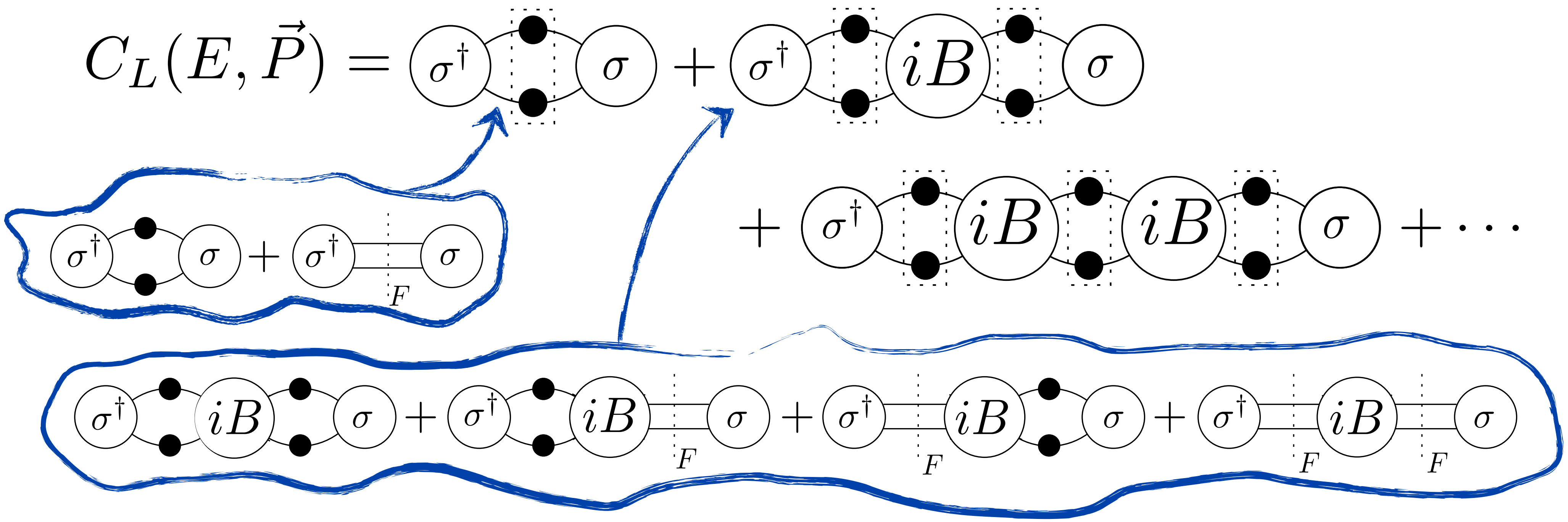
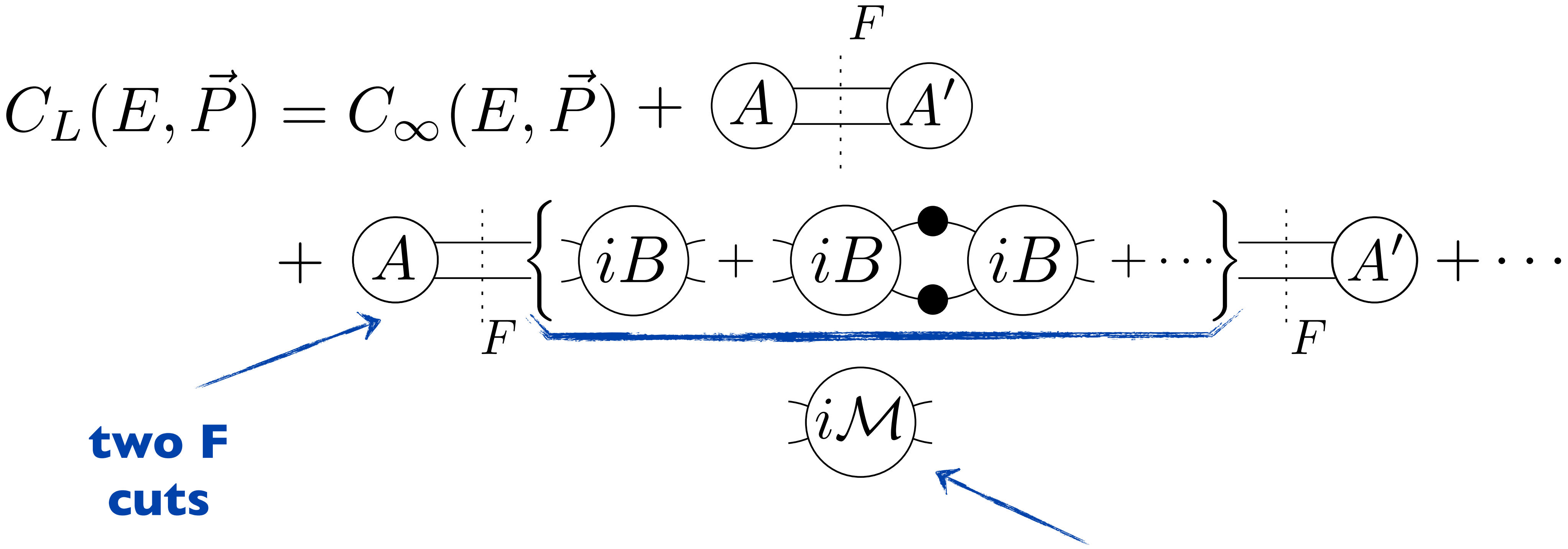


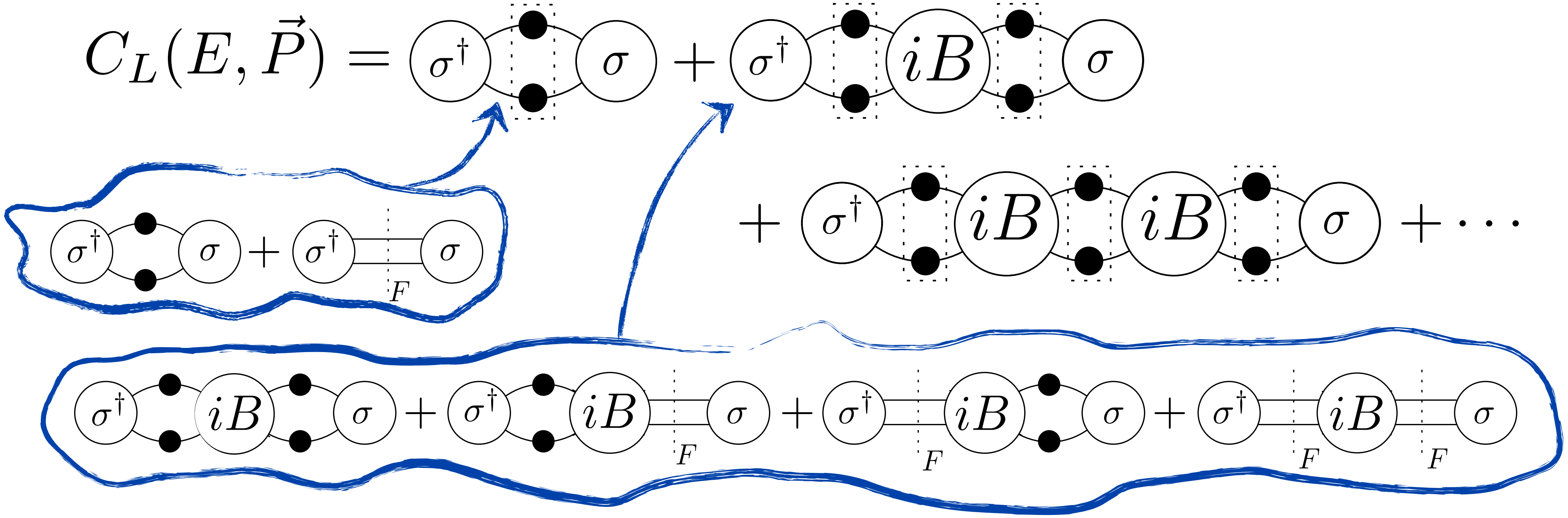
- And keep regrouping according to number of "F cuts"



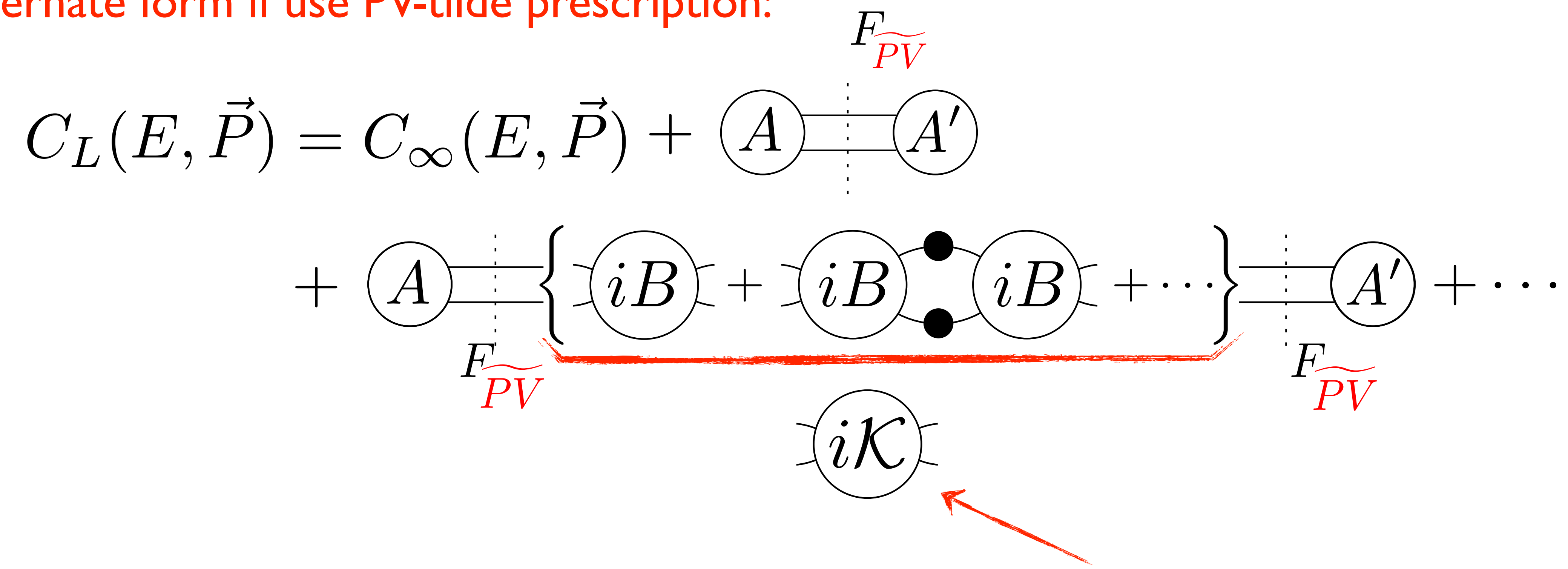
two F cuts

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

- Next use sum identity



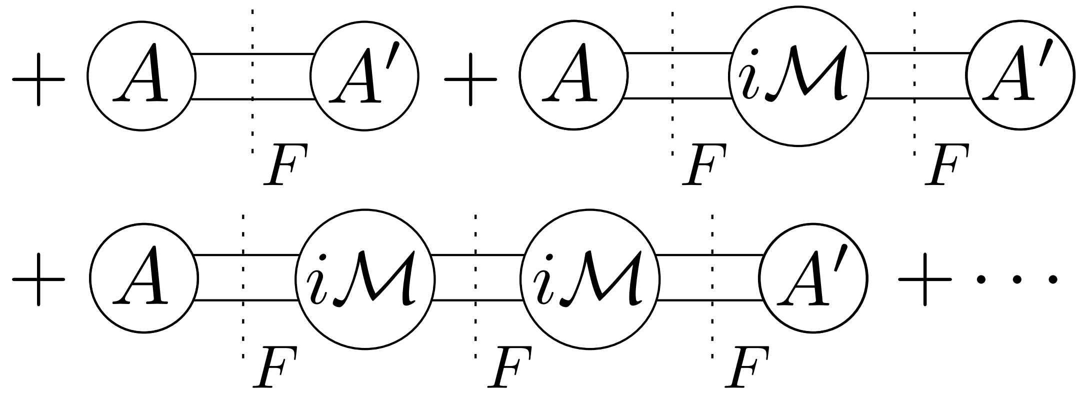
- Alternate form if use PV-tilde prescription:



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

- Final result:

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

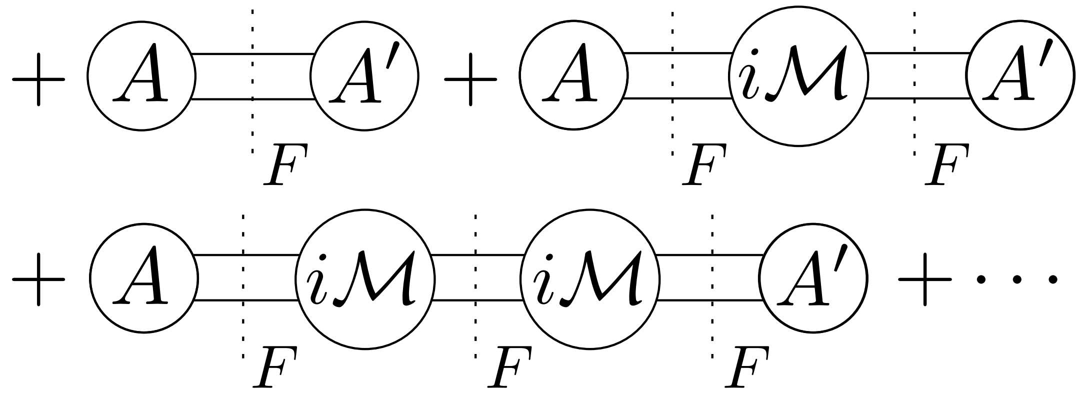


- $$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + \sum_{n=0}^{\infty} A' iF [i\mathcal{M}_{2\to 2} iF]^n A$$

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

- Final result:

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



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

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

no poles, only cuts

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

2-particle quantization condition

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

- At fixed L & **P**, the finite-volume spectrum E_1, E_2, ... is given by solutions to

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

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

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

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

Equivalent K-matrix form

$$C_L(E,\vec P) = C_\infty(E,\vec P) + A' \underbrace{iF_{\widetilde{\rm PV}} \frac{1}{1+\mathcal{K}_2 F_{\widetilde{\rm PV}}}}_{\propto\ [\mathcal{A}]} A$$

"dimer propagator"

- At fixed L & **P**, the finite-volume spectrum E_1, E_2, ... is given by solutions to

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

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

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

3-particle quantization condition

Following [Hansen & SS 14]

“Final” result

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

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

Infinite volume 3-particle scattering quantity

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

Known kinematical quantity: essentially the same as F_{PV} in 2-particle analysis

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

G is known kinematical quantity containing cut-off function H

- Superficially similar to 2-particle form ...

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

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

“Final” result

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

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

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

[finite volume “spectator” momentum: **k**=2π**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

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

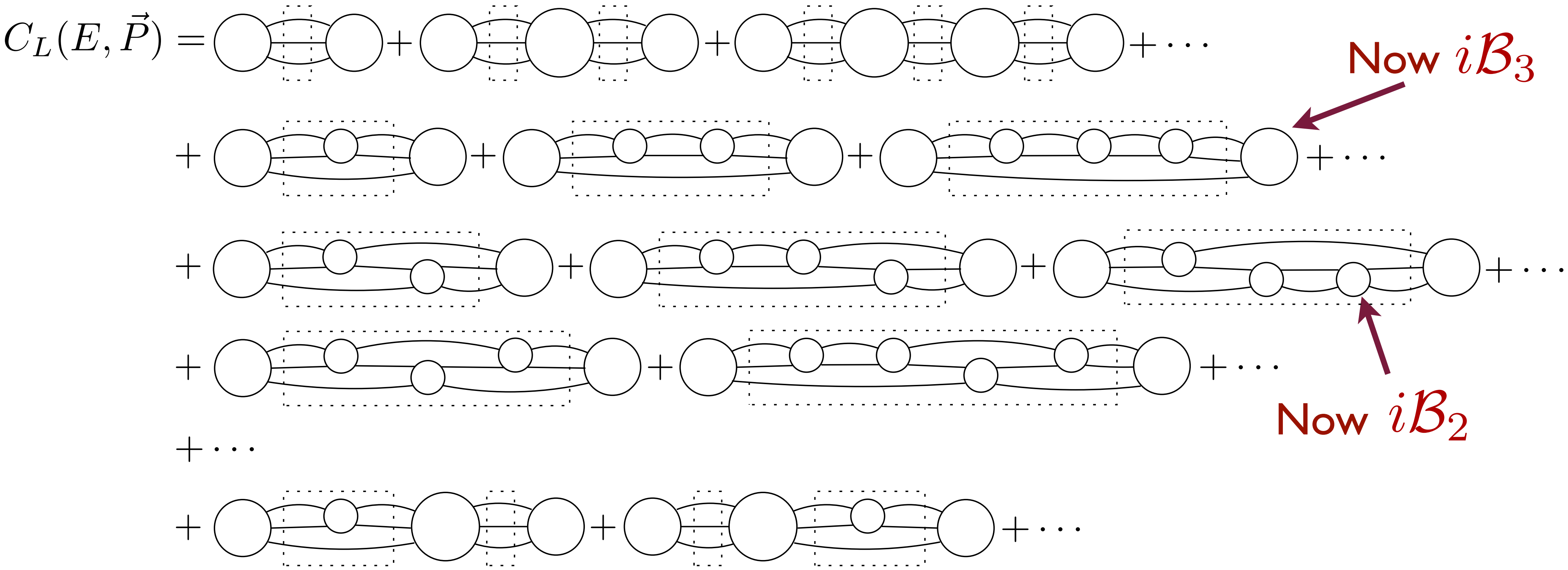
$$F_3 = \frac{F_{\widetilde{\mathrm{PV}}}}{2\omega L^3}\left[-\frac{2}{3} + \frac{1}{1 + (1 + \mathcal{K}_2 G)^{-1}\mathcal{K}_2 F_{\widetilde{\mathrm{PV}}}}\right]$$

- Successfully separated infinite volume quantities from finite volume kinematic factors
- But what is $\mathcal{K}_{\mathrm{df},3}$?
- 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
- 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

Skeleton expansion in terms of Bethe-Salpeter kernels



Now $i\mathcal{B}_3$

Now $i\mathcal{B}_2$

Key issue 4: dealing with cusps

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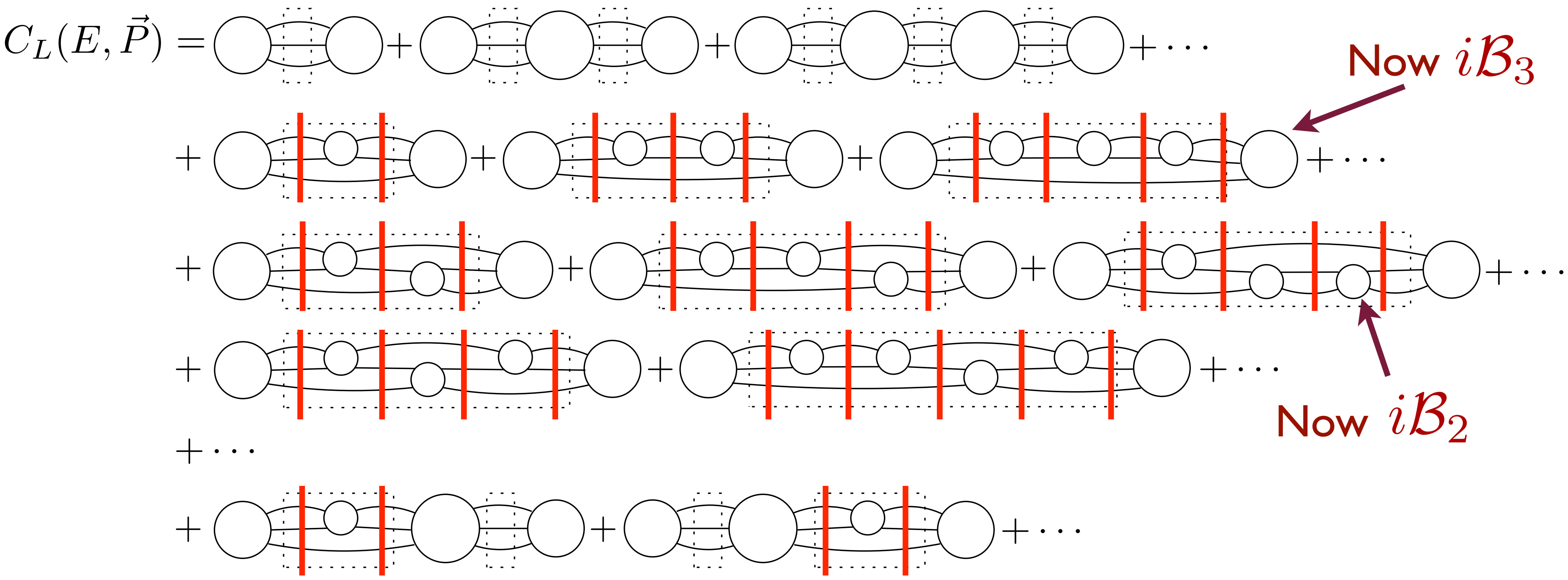
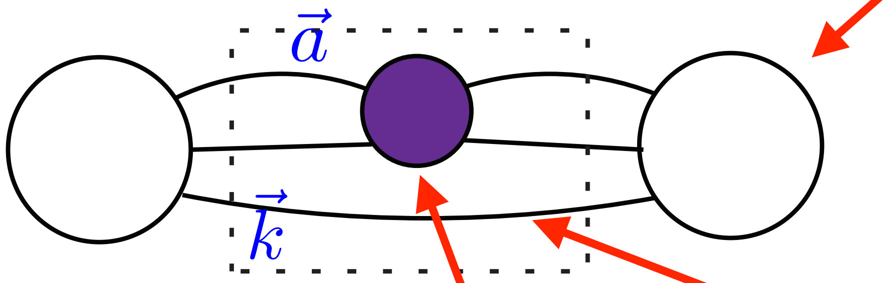


Cusp analysis (1)

- Aim: replace sums with integrals + finite-volume residue
- E.g.

$$(E, \vec{P}) \longrightarrow \qquad \frac{1}{L^6}\sum_{\vec{k}}\sum_{\vec{a}}$$



interpolating operator

2PI Bethe-Salpeter kernel

dressed propagators

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

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

smooth functions

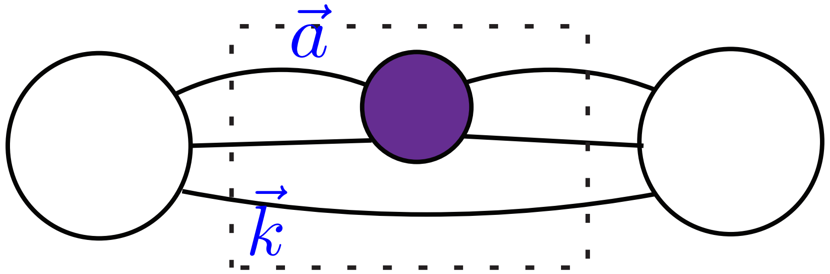
denominator vanishes on-shell

$\sqrt{\vec{k}^2+m^2}$

$\sqrt{\vec{a}^2+m^2}$

$\sqrt{(\vec{P}-\vec{k}-\vec{a})^2+m^2}$

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**

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

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

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

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
- iε prescription and standard principal value (PV) lead to cusps at threshold ⇒ sum-integral ~1/L^4 [Polejaeva & Rusetsky]
- Requires use of modified $\widetilde{\mathrm{PV}}$ prescription

Result:

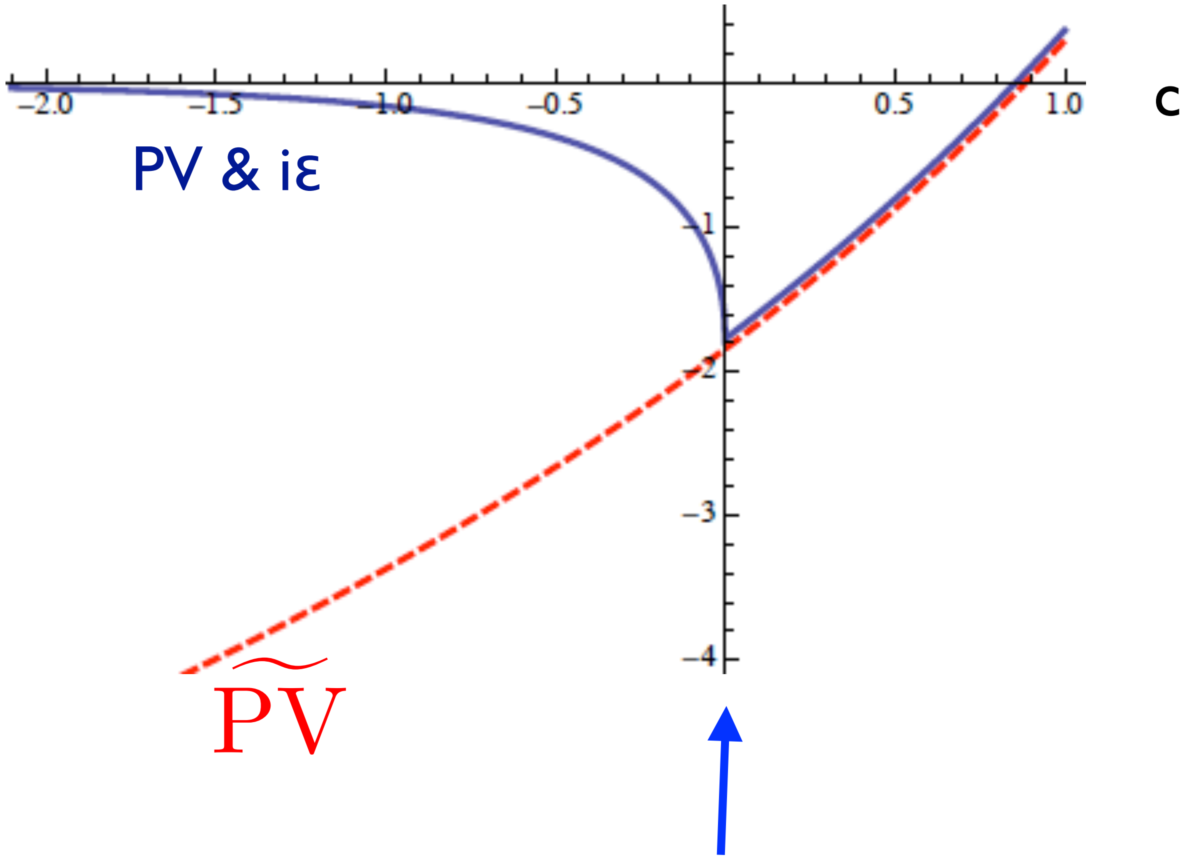
$$\frac{1}{L^6}\sum_{\vec k}\sum_{\vec a}=\int_{\vec k}\int_{\vec a}+\sum_{\vec k}\text{“F term”}$$

Cusp analysis (3)

$x \sim (a^*)^2$

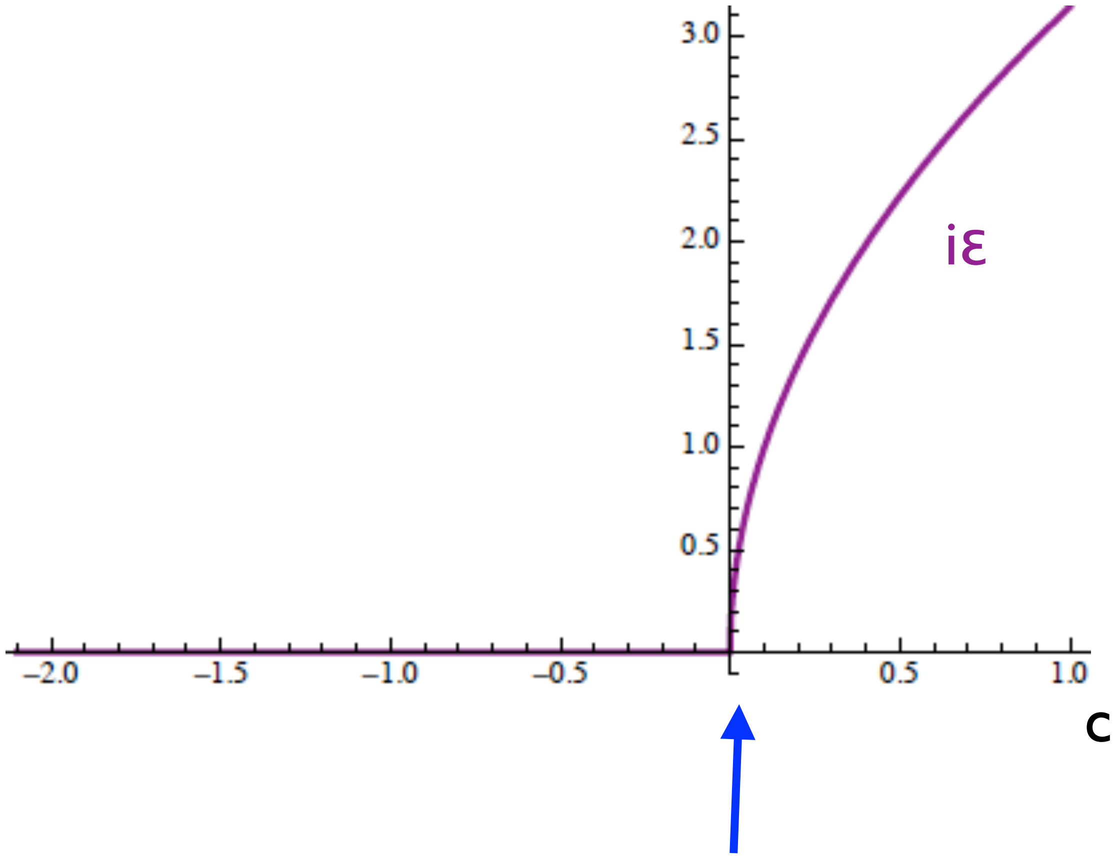
- Simple example: $\int_{\vec{a}} \frac{A(\vec{k},\vec{a})B(\vec{k},\vec{a})}{E-\omega_k-\omega_a-\omega_{ka}} \longrightarrow f(c) = \int_0^\infty dx \frac{\sqrt{x}e^{-(x-c)}}{c-x}$

Re f(c)



threshold

Im f(c)

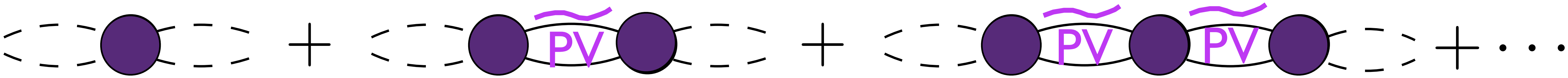


threshold

- Far below threshold, $\widetilde{\mathrm{PV}}$ smoothly turns back into PV

Cusp analysis (4)

- Bottom line: must use $\widetilde{\mathrm{PV}}$ 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)



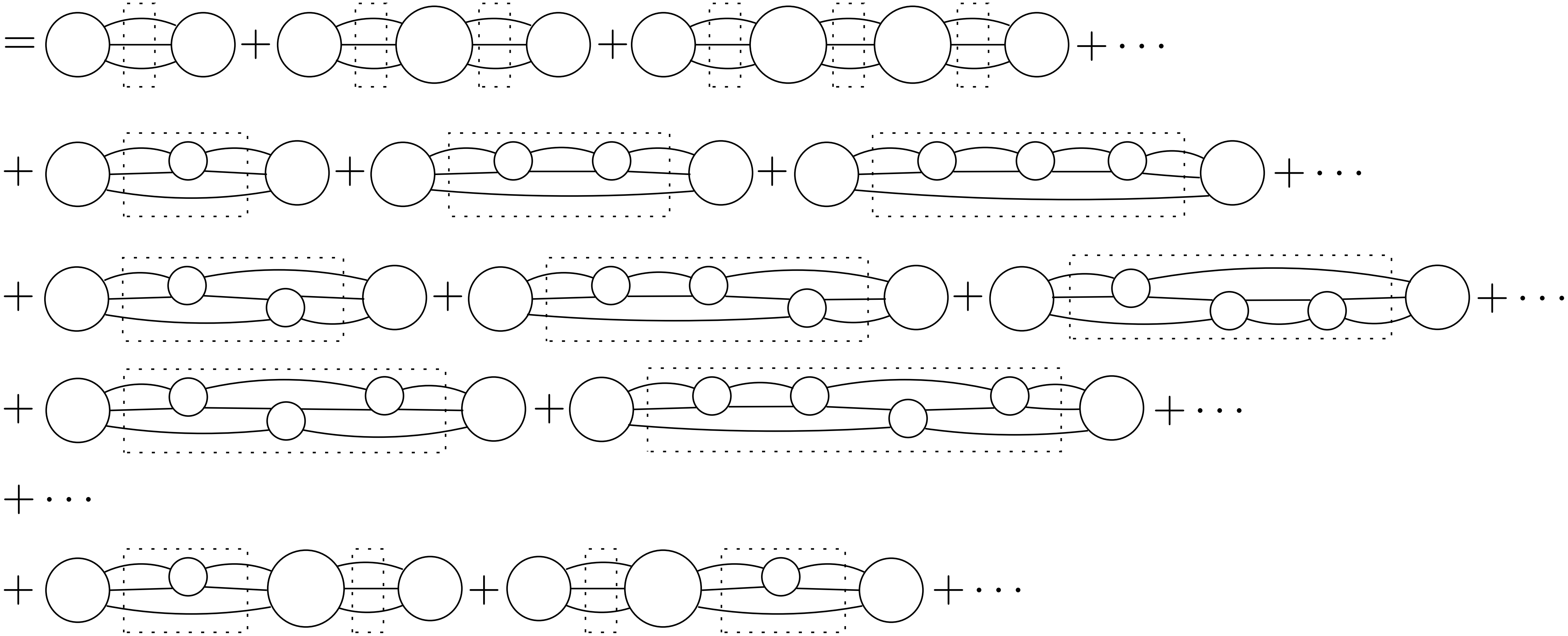
$$\mathcal{K}_2^\ell = \frac{16\pi E^*}{a^* \cot\delta_\ell(a^*)}$$

function of $(a^*)^2$

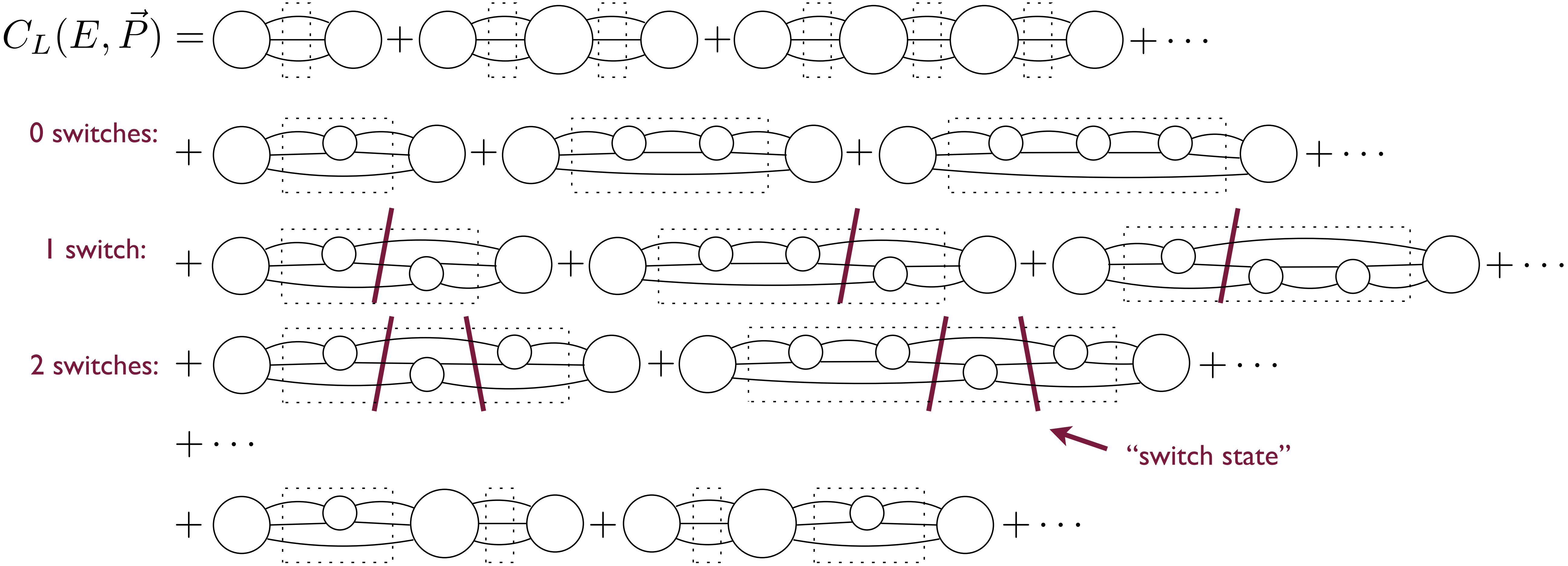
- This prescription is that used previously when studying finite-volume effects on bound-state energies using two-particle quantization condition [Detmold, Savage,...]
- Far below threshold smoothly turns into $\mathcal{M}_2{}^\ell$

Key issue 5: dealing with "switches"

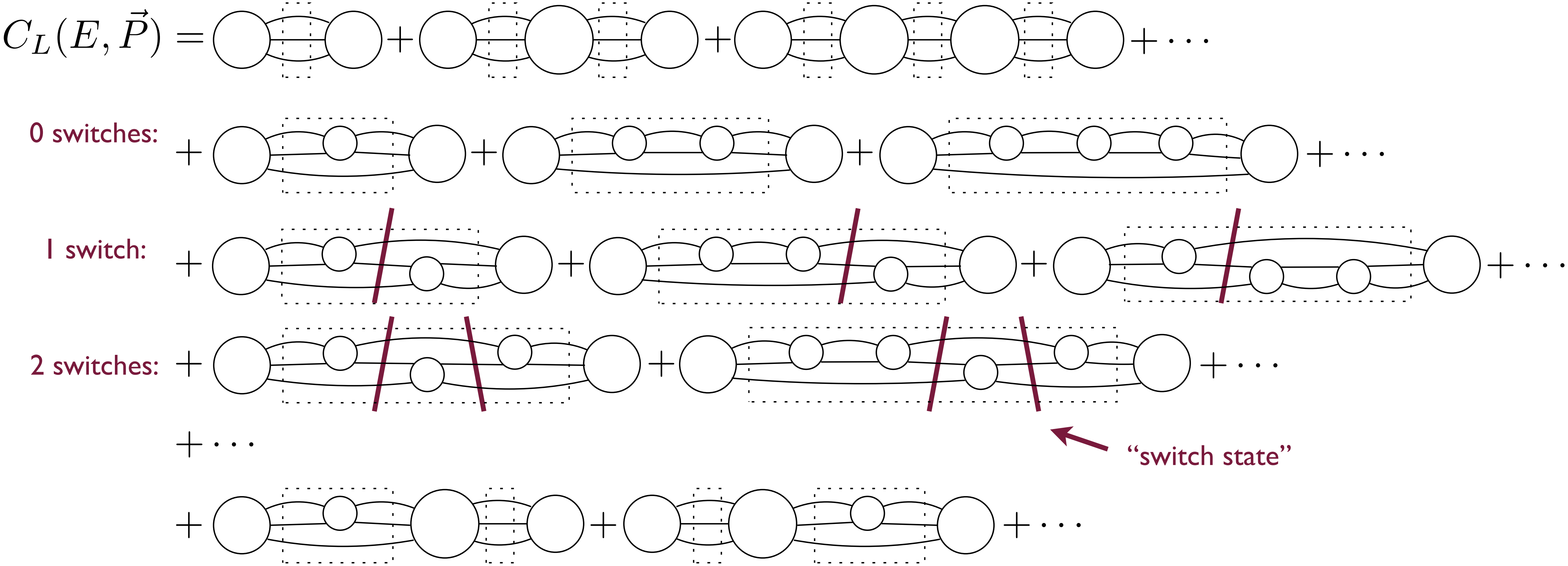
$C_L(E, \vec{P}) =$



Key issue 5: dealing with "switches"

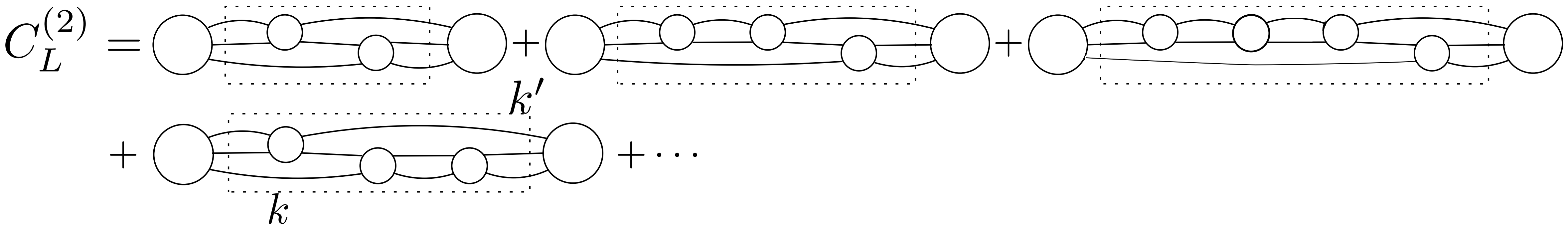


Key issue 5: dealing with “switches”

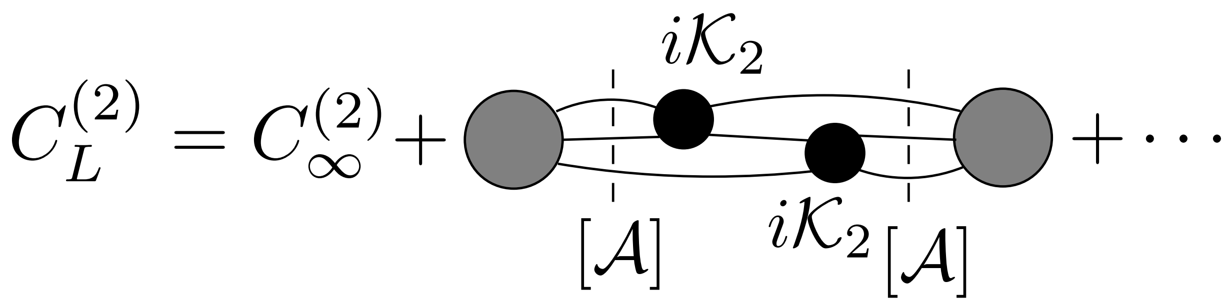


- With cusps removed, no-switch diagrams can be summed as for 2-particle case, leading to dimer propagator [$\mathcal{A}$]
- “Switches” present a new challenge

One-switch diagrams

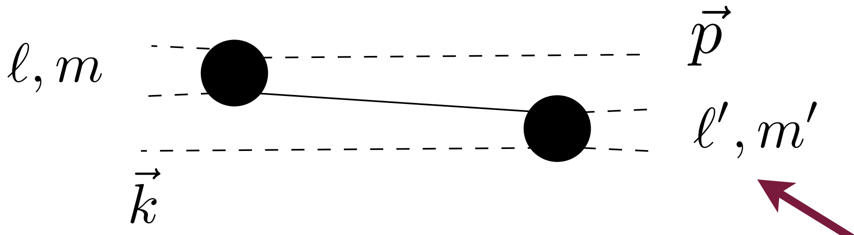


- There are now two spectator momenta, at least one of which must be on-shell to create a finite volume contribution
  - Only get new feature if **both** are on shell



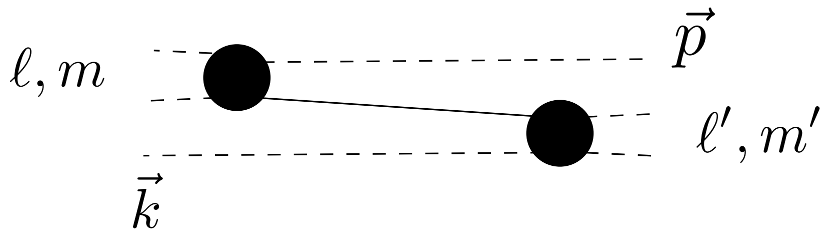
Terms with $C^{(1)}_L$ form, but with modified endcaps

- Term between $\mathcal{A}$'s is our first contribution to a 3→3 on-shell scattering qty

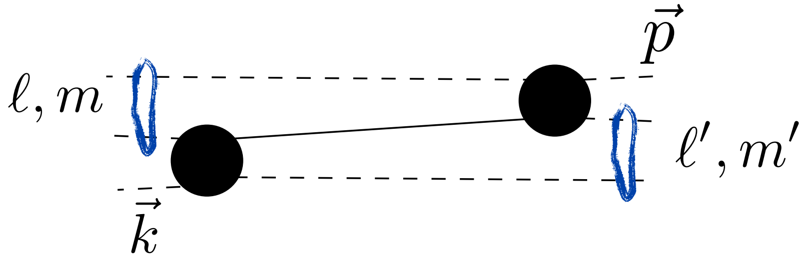


$Y_{l'm'}$ associated with lower pair of particles, due to switch

One-switch problem



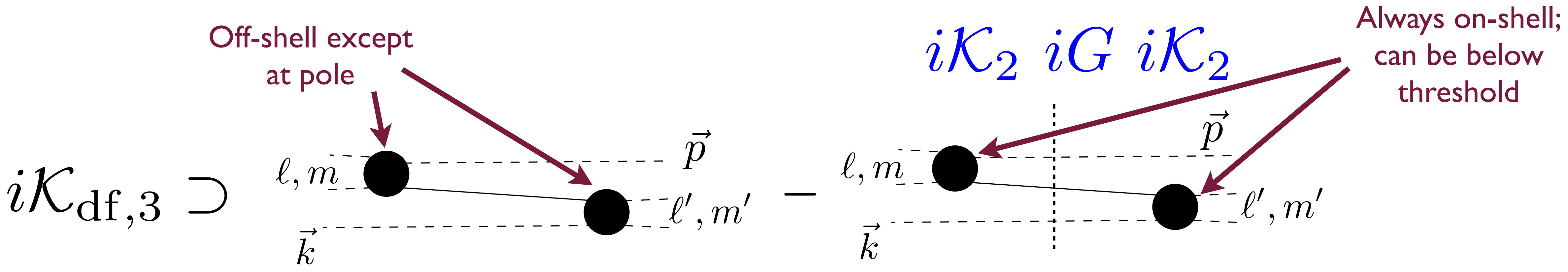
- Amplitude is **singular** for some choices of **k, p** in physical regime
  - Propagator goes on shell if top two (and thus bottom two) scatter elastically
- Not a problem per se, but leads to difficulties when amplitude is symmetrized
  - Occurs when include three-switch contributions



- 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]



Off-shell except at pole

$i\mathcal{K}_2 \; iG \; i\mathcal{K}_2$

Always on-shell; can be below threshold

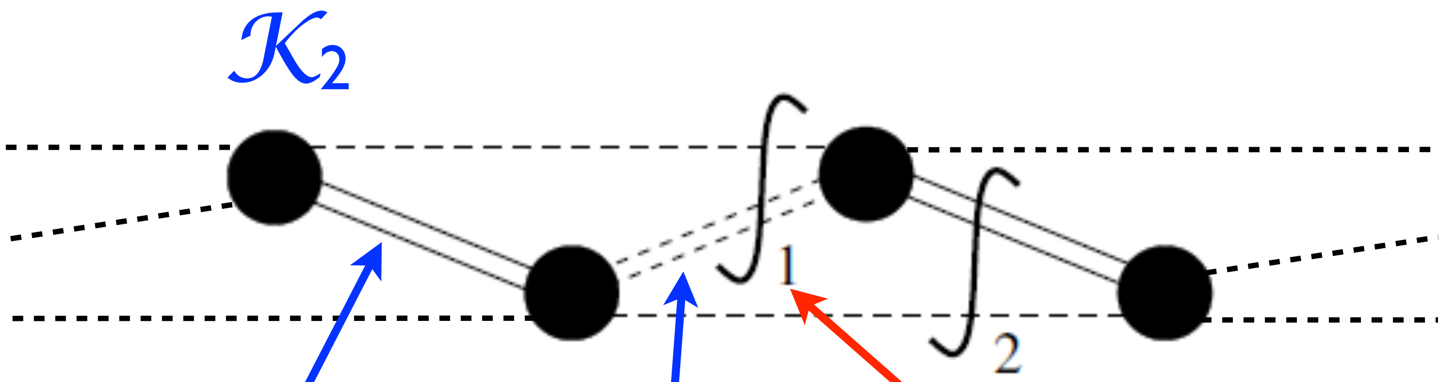
$$G_{p,\ell',m';k,\ell,m} \equiv \left(\frac{k^*}{q_p^*}\right)^{\ell'} \frac{4\pi Y_{\ell',m'}(\hat{k}^*) H(\vec{p}) H(\vec{k}) Y^*_{\ell,m}(\hat{p}^*)}{2\omega_{kp}(E-\omega_k-\omega_p-\omega_{kp})} \left(\frac{p^*}{q_k^*}\right)^{\ell} \frac{1}{2\omega_k L^3}$$

- 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

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

$$i\mathcal{K}_{\rm df,3} \supset$$



amputated external legs

propagator with divergence subtracted

divergent part of propagator

With PV-tilde prescription need to specify order of integrals diagram by diagram!

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

Key issue 6: symmetry breaking

- Final definition of $\mathcal{K}_{\text{df},3}$ 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) "decorations" (i.e. extra factors) to ensure external symmetrization
- $\mathcal{K}_{\text{df},3}$ is an UGLY infinite-volume quantity related to scattering
- At the time of our initial paper, we did not know the relation between $\mathcal{K}_{\text{df},3}$ and $\mathcal{M}_3$ & $\mathcal{M}_2$, although we had reasons to think that such a relationship exists
- We now think we know the relationship, which, if correct, completes the formal analysis for the three-particle quantization condition

“Final” result

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

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

- Successfully separated infinite volume quantities from finite volume kinematic factors
- But what is $\mathcal{K}_{\mathrm{df},3}$? ✔
- How do we obtain this result? ✔
- How can it be made useful?

Utility of result: truncation

Truncation in 2 particle case

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

- If $\mathcal{M}$ (which is diagonal in l,m) vanishes for $l > l_{\max}$ then can show that need only keep $l \le l_{\max}$ 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

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

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

- 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 $\mathcal{K}_2$ and $\mathcal{K}_{df,3}$ vanish for $l > l_{max}$
- Yields determinant condition truncated to $[N(2l_{max}+1)]^2$ block

Truncation in 3 particle case

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

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

- 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 $\mathcal{K}_{df,3\to3}$, in which case one would need at least as many levels as parameters at given energy
- If our preliminary result is correct, 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

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

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

- 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 (⇒ l_{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:

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

Sum over N^2 terms

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

Important check: threshold expansion

Threshold expansion

- For **P**=0 and near threshold: $E=3m+\Delta E$, with $\Delta E \sim 1/L^3+\ldots$
- In other words, study energy shift of three particles (almost) at rest
- Dominant effects (L^{-3}, L^{-4}, L^{-5}) involve 2-particle interactions, but 3-particle interaction enters at L^{-6}
- For large L, particles are non-relativistic ($\Delta E \ll m$) and can use NREFT methods
- This has been done previously by [Beane, Detmold & Savage, 0707.1670] and [Tan, 0709.2530]

NR EFT results

[Beane, Detmold & Savage, 0707.1670]

2 particles

$$E_0(2,L) = \frac{4\pi a}{ML^3}\left\{1 - \left(\frac{a}{\pi L}\right)\mathcal{I} + \left(\frac{a}{\pi L}\right)^2[\mathcal{I}^2 - \mathcal{J}] + \left(\frac{a}{\pi L}\right)^3[-\mathcal{I}^3 + 3\mathcal{I}\mathcal{J} - \mathcal{K}]\right\} + \frac{8\pi^2 a^3}{ML^6} r + \mathcal{O}(L^{-7}), \qquad (11)$$

- 2-particle result agrees with [Luscher]
- Scattering length *a* is in nuclear physics convention
- *r* is effective range
- $\mathcal{I}$, $\mathcal{J}$, $\mathcal{K}$ are zeta-functions

3 particles

$$E_0(3,L) = \frac{12\pi a}{ML^3}\left\{1 - \left(\frac{a}{\pi L}\right)\mathcal{I} + \left(\frac{a}{\pi L}\right)^2[\mathcal{I}^2 + \mathcal{J}] + \left(\frac{a}{\pi L}\right)^3[-\mathcal{I}^3 + \mathcal{I}\mathcal{J} + 15\mathcal{K} - 8(2\mathcal{Q} + \mathcal{R})]\right\} + \frac{64\pi a^4}{ML^6}(3\sqrt{3} - 4\pi)\log(\mu L) + \frac{24\pi^2 a^3}{ML^6} r + \frac{1}{L^6}\eta_3(\mu) + \mathcal{O}(L^{-7}), \qquad (12)$$

- 3 particle result through L^{-4} is 3x(2-particle result) from number of pairs
- Not true at L^{-5},L^{-6} where additional finite-volume functions $\mathcal{Q}$, $\mathcal{R}$ enter
- $\eta_3(\mu)$ is 3-particle contact potential, which requires renormalization

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Tan has 36 instead of 24,
but a different definition of η_3

- 3 particle result through L^{-4} is 3x(2-particle result) from number of pairs
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- $\eta_3(\mu)$ is 3-particle contact potential, which requires renormalization

NR EFT results

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zeta-functions

$$\mathcal{I} = Z_{00}(1,0) = \sum_{\vec{n}\neq 0}^{\Lambda}\frac{1}{\vec{n}^2} - 4\pi\Lambda\,, \quad \mathcal{J} = Z_{00}(2,0) = \sum_{\vec{n}\neq 0}\frac{1}{(\vec{n}^2)^2}\,, \quad \mathcal{K} = Z_{00}(3,0) = \sum_{\vec{n}\neq 0}\frac{1}{(\vec{n}^2)^3}$$

additional finite-volume quantities

dim. reg.

$$\hat{\mathcal{Q}} = \sum_{\mathbf{i}\neq\mathbf{0}}\sum_{\mathbf{j}\neq\mathbf{0}}\frac{1}{|\mathbf{i}|^2|\mathbf{j}|^2(|\mathbf{i}|^2 + |\mathbf{j}|^2 + |\mathbf{i}+\mathbf{j}|^2)} \to \mathcal{Q} + \frac{4}{3}\pi^4\log(\mu L) - \frac{2\pi^4}{3(d-3)}$$

$$\hat{\mathcal{R}} = \sum_{\mathbf{j}\neq\mathbf{0}}\frac{1}{|\mathbf{j}|^4}\left[\sum_{\mathbf{i}}\frac{1}{|\mathbf{i}|^2 + |\mathbf{j}|^2 + |\mathbf{i}+\mathbf{j}|^2} - \frac{1}{2}\int d^d\mathbf{i}\,\frac{1}{|\mathbf{i}|^2}\right] \to \mathcal{R} - 2\sqrt{3}\pi^3\log(\mu L) + \frac{\sqrt{3}\pi^3}{d-3}$$

Expanding our result

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

$$F_3 = \frac{1}{L^3}\frac{1}{2\omega}\left[\frac{F}{3} - F\frac{1}{\mathcal{K}_2{}^{-1} + F + G}F\right]$$

Means F_{PV}

- Only terms with l=m=0 contribute to the desired order
- $[F_3]_{\mathbf{0,0}}$ dominates other terms in F_3 by ~L^3, so quantization condition becomes

Evaluated at threshold

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

- F, G & $\mathcal{K}_2$ are matrices with indices **k,p**, truncated by cutoff function H
- F is $O(L^0)$, so to cancel the $1/L^3$ in F_3 need $[\mathcal{K}_2{}^{-1}+F+G]^{-1}$~$L^3$
- Roughly speaking this requires the cancellation of L^0, L^{-1} & L^{-2} terms in $[\mathcal{K}_2{}^{-1}+F+G]$, which requires tuning E and determines the L^{-3}, L^{-4} & L^{-5} in ΔE
- The L^{-6} term in ΔE is then determined by the quantization condition

Our threshold expansion

- L^{-3}, L^{-4}, L^{-5} terms agree with previous results, which checks details of F & G
- L^{-6} relates $\mathcal{K}_{\rm df,3}$ to 3-body contact potential of NREFT

$$\frac{\mathcal{K}_{\rm df,3;00}}{48m^3} = -\eta_3(\mu) + \frac{36\pi^2 a^2}{m^3} + \frac{48\pi^2 r a^3}{m}$$
$$+ \left(\frac{a}{\pi}\right)^3 \left[\frac{32\pi^3}{am}\widetilde{d}_3 + 16\pi^4(\widetilde{e}_2 + \widetilde{f}_2) + 16Q + 8R + \frac{16\pi^3}{3}(3\sqrt{3} - 4\pi)\log\left(\frac{m}{2\pi\mu}\right)\right]$$

- Agreement of coefficient of logarithm is another non-trivial check
- Final step will be to relate this to $\mathcal{M}_3$

Conclusions & Outlook

Summary: successes

- Confirmed that 3-particle spectrum determined by infinite-volume scattering quantities
- Obtained an "algebraic" result directly in terms of these amplitudes
- Derivation leads us to introduce divergence-free 3→3 scattering quantity
- Threshold expansion and other checks give us confidence in the expression
- Truncation to obtain finite problem occurs naturally

Summary: limitations

- $\mathcal{K}_{\mathrm{df},3}$ is not physical---rather an intermediate infinite-volume quantity
    - We now think we can relate it to $\mathcal{M}_3$
- $\mathcal{K}_2$ is needed below (as well as above) 2-particle threshold
- Formalism fails when K_2 is singular ⇒ each two-particle channel must have no resonances within kinematic range
- Warning (in case you want to run off and apply this!): σ couples also to the single "pion" state (which is why we kept $E^* > M$). In Euclidean space this pole will be the lowest lying state. All "3 pion" states will thus be excited states.
- Applies to identical, spinless particles, with Z_2 symmetry
    - We expect generalizing to other cases to be (relatively) straightforward

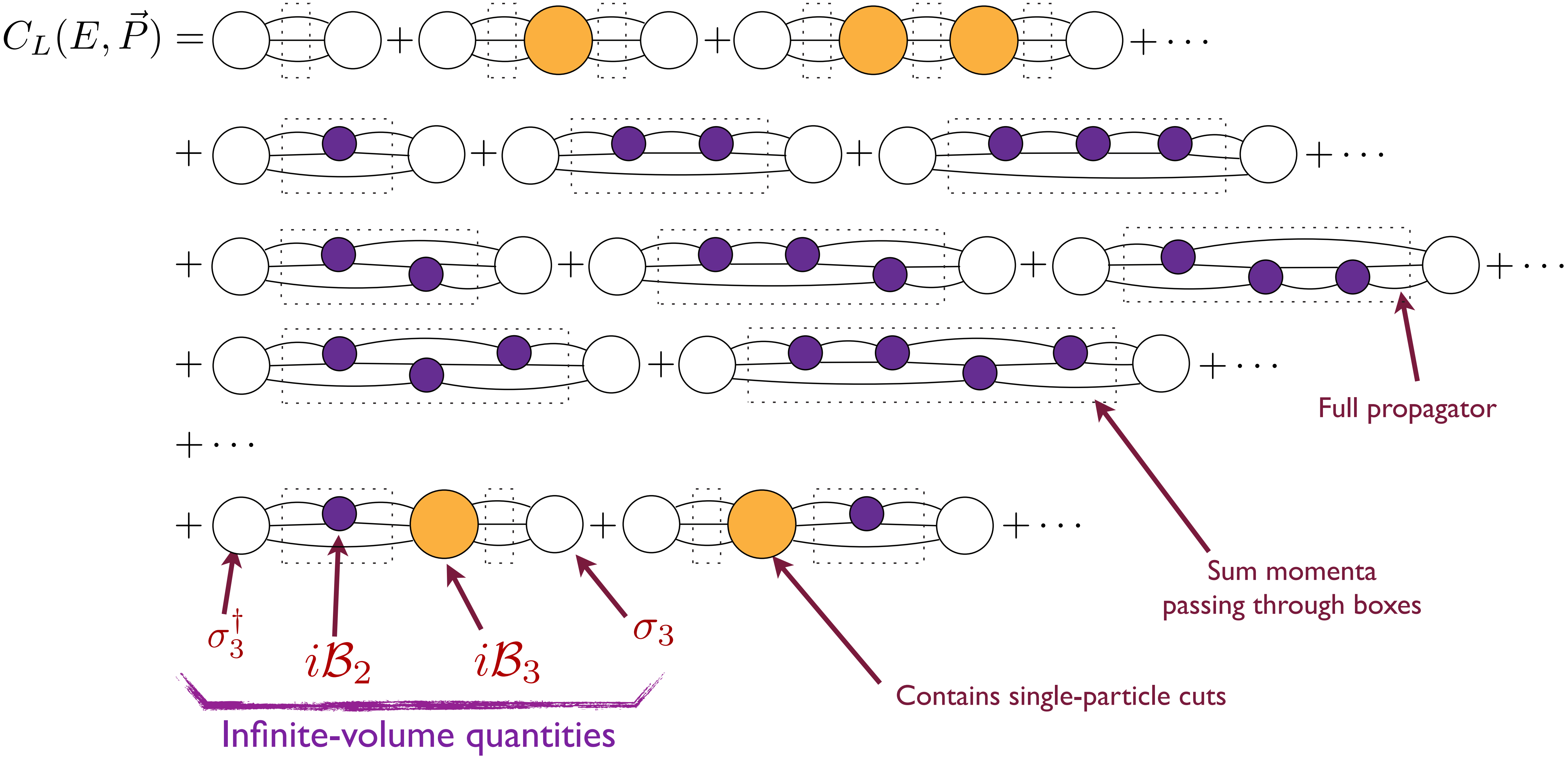
Plans

- Extend result to non-degenerate masses & other spins
- Detailed studies of practical utility using simple forms for amplitudes
- Detailed comparison with [Polejaeva & Rusetsky] and [Briceno & Davoudi]
- Derive generalization of Lellouch-Lüscher formula (for K→3π, etc.)
- Efimov states?
- Include 2→3 vertices and other Z_2 violating interactions
- Onward to four particles ?!

Thank you!
Questions?

Backup Slides

Skeleton expansion



$C_L(E,\vec{P}) =$

Full propagator

Sum momenta passing through boxes

Contains single-particle cuts

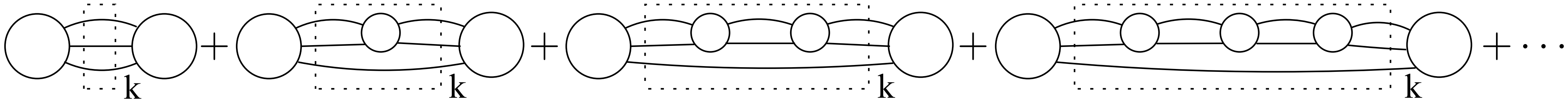
$\sigma_3^\dagger$ $i\mathcal{B}_2$ $i\mathcal{B}_3$ σ_3

Infinite-volume quantities

- If remove "endcaps", drop first diagram, and change internal sums to integrals, then have skeleton expansion for $\mathcal{M}_{3\to3}$

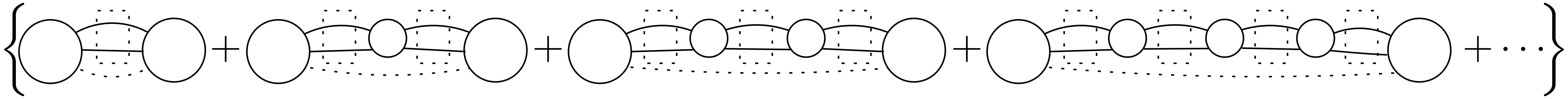
“No switch” diagrams

$C_L^{(1)} \equiv$

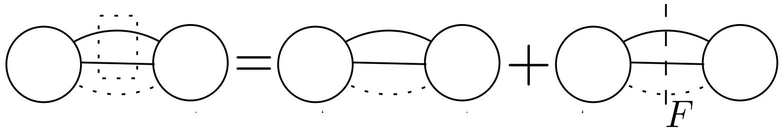


- Do k_0 integral, keeping only on-shell pole at $k_0=\omega_k$
  - Other poles give terms in which remaining sums can be replaced by integrals, and thus contribute to $C^{(1)}_\infty$

$C_L^{(1)} \supset \frac{1}{L^3}\sum_{\vec{k}}\frac{1}{2\omega_k}\Big\{$



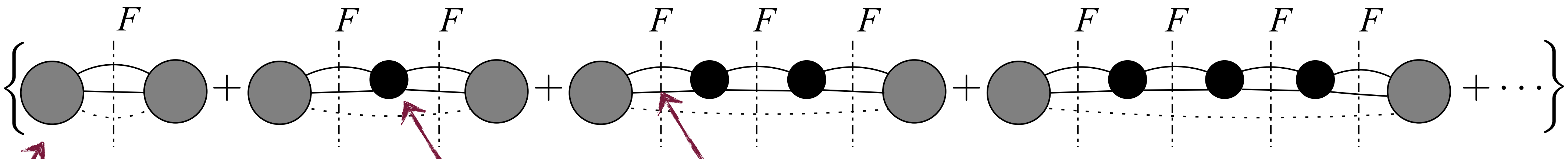
- Substitute identity

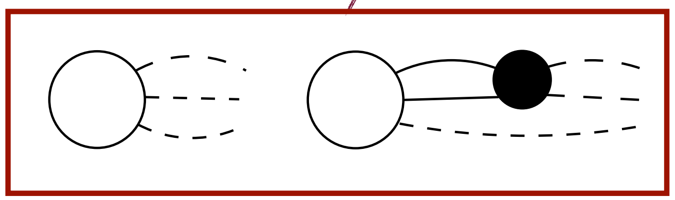


& proceed as for 2-particle case

$$C_L^{(1)} = C_\infty^{(1)} + \frac{1}{L^3}\sum_{\vec{k}}\frac{1}{2\omega_k}\Big\{$$

All F’s use PV-tilde prescription



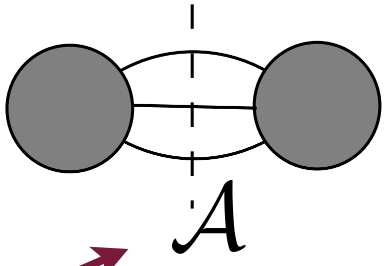


$i\mathcal{K}_2$

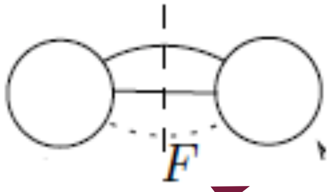
Quantities on either side of F’s are on-shell

“No switch” diagrams

$C_L^{(1)} = C_\infty^{(1)} +$



$-\frac{2}{3}$



“Dimer” propagator $[\mathcal{A}] = \frac{iF}{2\omega L^3}\frac{1}{1+\mathcal{K}_2 F}$

Present due to
mismatch of symmetry factors.
Absent if bottom particle non-interacting

- Matrix notation: indices are expanded compared to 2-particle case

[“spectator” momentum: **k**=2π**n**/L] x [2-particle CM angular momentum: *l*,*m*]

e.g. $iF_{k',\ell',m';k,\ell,m} = \delta_{k,k'}\ iF_{\ell',m';\ell,m}\underbrace{(E-\omega_k,\vec{P}-\vec{k})}_{\text{4-momentum of non-spectator pair}}$

- Obtain correct quantization condition if bottom particle is non-interacting