Three particles in a box: Mapping the finite-volume spectrum to the S-matrix

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MTH and Stephen R. Sharpe, arXiv:1408.5933, 2014
(published in PRD)

The three-particle quantization condition is a necessary first step for using LQCD to investigate...

resonances decaying to three or more hadrons

$\omega(782) \to \pi\pi\pi$ $\qquad$ $N(1440) \to N\pi\pi$

three-body forces

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

The three-particle quantization condition is a necessary first step for using LQCD to investigate...

weak decays coupling to three or more hadrons

$K \to \pi\pi\pi$ $\quad$ $D \to \pi\pi$ $\quad$ $D \to K\overline{K}$

(couples to $\pi\pi\pi\pi$)

Need QCD scattering amplitudes to relate finite-volume lattice matrix elements to physical decay amplitudes

Lellouch, L. & Lüscher, M.
Commun. Math. Phys. 219, 31-44 (2001)

Outline

Two particle review

Three particle quantization condition

Relation to scattering amplitude

Conclusion

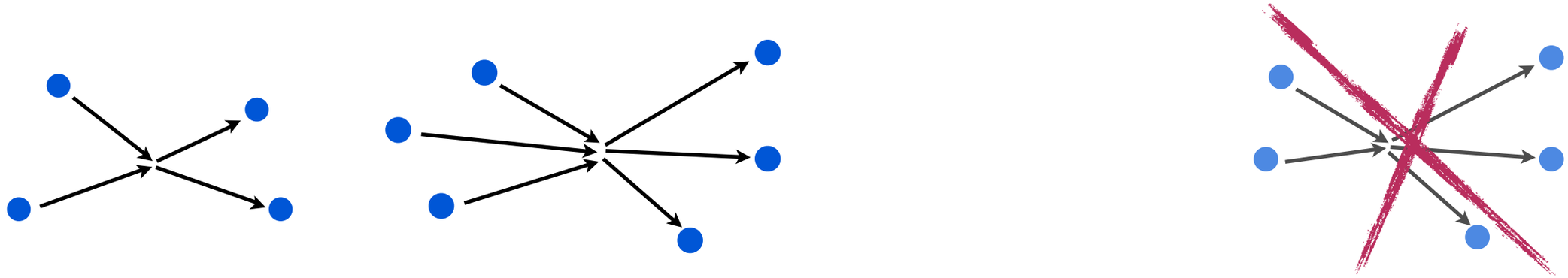
Particle content

Single scalar, mass m

all results for identical scalars

Relativistic field theory

$\mathbb{Z}_2$ **symmetry**

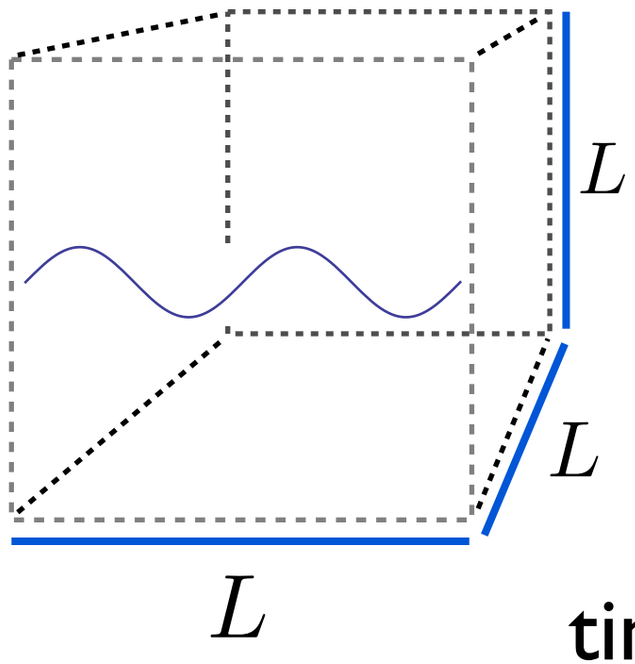


(For pions in QCD this is G-parity)

Include all vertices

with even number of legs

Finite volume



cubic, spatial volume (extent L)

periodic boundary conditions

$\vec{p} \in (2\pi/L)\mathbb{Z}^3$

time direction **infinite** and **Minkowski**

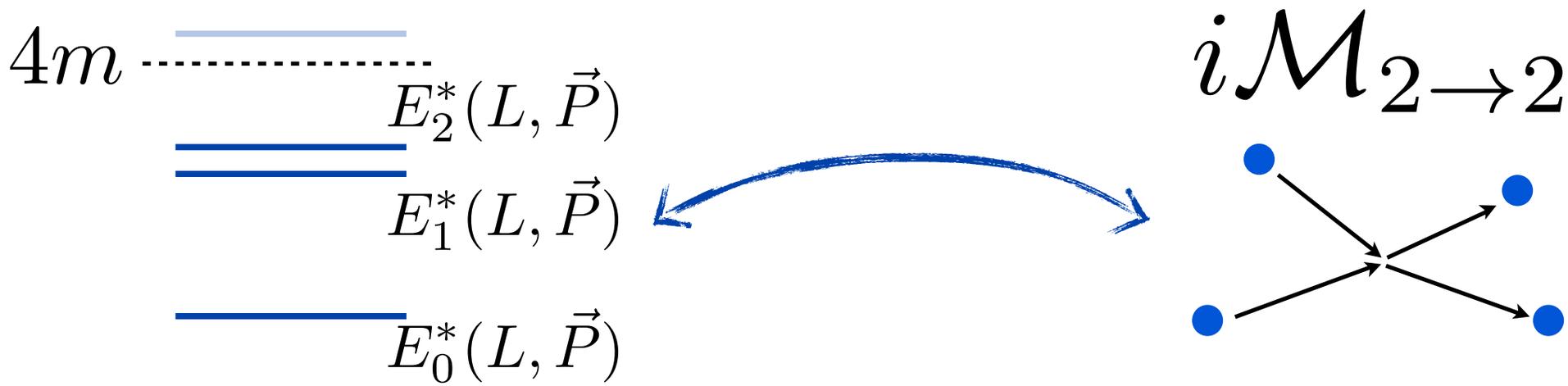
Take L large enough to ignore e^{-mL}

dropped throughout!

Take space to be continuous

lattice spacing set to zero

Two particles in a box



$$C_L(E,\vec{P}) \equiv \int_L d^4x\, e^{i(Ex^0 - \vec{P}\cdot\vec{x})} \langle 0|\mathrm{T}\sigma(x)\sigma^\dagger(0)|0\rangle$$

Require $E^* < 4m$ **even-particle quantum numbers**

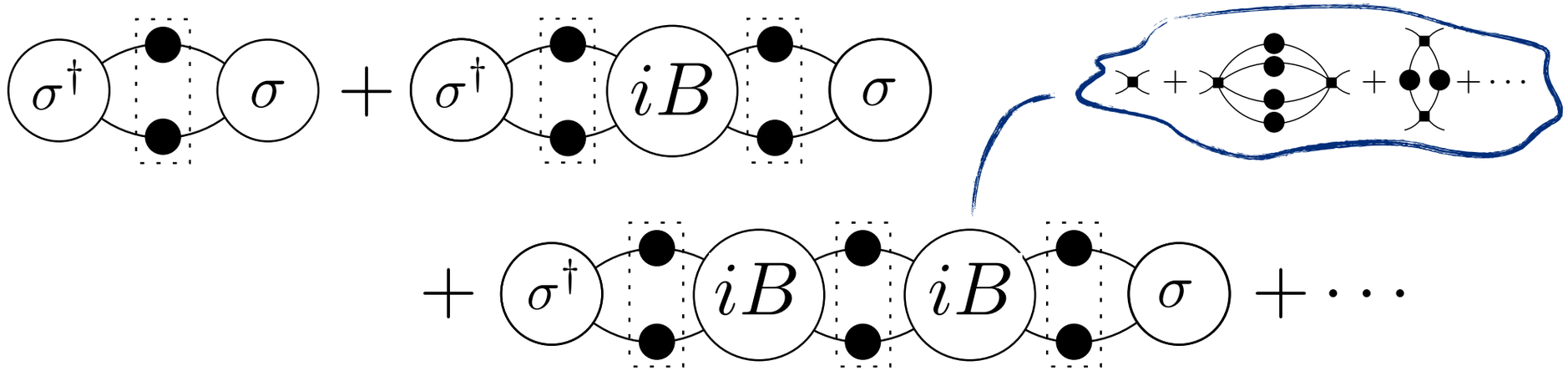
Calculate $C_L(E,\vec{P})$ to all orders in perturbation theory and determine condition of divergence.

Following Kim, Sachrajda and Sharpe. *Nucl. Phys.* B727, 218-243 (2005)

Two particles in a box

1

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



Two particles in a box

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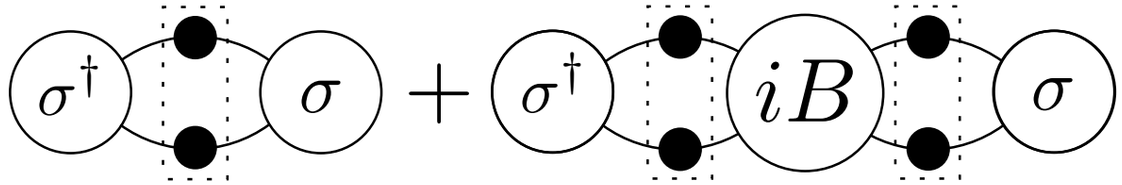
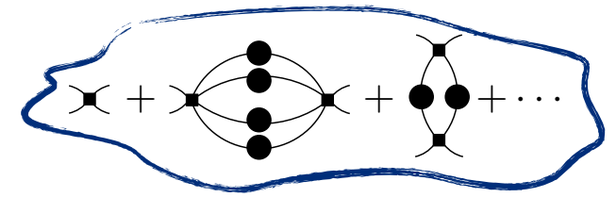
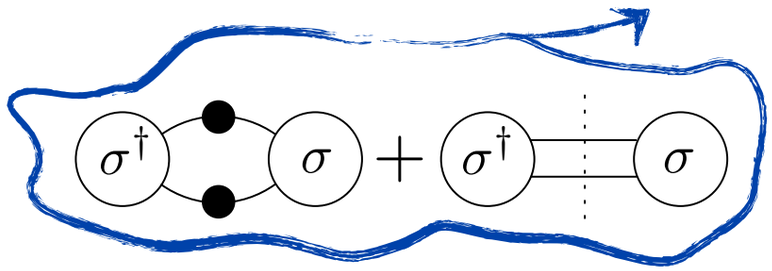
$C_L(E,\vec{P}) =$

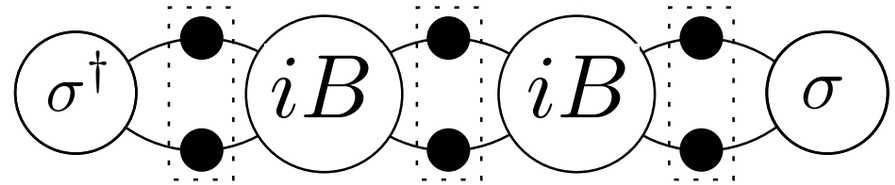




2



$+$

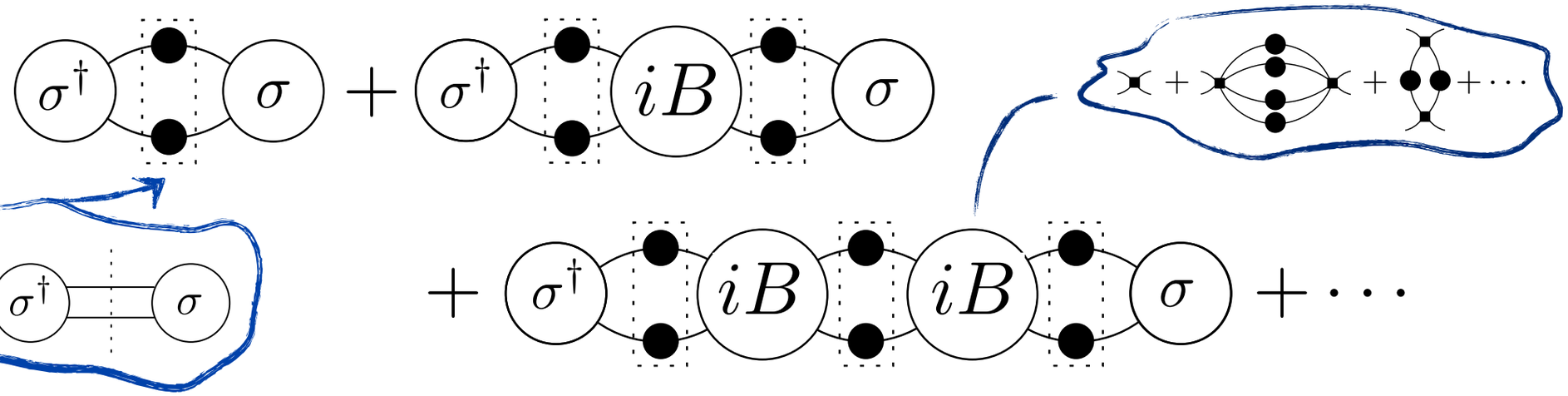


$+ \cdots$

Two particles in a box

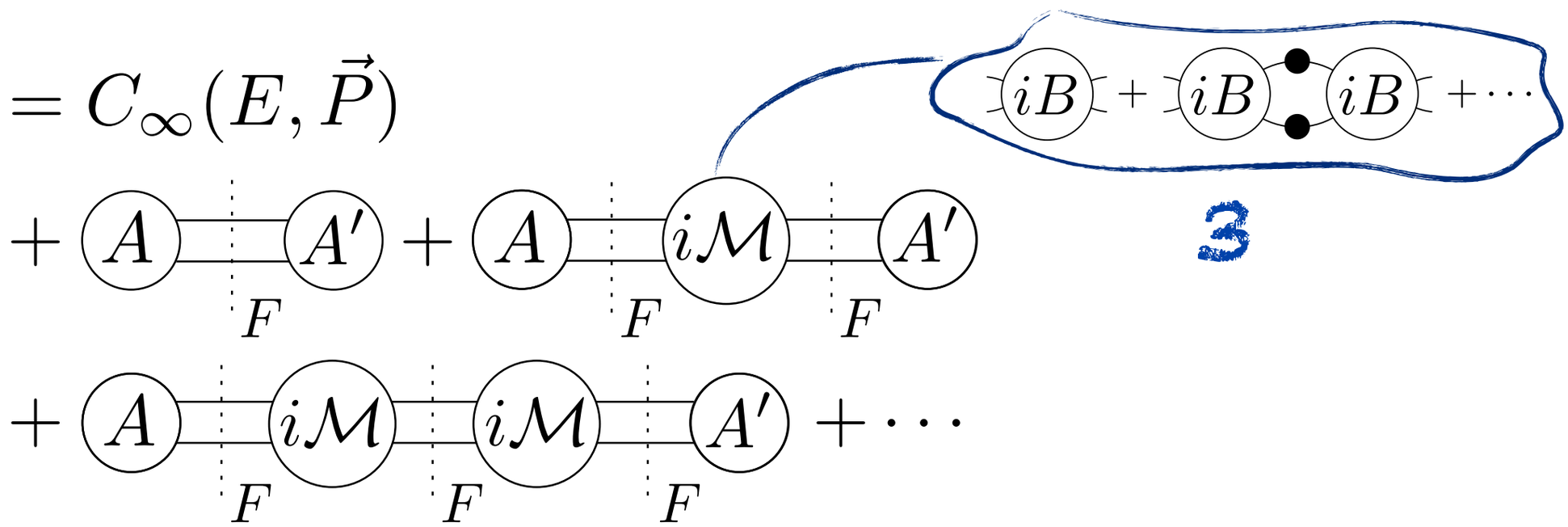
1

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



2

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

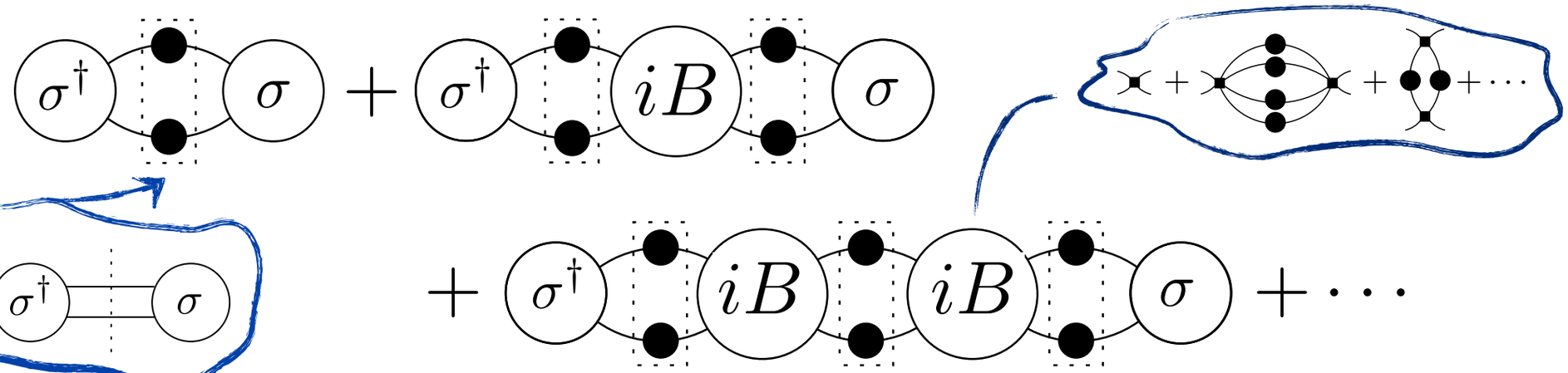


3

Two particles in a box

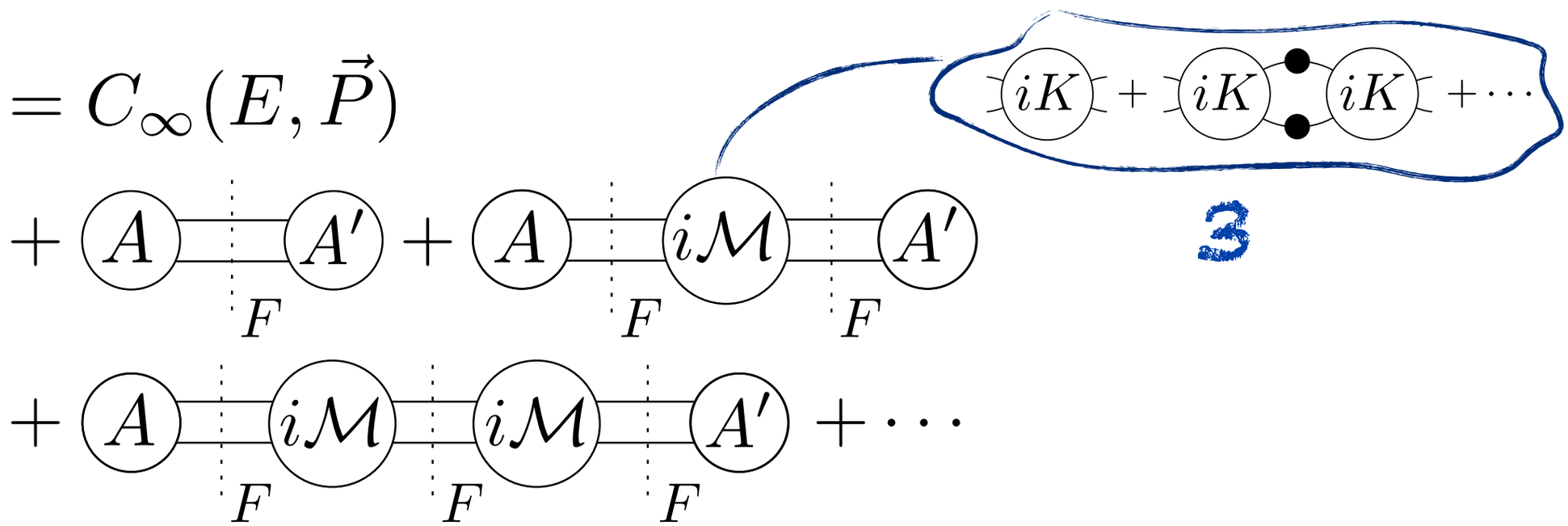
1

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



2

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



3

4

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

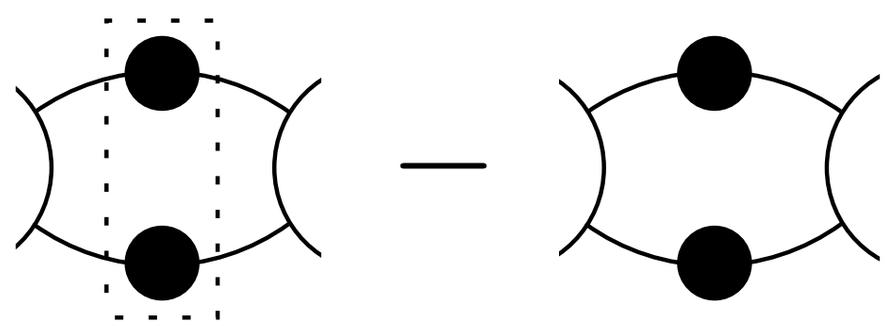
Two-particle result

At fixed $(L, \vec{P})$, finite-volume spectrum is all solutions to

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

diagonal matrix in angular momentum space

kinematic (related to Lüscher Zeta function)

$F \equiv$ 

Two-particle result

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

...is it useful?

At low energies, s-wave dominates

$$[\mathcal{M}^s_{2\to 2}(E^*_n)]^{-1} = -F^s(E_n, \vec{P}, L)$$

$$F^s(E, \vec{P}, L) \equiv \frac{1}{2}\left[\frac{1}{L^3}\sum_{\vec{k}} - \int \frac{d^3k}{(2\pi)^3}\right] \frac{1}{2\omega_k 2\omega_{P-k}(E - \omega_k - \omega_{P-k} + i\epsilon)}$$

Two-particle result

Note also, equation is real

$$[\mathcal{M}^s_{2\to 2}(E^*_n)]^{-1} = -F^s(E_n, \vec{P}, L)$$

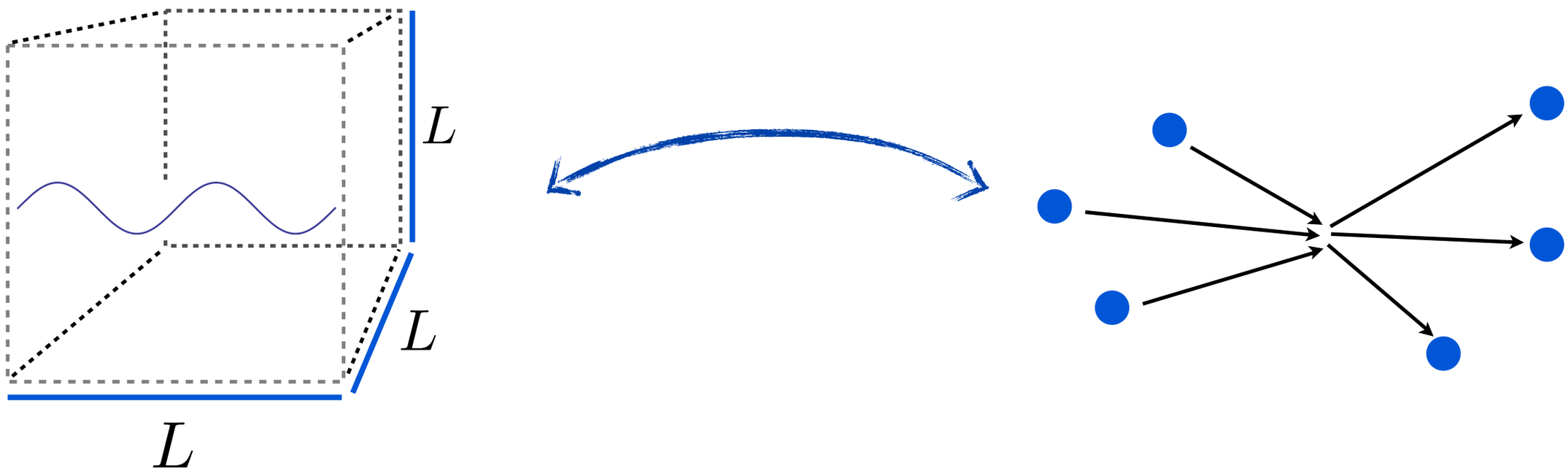
$$\boxed{p_n \cot\delta^s(p_n) - i\cancel{p}_n = -16\pi E^*_n \,\mathrm{Re}F^s - i\cancel{p}_n}$$

This can also be seen by **replacing i-epsilon with principal value** everywhere in derivation.

$$\mathcal{M}_{2\to 2} \longrightarrow \mathcal{K}_{2\to 2} \qquad\qquad F \longrightarrow \mathrm{Re}\, F$$

Important for three-particle case

Now, three particles in a box

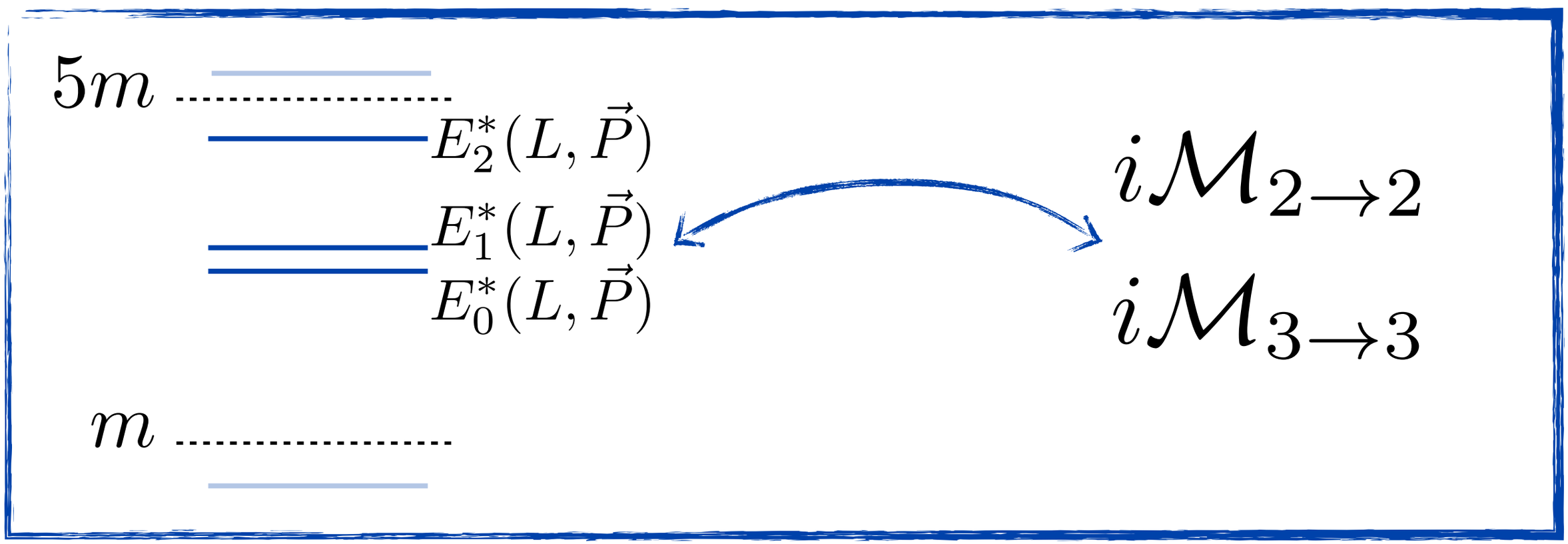


Three particles in a box

$$C_L(E,\vec{P}) \equiv \int_L d^4x\, e^{i(Ex^0-\vec{P}\cdot\vec{x})}\langle 0|\mathrm{T}\sigma(x)\sigma^\dagger(0)|0\rangle$$

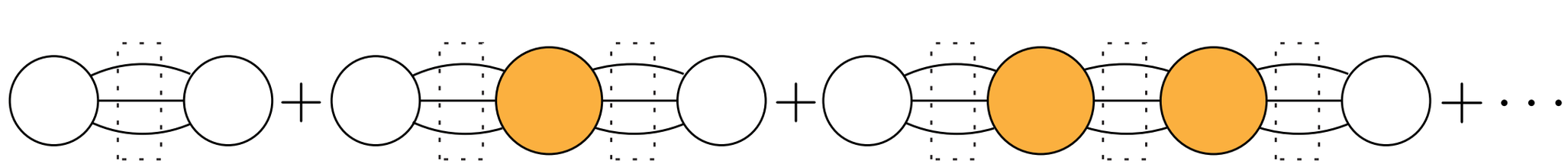
Require $m < E^* < 5m$

odd-particle quantum numbers



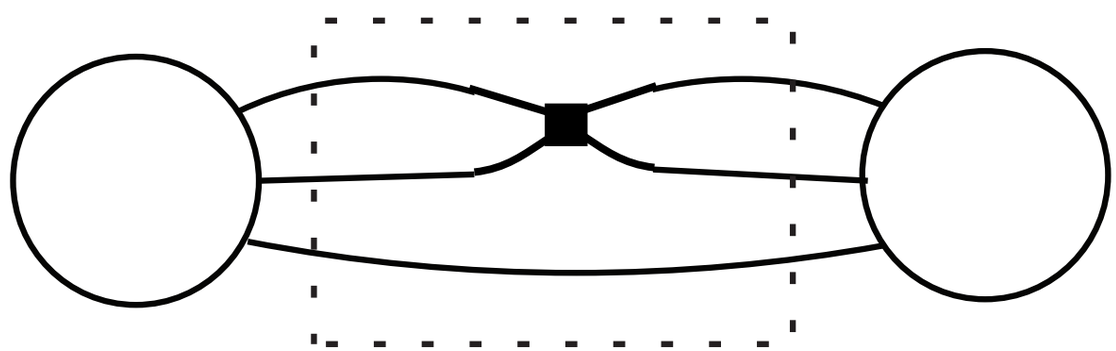
Assume no two-particle bound state

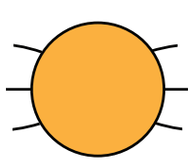
New skeleton expansion

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

(propagators still fully dressed)

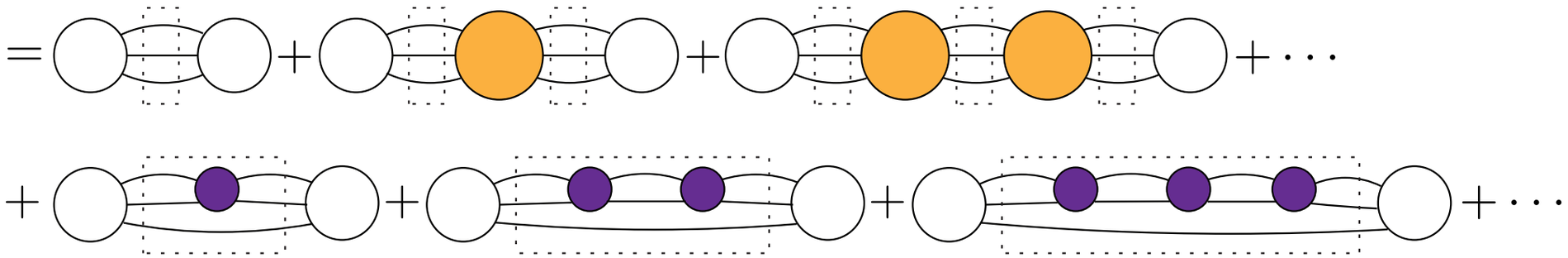
No! We also need diagrams like



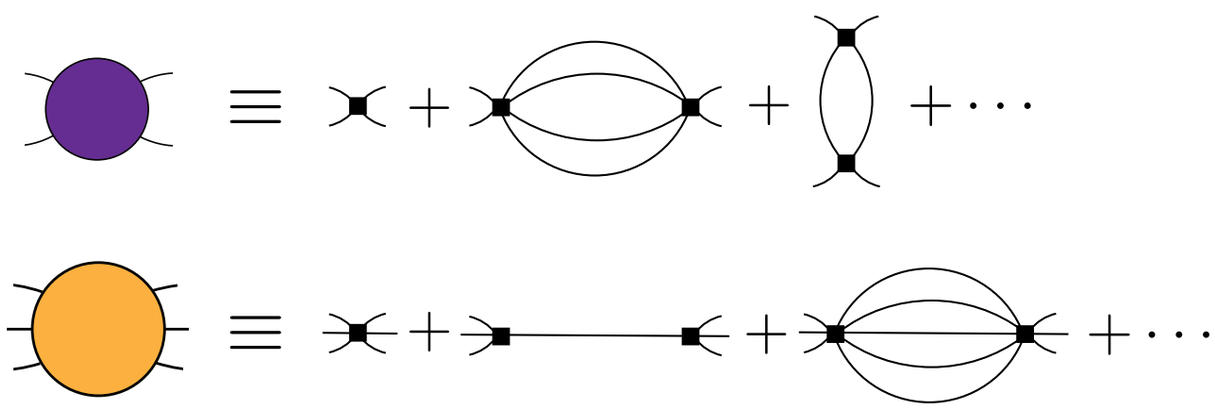
( **should only contain connected diagrams)**

New skeleton expansion

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

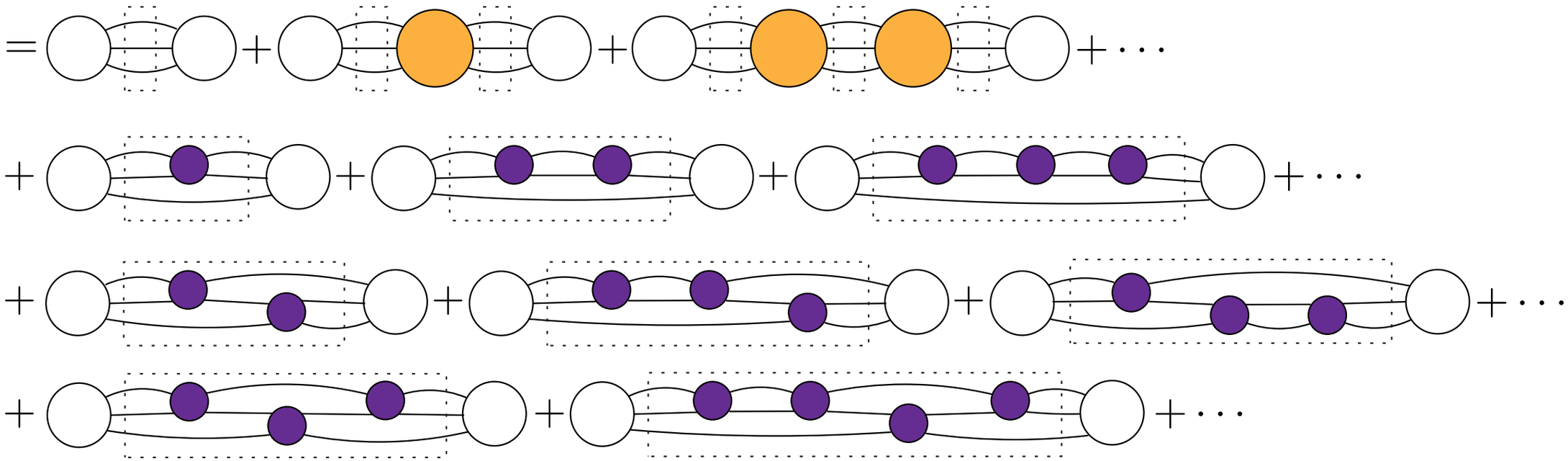


Kernel definitions:



New skeleton expansion

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



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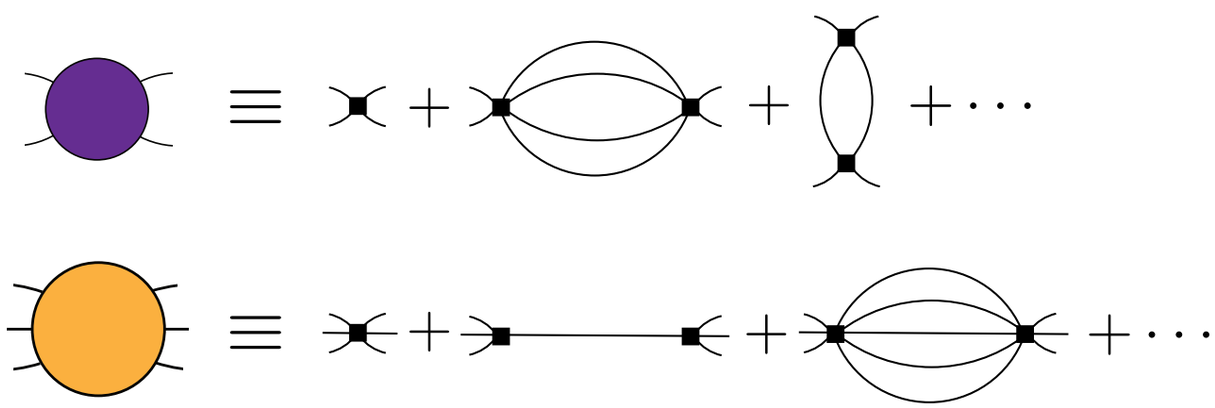

New skeleton expansion

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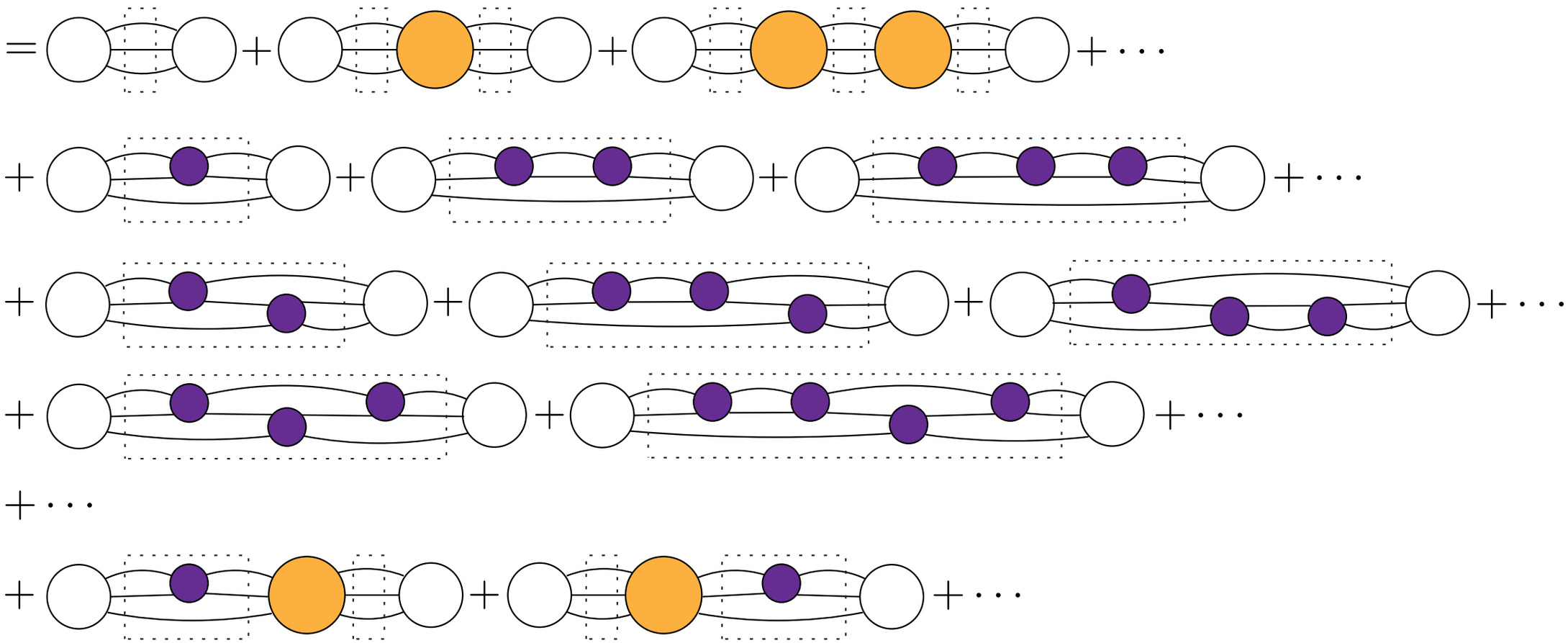

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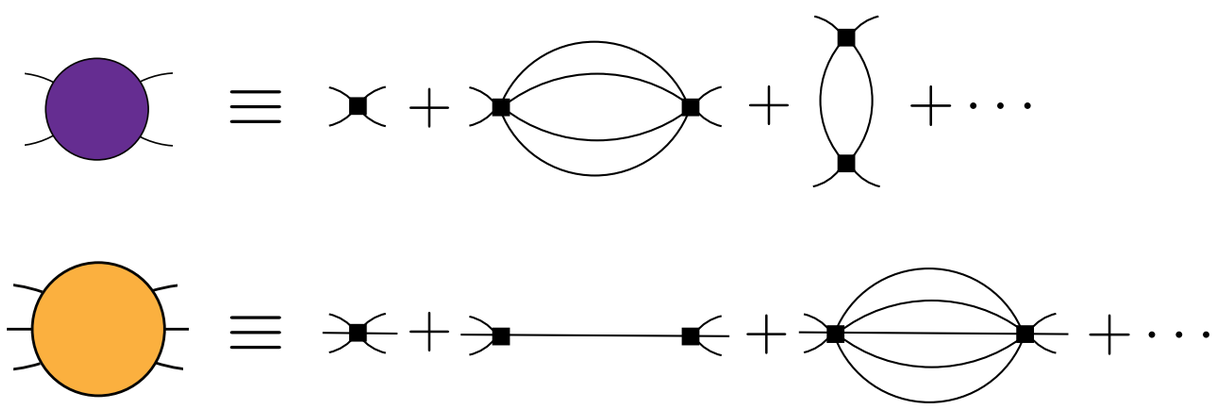

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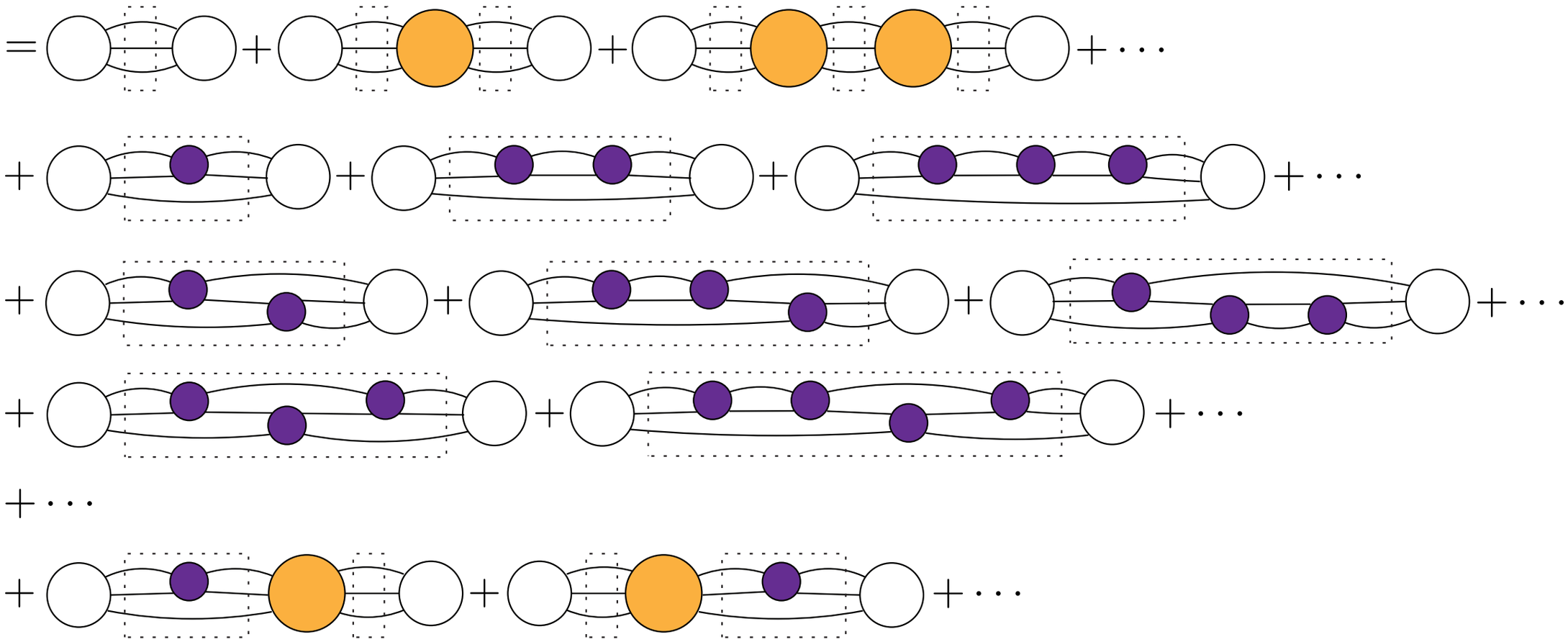
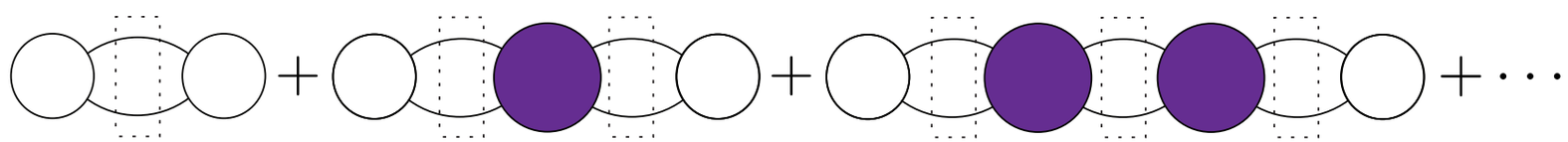


Compare to two-particle skeleton expansion

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



What is new here?

1. Degrees of freedom are different

two particles

two-particle angular momentum

three particles

$\vec{k}$ + **two-particle angular momentum**

Our result only depends on finite-volume $\vec{k}$

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

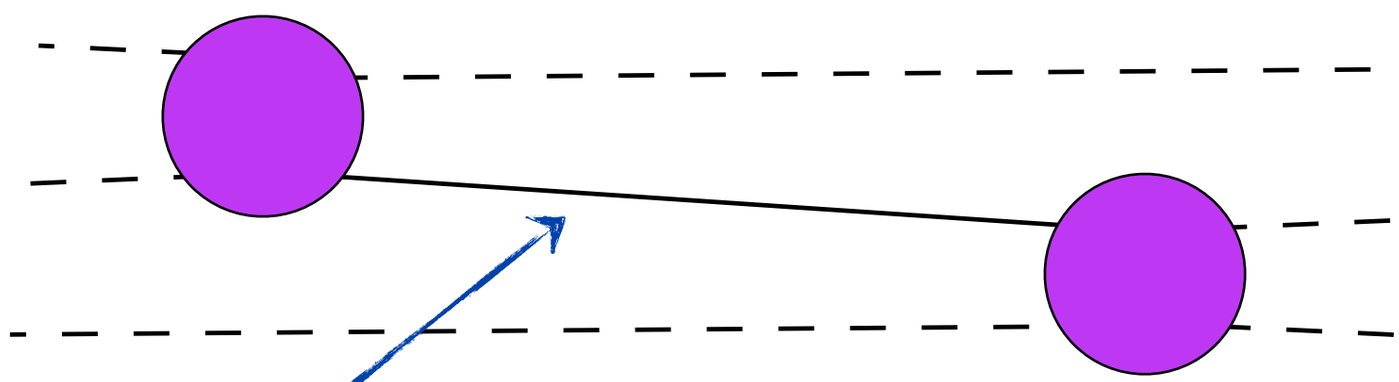
integer vector

What is new here?

2. Three particle divergences

Three particle observable $i\mathcal{M}_{3\to 3}$

contains the diagram



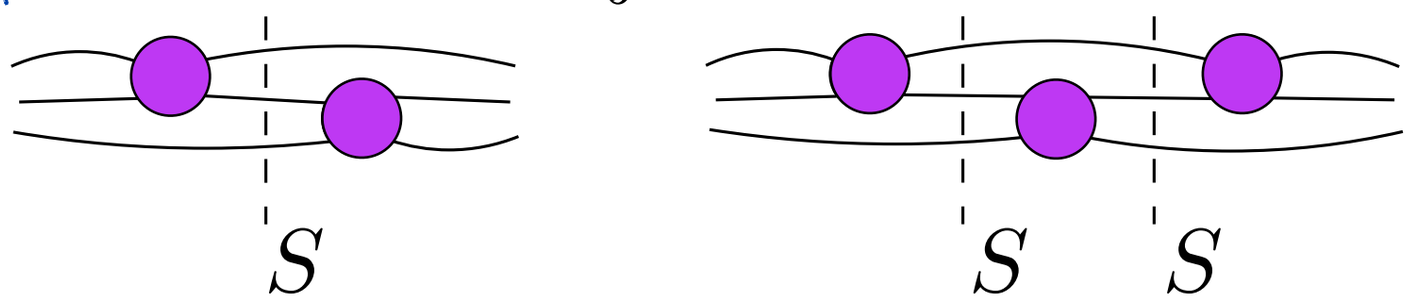
Certain external momenta put this on-shell → $i\mathcal{M}_{3\to 3}$ **has singularities**

What is new here?

2. Three particle divergences

Define $i\mathcal{M}_{\mathrm{df},3\to3}$

$$\equiv i\mathcal{M}_{3\to3} - \left[i\mathcal{M}_{2\to2} S i\mathcal{M}_{2\to2} + \int i\mathcal{M}_{2\to2} S i\mathcal{M}_{2\to2} S i\mathcal{M}_{2\to2} + \cdots \right]$$



only on-shell amplitudes here

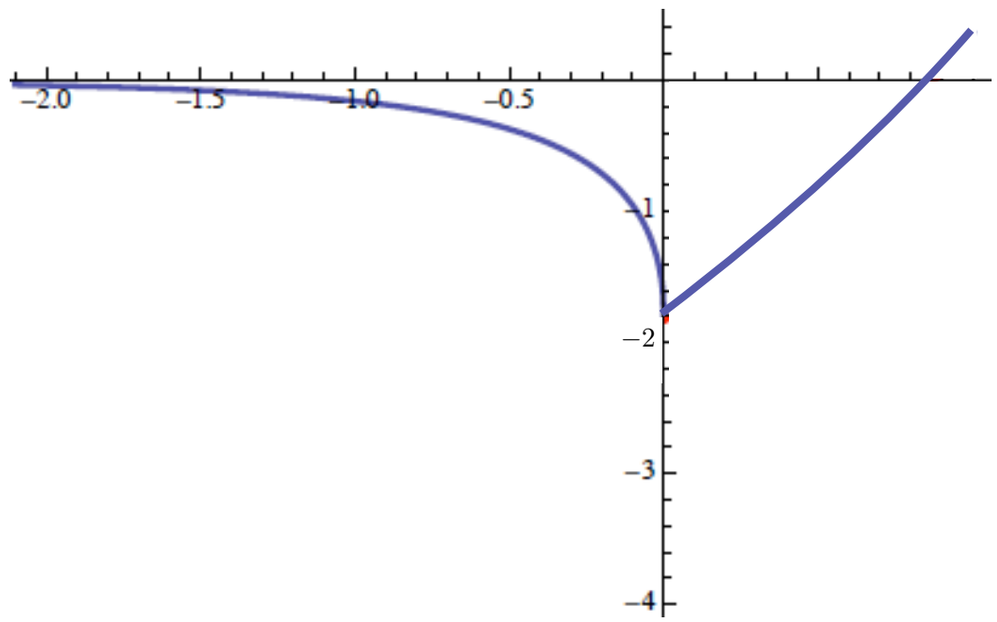
infinite series built with factors of $Si\mathcal{M}_{2\to2}$

This subtraction emerges naturally in our finite-volume analysis

What is new here?

3. Must now worry about sum crossing two-particle unitary cusp

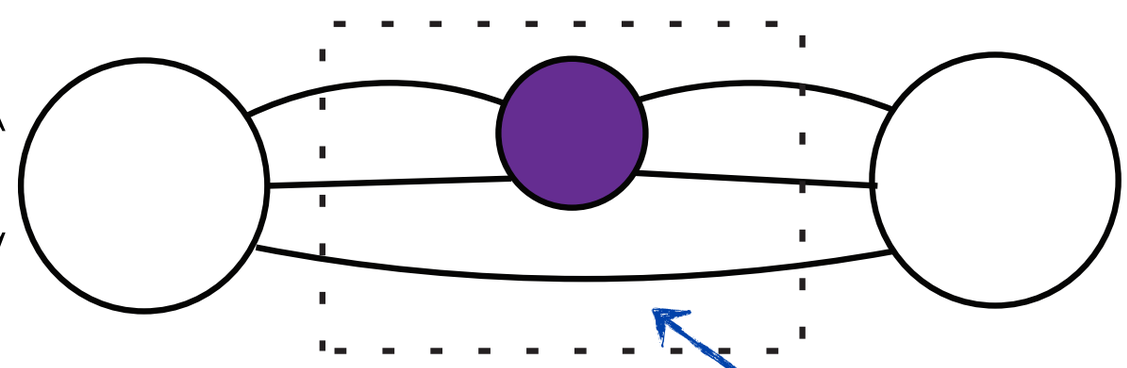
two-particle scattering (real part)



depends on k

two particle energy

$$\frac{1}{L^3}\sum_{\vec{k}}$$



k

What is new here?

3. Must now worry about sum crossing two-particle unitary cusp

To remove cusp

$i\epsilon$ prescription → principal value $\widetilde{\mathrm{PV}}$

Analytically continue principal value below threshold then interpolate to prescription-free subthreshold form

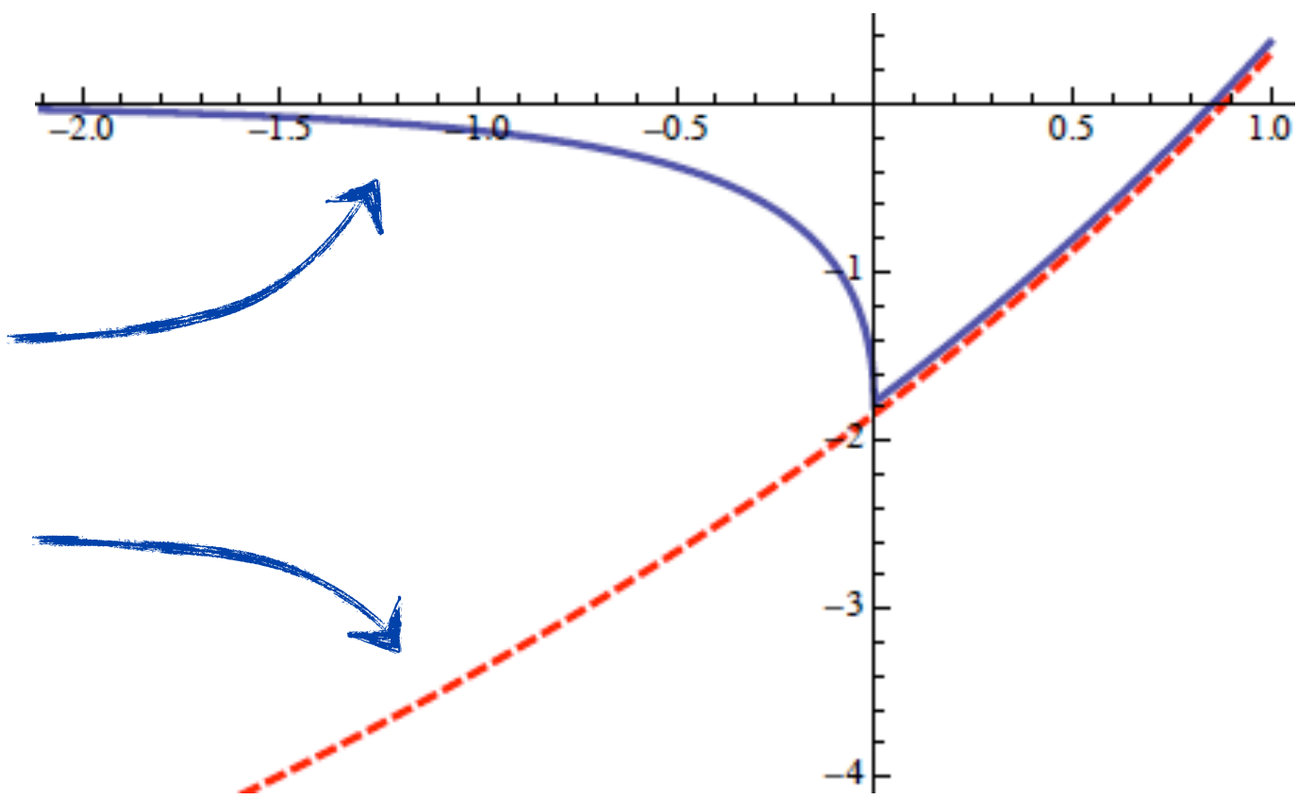
Polejaeva, K. and Rusetsky, A. *Eur. Phys. J.* A48 (2012) 67

What is new here?

3. Must now worry about sum crossing two-particle unitary cusp

To remove cusp

$i\epsilon$ prescription → principal value $\widetilde{\mathrm{PV}}$

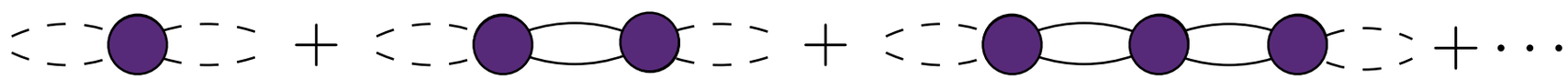


standard definition

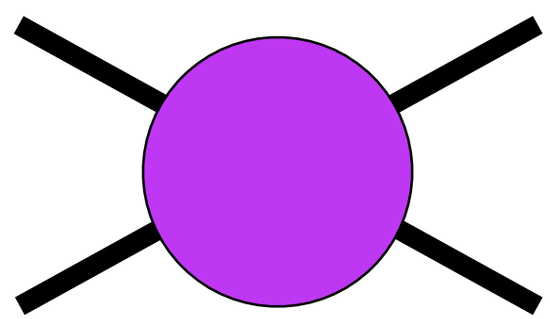
modification $\widetilde{\mathrm{PV}}$

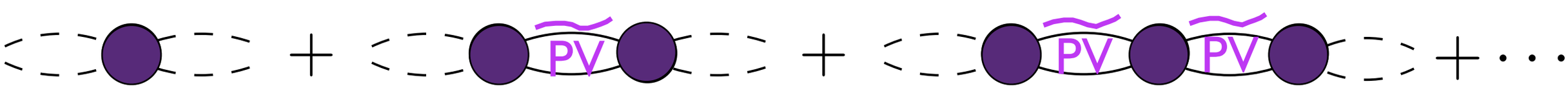
What is new here?

3. Must now worry about sum crossing two-particle unitary cusp

$i\mathcal{M}_{2\to 2} =$ 

has cusp

$i\mathcal{K}_{2\to 2} =$  $=$



has no cusp

What is new here?

3. Must now worry about sum crossing two-particle unitary cusp

$$i\mathcal{M}_{2\to 2} \longrightarrow i\mathcal{K}_{2\to 2}$$

$$i\mathcal{M}_{\mathrm{df},3\to 3} \qquad i\mathcal{K}_{\mathrm{df},3\to 3}$$

We relate these infinite-volume quantities to the finite-volume spectrum

Three-particle result

$$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A_3' i F_3 \frac{1}{1 - i\mathcal{K}_{\mathrm{df},3\to3}\ iF_3} A_3$$

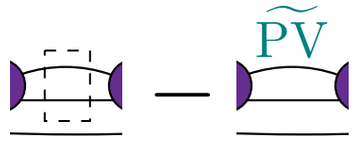
$$iF_3 \equiv \frac{iF}{2\omega L^3}\left[\frac{1}{3} + \frac{1}{1 - i\mathcal{M}_{L,2\to2}\ iG}\ i\mathcal{M}_{L,2\to2}\ iF\right]$$

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

Three-particle result

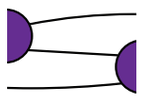
$$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A_3' iF_3 \frac{1}{1 - i\mathcal{K}_{\mathrm{df},3\to3}\, iF_3} A_3$$

sum-integral difference



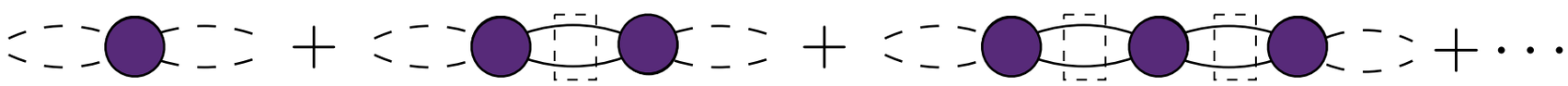
$$iF_3 \equiv \frac{iF}{2\omega L^3}\left[\frac{1}{3} + \frac{1}{1 - i\mathcal{M}_{L,2\to2}\, iG}\, i\mathcal{M}_{L,2\to2}\, iF\right]$$

encodes switches



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

sum of all two-particle loops (with summed momenta)



Three-particle result

$$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A_3' i F_3 \frac{1}{1 - i\mathcal{K}_{\mathrm{df},3\to3}\; iF_3} A_3$$

row matrices column

all in $\vec{k}, \ell, m$ space

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

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

Three-particle result

$$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A_3' iF_3 \frac{1}{1 - i\mathcal{K}_{\mathrm{df},3\to3}\ iF_3} A_3$$

no poles **no poles** **no poles**

$C_L(E,\vec{P})$ **diverges whenever** $iF_3 \dfrac{1}{1 - i\mathcal{K}_{\mathrm{df},3\to3}\ iF_3}$ **diverges**

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

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

Three-particle result

At fixed $(L, \vec{P})$, finite-volume spectrum is all solutions to

$$\Delta_{L,P}(E) = \det\left[1 - \underline{i\mathcal{K}_{\mathrm{df},3\to3}}\,\underline{iF_3}\right] = 0$$

matrix in space $\vec{k}, \ell, m$

depends on kinematics and two-particle scattering

Three-particle result

$$\Delta_{L,P}(E) = \det\left[1 - i\mathcal{K}_{\mathrm{df},3\to3} iF_3\right] = 0$$

...is it useful?

truncate in angular momentum to reduce to finite matrices ✓

need relation between $i\mathcal{M}_{3\to3}$ **and** $i\mathcal{K}_{\mathrm{df},3\to3}$

need to explore parametrizations of $i\mathcal{K}_{\mathrm{df},3\to3}$

Threshold expansion

At weak coupling, perturbatively study finite-volume shift from threshold

$$E = 3m + \mathcal{O}(1/L^3)$$ ← **finite-volume shift**

We find…

$$E = 3m + \frac{12\pi a}{mL^3}\left[1 + A\frac{a}{L} + B\frac{a^2}{L^2}\right] + C_1\frac{1}{L^6} - \frac{\mathcal{K}_{\mathrm{df},3\to3,\mathrm{thresh}}}{48m^3L^6} + C_2\frac{\log(mL)}{L^6}$$

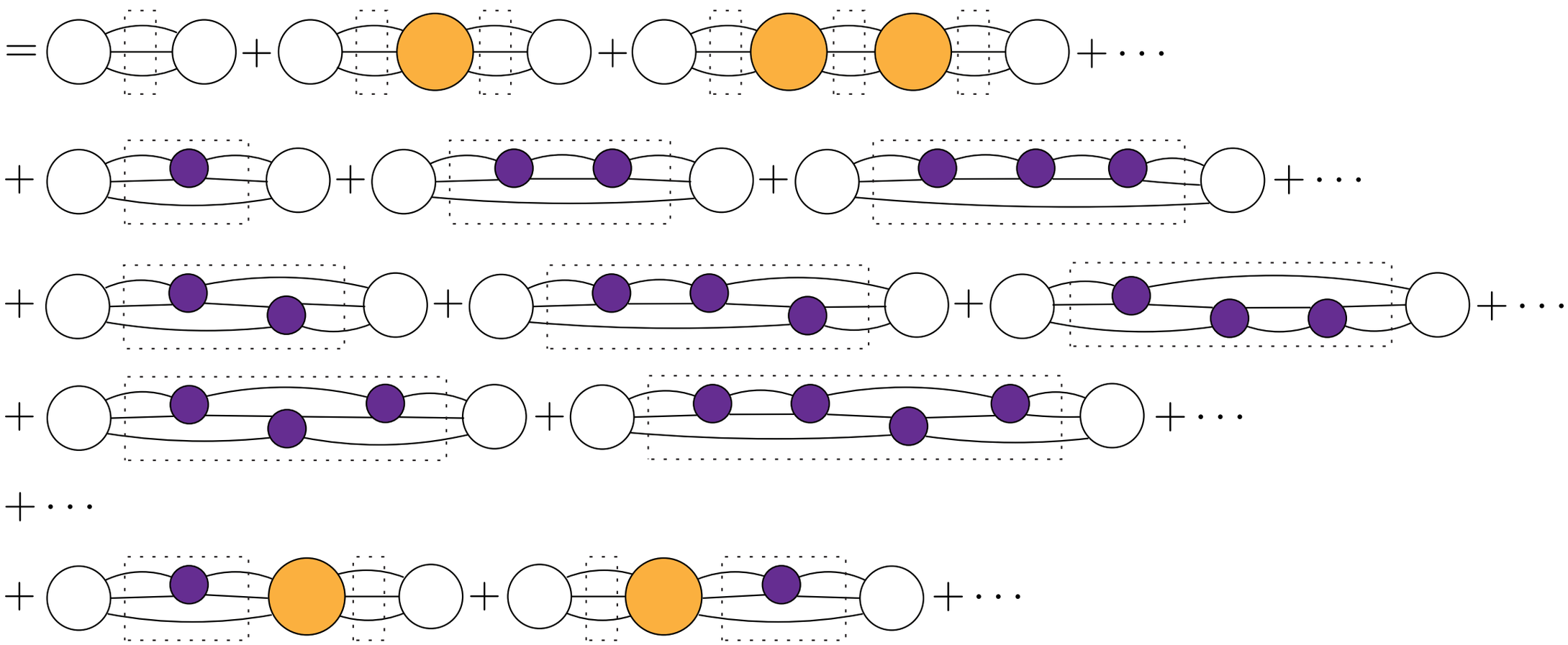
A, B, C_2 **agree unambiguously with earlier work**

Beane, S., Detmold, W. & Savage, M. *Phys. Rev.* D76 (2007) 074507
Tan, S. Phys. Rev. A78 (2008) 013636

$$C_1 - \frac{\mathcal{K}_{\mathrm{df},3\to3,\mathrm{thresh}}}{48m^3}$$ **related to non-relativistic contact interaction**

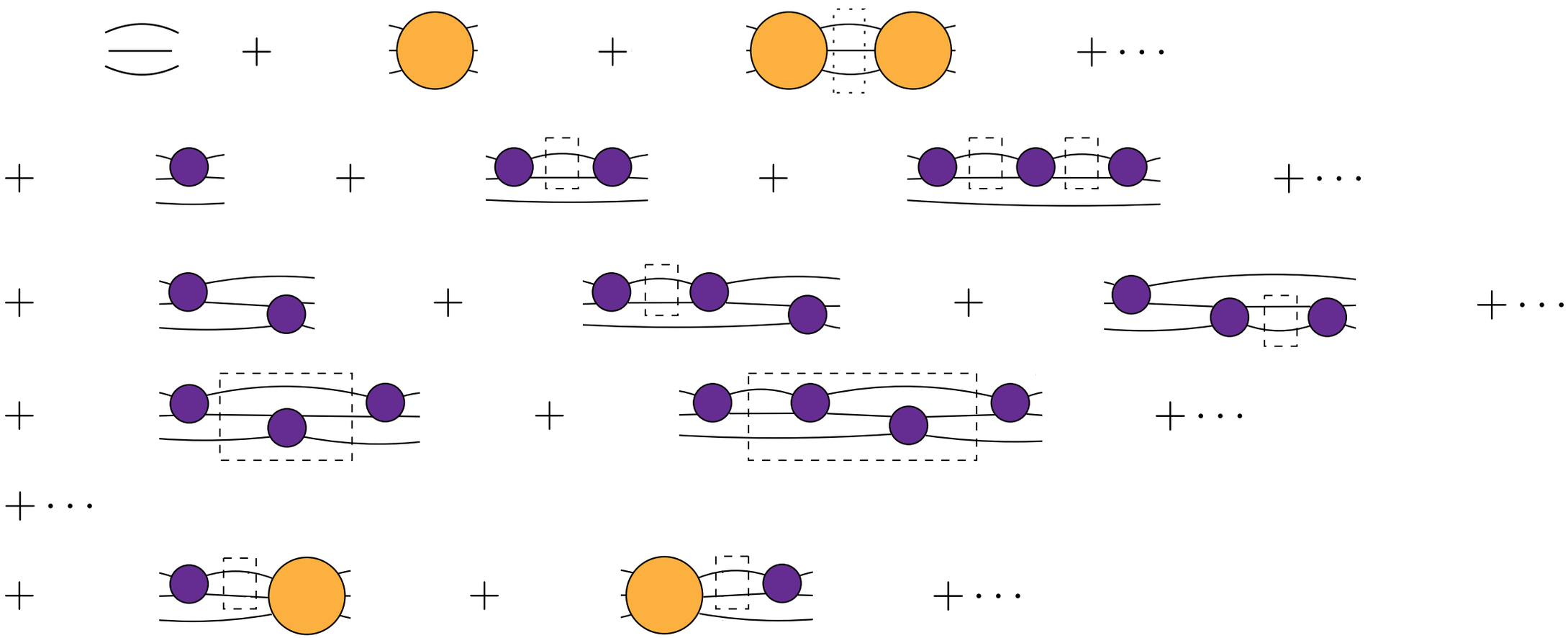
Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

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



First we modify $C_L(E,\vec{P})$ to define $i\mathcal{M}_{L,3\to3}$

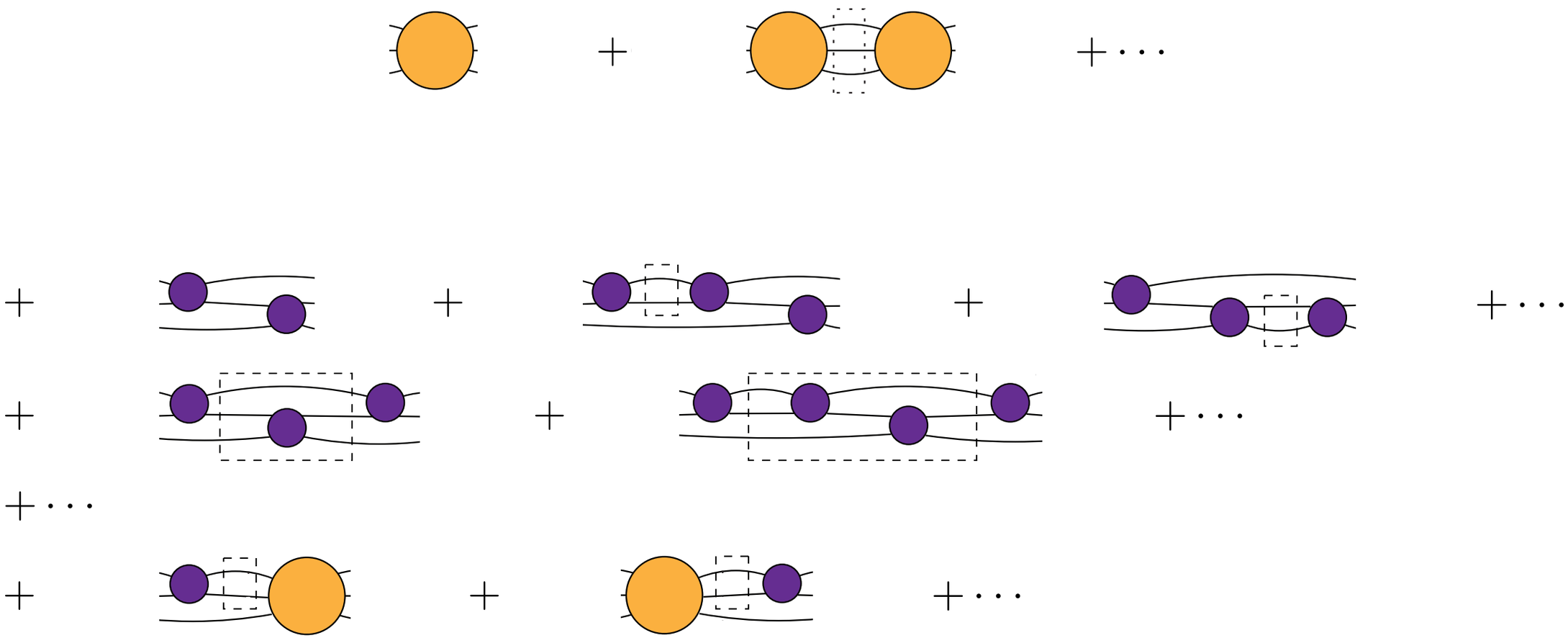
Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$



First we modify $C_L(E,\vec{P})$ to define $i\mathcal{M}_{L,3\to3}$

1. Amputate interpolating fields

Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

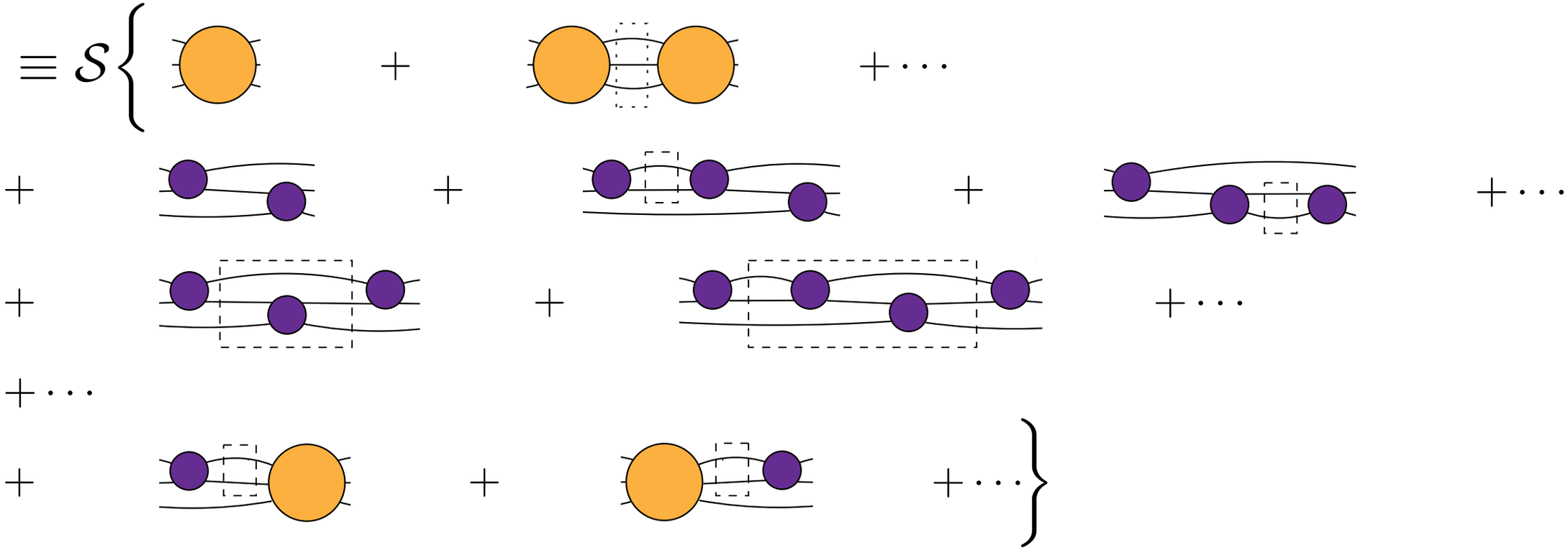


First we modify $C_L(E,\vec{P})$ to define $i\mathcal{M}_{L,3\to3}$

2. Drop disconnected diagrams

Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

$i\mathcal{M}_{L,3\to3} \equiv \mathcal{S}\Big\{$

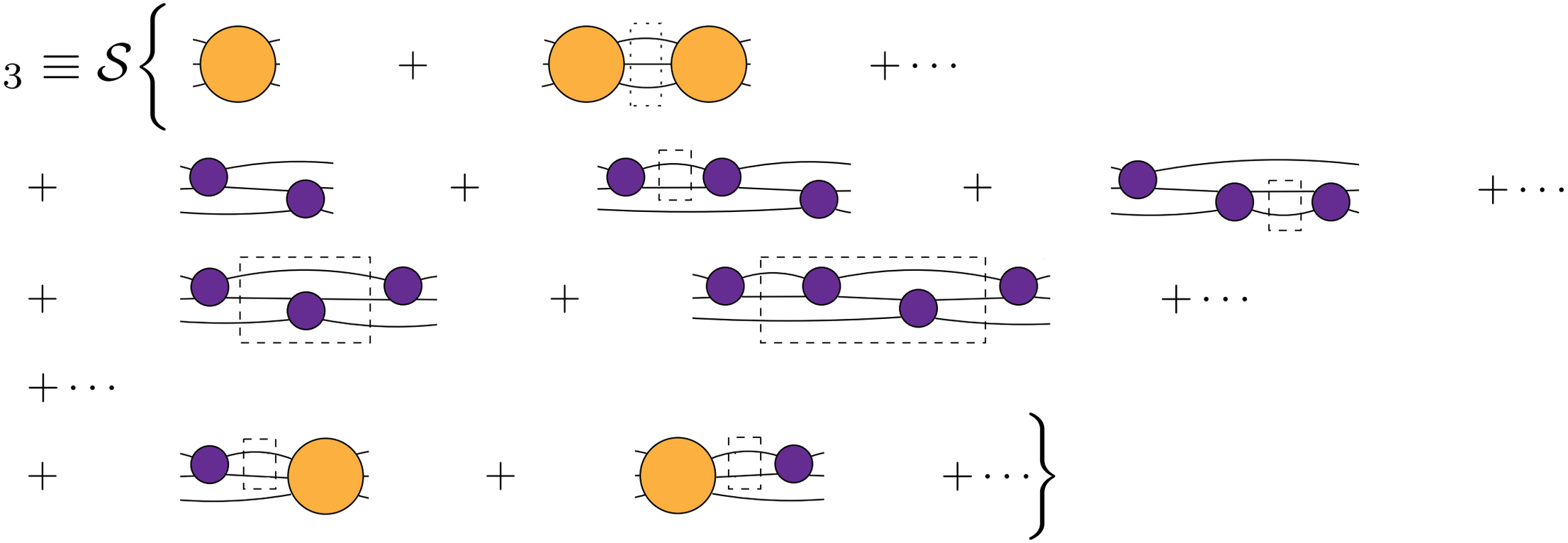


First we modify $C_L(E,\vec{P})$ to define $i\mathcal{M}_{L,3\to3}$

3. Symmetrize

Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

$i\mathcal{M}_{L,3\to3} \equiv \mathcal{S}\Big\{$



$\Big\}$

Replacing all loop momentum sums with i-epsilon prescription integrals would give physical three-to-three scattering amplitude

Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

We find a simple form for $i\mathcal{M}_{L,3\to3}$

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

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

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

$$\equiv \frac{iF}{2\omega L^3}\mathcal{L}_L \equiv \mathcal{R}_L \frac{iF}{2\omega L^3}$$

Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

We find a simple form for $i\mathcal{M}_{L,3\to3}$

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

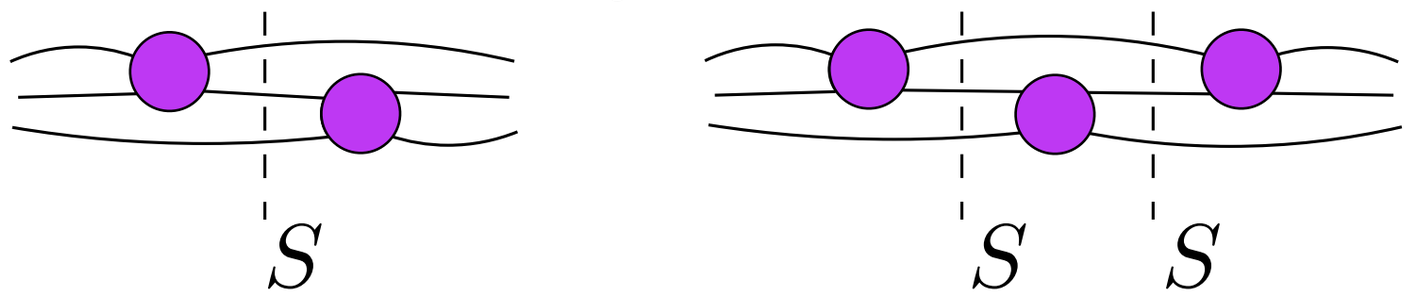
Complete analysis with infinite volume limit

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

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

Recall $i\mathcal{M}_{\mathrm{df},3\to3}$

$$\equiv i\mathcal{M}_{3\to3} - \left[i\mathcal{M}_{2\to2} S i\mathcal{M}_{2\to2} + \int i\mathcal{M}_{2\to2} S i\mathcal{M}_{2\to2} S i\mathcal{M}_{2\to2} + \cdots\right]$$



It reappears here… $i\mathcal{M}_{df,3\to3} \equiv \lim_{L\to\infty} \Big|_{i\epsilon} \left[i\mathcal{M}_{L,3\to3} - i\mathcal{D}_L\right]$

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

encodes switches

Relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

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

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

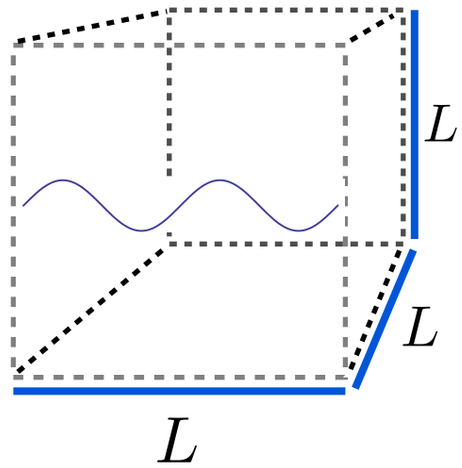
Gives integral equation relating $i\mathcal{K}_{\mathrm{df},3\to3}$ to $i\mathcal{M}_{3\to3}$

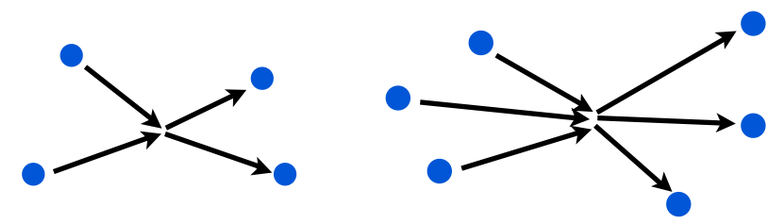
Completes formal story (for the setup considered!)

Relation only depends on on-shell scattering quantities

Summary

Presented work relating finite-volume spectrum and three-to-three scattering.





Necessary first step for extracting any decay or scattering amplitude with more than two hadrons from Lattice QCD.

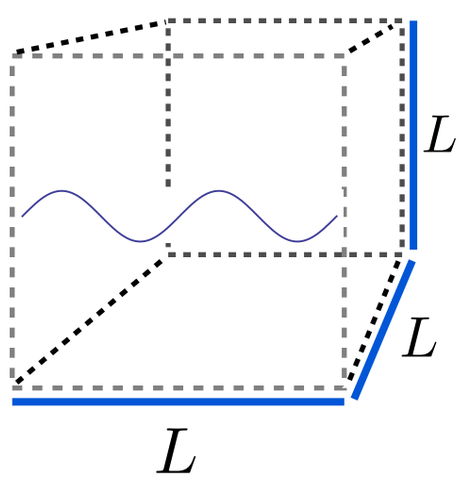
Future work and Applications

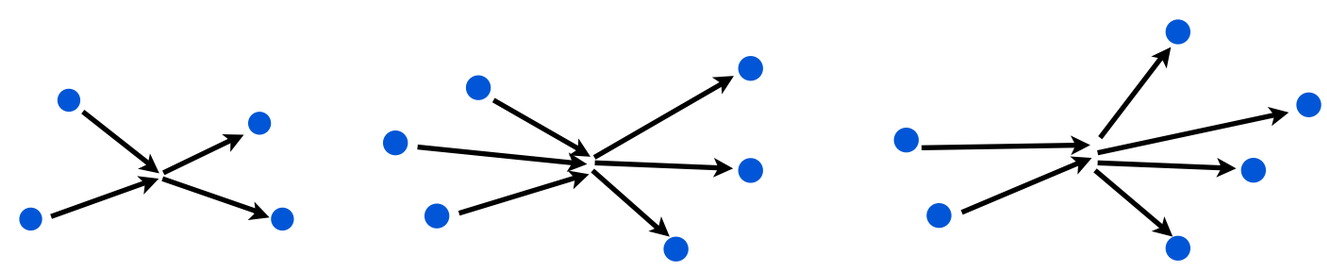
Generalize Lellouch-Lüscher method, to extract three-particle weak decays

$$K \longrightarrow \pi\pi\pi$$

Include non-identical, non-degenerate and spin-half particles

Extend mapping to four-particle states





Isotropic approximation

Following two particle case, suppose $\mathcal{K}_{\mathrm{df},3\to3}$ can be approximated to be isotropic (only depends on E^*)

$$\mathcal{K}_{\mathrm{df},3\to3}(E_n^*) = -[F_{3,\mathrm{iso}}(E_n, \vec{P}, L)]^{-1}$$

$$F_{3,\mathrm{iso}} \equiv \sum_{\vec{k},\vec{p}} F_{3;k,p}$$

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

Three-particle result

At fixed $(L, \vec{P})$ the finite-volume spectrum $E_1, E_2, \cdots$ is the set of solutions to

$$\Delta_{L,P}(E) = \det[1 - i\widetilde{\mathcal{K}}_{df,3\to3} iF_3] = 0$$

where

$$iF_3 \equiv \frac{1}{2\omega L^3}\left[-(2/3)iF_{\widetilde{\mathrm{PV}}} + \frac{1}{[iF_{\widetilde{\mathrm{PV}}}]^{-1} - [1 - i\widetilde{\mathcal{K}}_{2\to2} iG]^{-1} i\widetilde{\mathcal{K}}_{2\to2}}\right]$$

$$iF_{\widetilde{\mathrm{PV}};k,k'} \equiv \delta_{k,k'}\frac{1}{2}\left[\frac{1}{L^3}\sum_{\vec{a}} - \widetilde{\mathrm{PV}}\int_{\vec{a}}\right]\frac{iQ(\vec{a}^*)Q^*(\vec{a}^*)}{2\omega_a 2\omega_{P-k-a}(E - \omega_k - \omega_a - \omega_{P-k-a})}$$

$$iG_{k,p} \equiv \frac{1}{2\omega_p L^3}\frac{iQ(\vec{p}^*)Q^*(\vec{k}^*)}{2\omega_{P-p-k}(E - \omega_p - \omega_k - \omega_{P-p-k})}$$

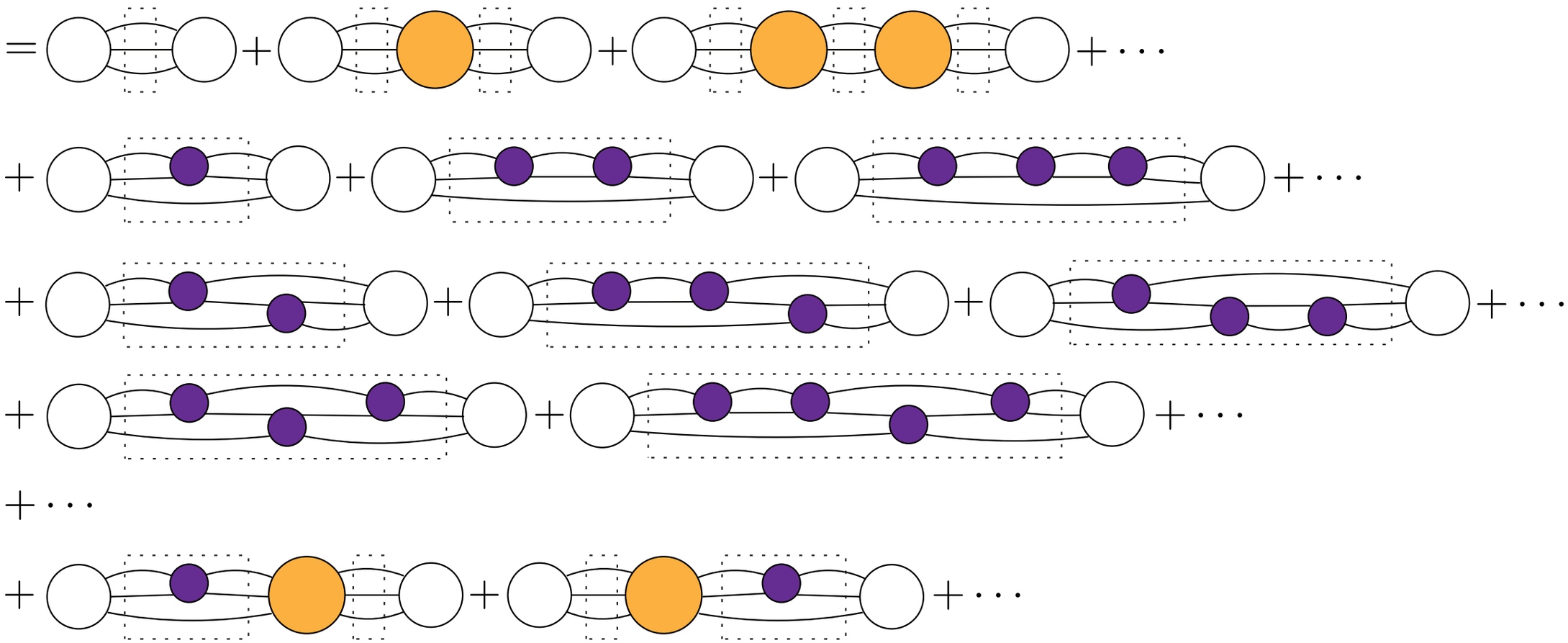
$$Q_{\ell,m}(\vec{k}^*) \equiv \sqrt{4\pi}Y_{\ell,m}(\hat{k}^*)(k^*/q^*)^\ell$$

with $\omega_k^2 = \vec{k}^2 + m^2$ and $q^{*2} = (1/4)[E^2 - \vec{P}^2] - m^2$

Additional Material Concerning Differences Between Two- and Three-Particle Quantization

New skeleton expansion

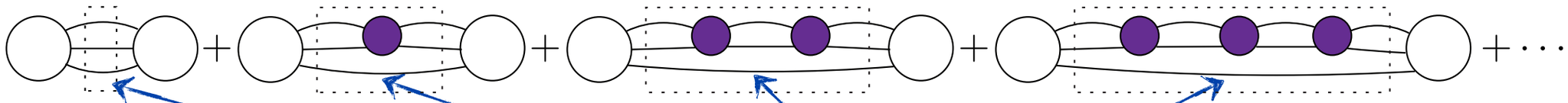
$C_L(E, \vec{P}) =$



Here I will only give first parts of derivation.

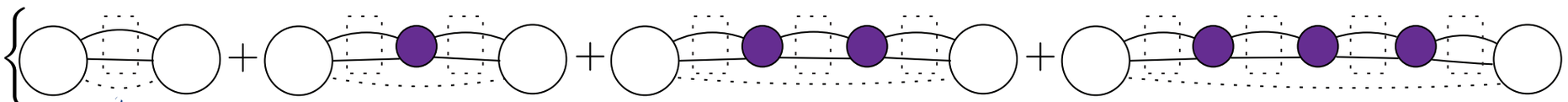
This is to illustrate certain points, needed to understand the final result.

First Part: Sum "no-switch" diagrams

$C_L^{(1)} \equiv$ 

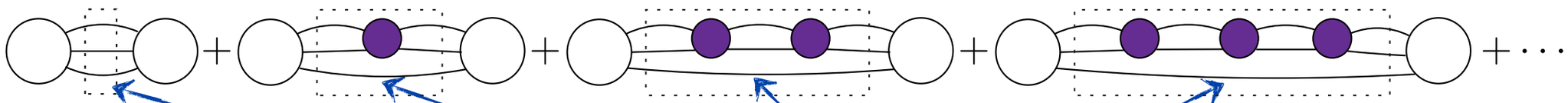
call the bottom momentum k

important finite-volume corrections only arise from $k^0 = \omega_k$

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

bottom propagator replaced with $1/(2\omega_k)$

First Part: Sum "no-switch" diagrams

$C_L^{(1)} \equiv$ 

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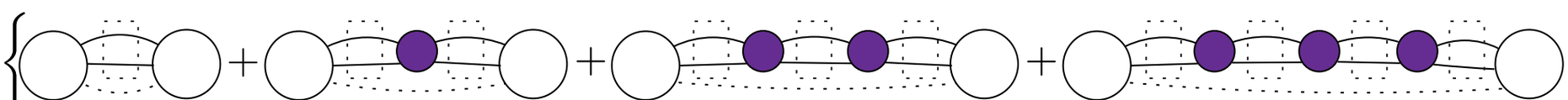
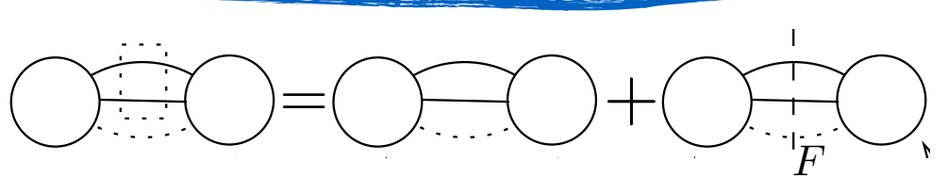
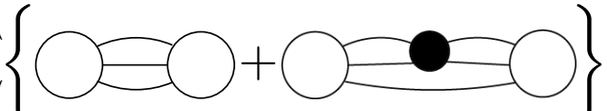
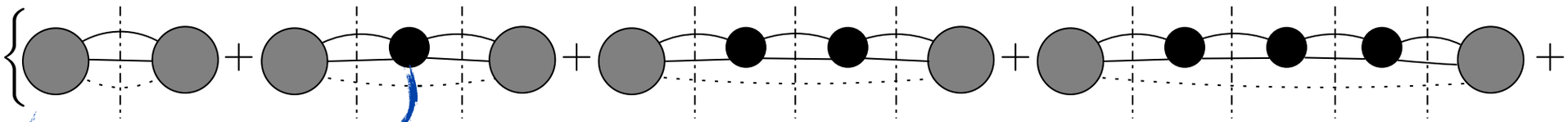
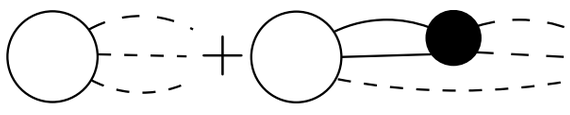
$C_L^{(1)} = \frac{1}{L^3}\sum_{\vec{k}} \frac{1}{2\omega_k}\Big\{$  $\Big\}$

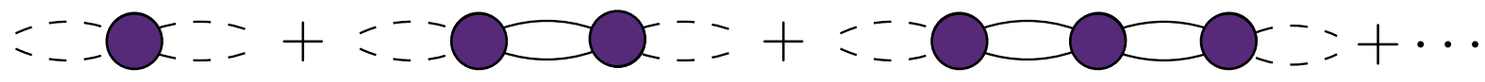
bottom propagator replaced with $1/(2\omega_k)$

Next substitute  and regroup by F-cuts

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

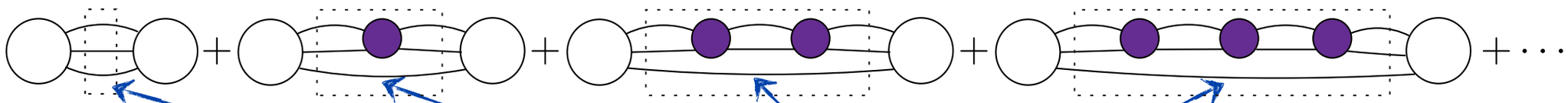
$+ \frac{1}{L^3}\sum_{\vec{k}} \frac{1}{2\omega_k}\Big\{$  $\Big\}$

$=$ 

$=$ 

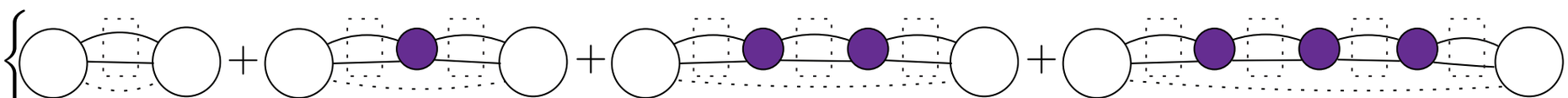
$= i\mathcal{M}_{2\to 2}$

First Part: Sum "no-switch" diagrams

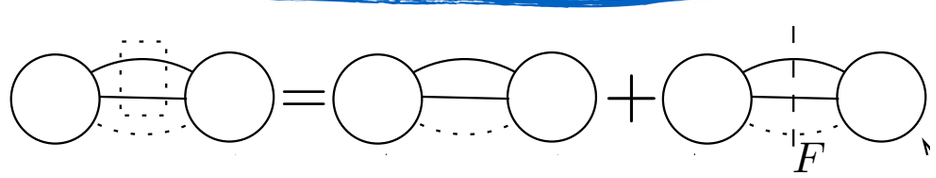
$C_L^{(1)} \equiv$ 

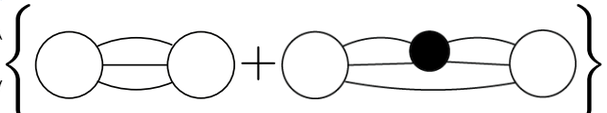
call the bottom momentum k

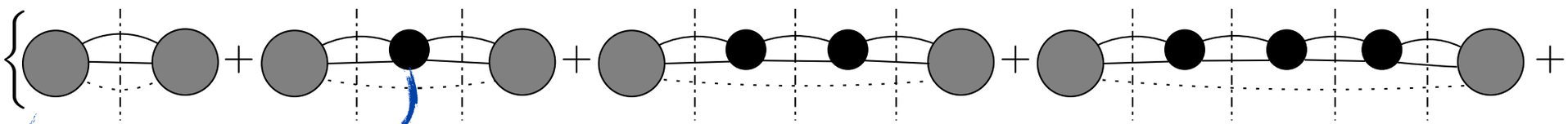
important finite-volume corrections only arise from $k^0 = \omega_k$

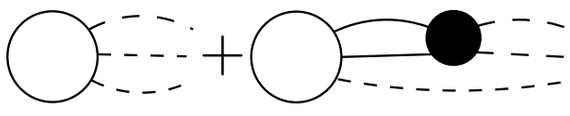
$C_L^{(1)} = \frac{1}{L^3}\sum_{\vec{k}} \frac{1}{2\omega_k}\Big\{$  $\Big\}$

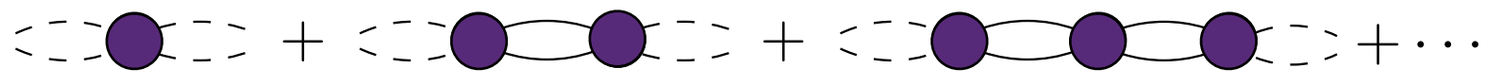
bottom propagator replaced with $1/(2\omega_k)$

Next substitute  and regroup by F-cuts

$C_L^{(1)} = \frac{1}{L^3}\sum_{\vec{k}}\Big\{$  $\Big\}$ **Can this be replaced with an integral?** **No!**

$+ \frac{1}{L^3}\sum_{\vec{k}} \frac{1}{2\omega_k}\Big\{$  $\Big\}$

$=$ 

$=$ 

$= i\mathcal{M}_{2\to 2}$

Main Lesson Number 1: Cusp effects

$$\frac{1}{L^3}\sum_{\vec{k}} f(\vec{k}) = \int_{\vec{k}} f(\vec{k}) + \mathcal{O}(e^{-mL})$$

only holds if $f(\vec{k})$ is an infinitely differentiable function with width $\sim m$.

$C_\infty^{(1)}(\vec{k}) \equiv$

has a unitary cusp at threshold

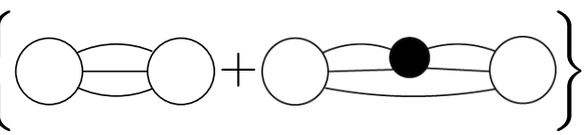
$$(E-\omega_k)^2 - (\vec{P}-\vec{k})^2 = 4m^2$$

To remove cusp

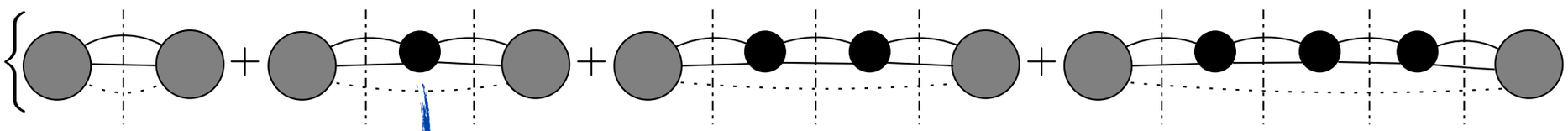
$i\epsilon$ prescription → principal value $\widetilde{\mathrm{PV}}$

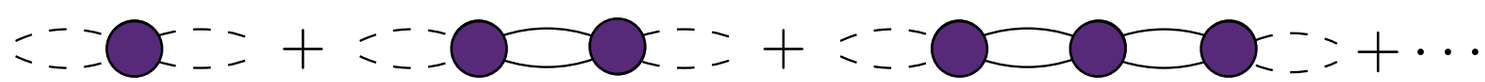
(analytically continue below threshold, then interpolate to standard subthreshold form)

Polejaeva, K. and Rusetsky, A. *Eur. Phys. J.* A48 (2012) 67

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

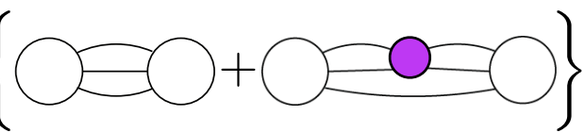
Can this be replaced with an integral? No!

$$+\frac{1}{L^3}\sum_{\vec{k}}\frac{1}{2\omega_k}\Big\{$$  $$+\cdots\Big\}$$

$$=$$  $$+\cdots$$

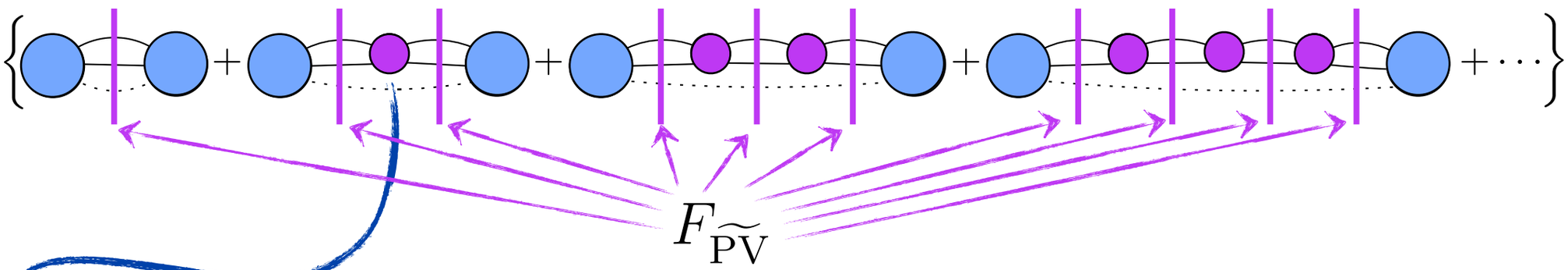
$$= i\mathcal{M}_{2\to 2}$$

$$C_L^{(1)} = \frac{1}{L^3}\sum_{\vec{k}}$$

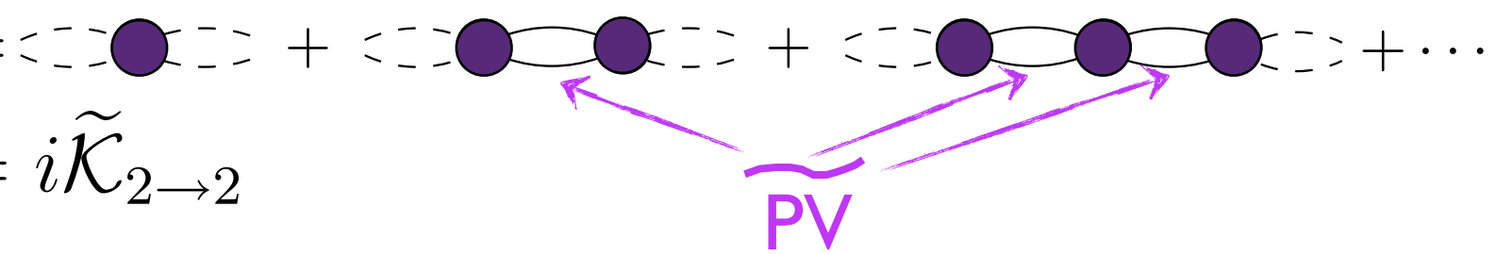


But if we change pole prescription, then we can make the replacement

$$+\frac{1}{L^3}\sum_{\vec{k}}\frac{1}{2\omega_k}$$



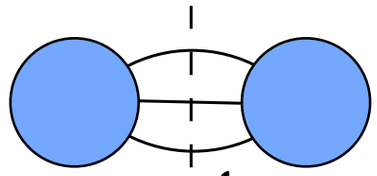
$$= i\widetilde{\mathcal{K}}_{2\to 2}$$



All three-particle poles now have principal-value prescription

Deduce

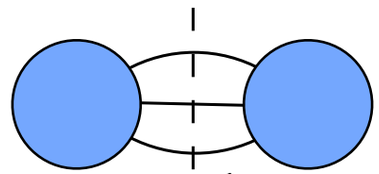
$$C_L^{(1)} = \widetilde{C}_\infty^{(1)} +$$



$$[\mathcal{A}] \equiv \frac{iF_{\widetilde{\mathrm{PV}}}}{2\omega L^3} \frac{1}{1 + \widetilde{\mathcal{K}}_{2\to 2} F_{\widetilde{\mathrm{PV}}}}$$

think of this as a new cut,
like F it puts neighbors on-shell

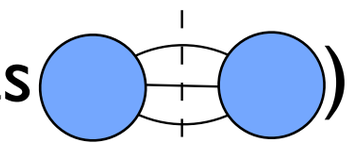
Deduce

$$C_L^{(1)} = \widetilde{C}_\infty^{(1)} +$$ 

$$[\mathcal{A}] \equiv \frac{iF_{\widetilde{\mathrm{PV}}}}{2\omega L^3} \frac{1}{1+\widetilde{\mathcal{K}}_{2\to 2} F_{\widetilde{\mathrm{PV}}}}$$

think of this as a new cut, like F it puts neighbors on-shell

Main Lesson Number 2: Matrix structure

Finite volume residue terms (such as ) are of the form:

(row vector)x(matrix)x(column vector), acting on product space

[finite-volume momentum]x[angular momentum]

For example, $[\mathcal{A}]$ is built from

$$F_{\widetilde{\mathrm{PV}};k',\ell',m';k,\ell,m} \equiv \delta_{k',k}\, F_{\widetilde{\mathrm{PV}};\ell',m';\ell,m}(E-\omega_k, \vec{P}-\vec{k}) \qquad \vec{k}=\vec{k}' \in (2\pi/L)\mathbb{Z}^3$$

$$\widetilde{\mathcal{K}}_{2\to 2;k',\ell',m';k,\ell,m} \equiv \delta_{k',k}\, \widetilde{\mathcal{K}}_{2\to 2;\ell',m';\ell,m}(E-\omega_k, \vec{P}-\vec{k})$$

Deduce

$$C_L^{(1)} = \widetilde{C}_\infty^{(1)} + \quad \mathcal{A} \qquad [\mathcal{A}] \equiv \frac{iF_{\widetilde{\mathrm{PV}}}}{2\omega L^3} \frac{1}{1 + \widetilde{\mathcal{K}}_{2\to 2} F_{\widetilde{\mathrm{PV}}}}$$

think of this as a new cut,
like F it puts neighbors on-shell

Main Lesson Number 2: Matrix structure

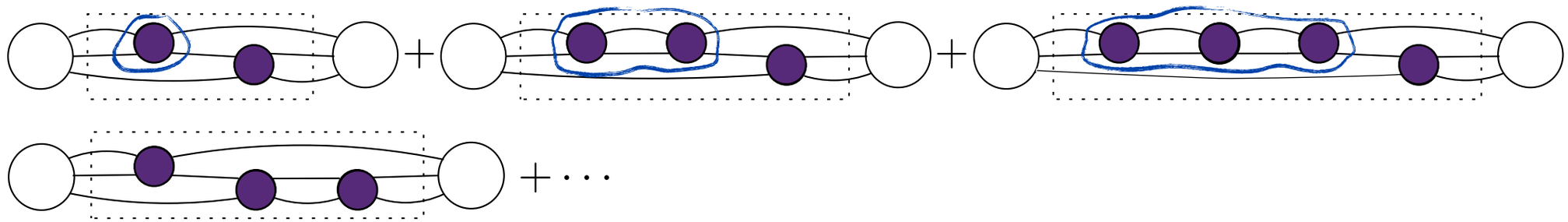
Finite volume residue terms (such as) are of the form:

(row vector)x(matrix)x(column vector), acting on product space

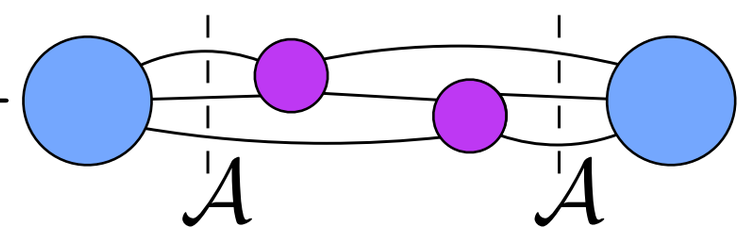
[finite-volume momentum]x[angular momentum]

Observe that $\vec{k}, \ell, m$ parametrizes three particles with fixed $(E, \vec{P})$

Second part: Sum "one-switch" diagrams

$C_L^{(2)} =$ 

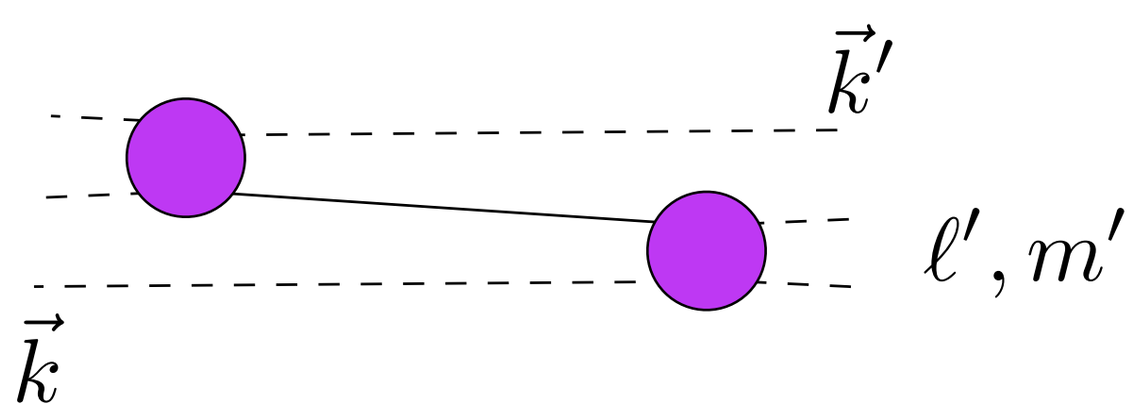
In this case we have two "spectator-momenta"
(momenta that do not appear in two-particle loops)

$C_L^{(2)} = \widetilde{C}_\infty^{(2)} +$ 

$+ \cdots$

stands for terms that modify endcaps of $C_L^{(1)}$

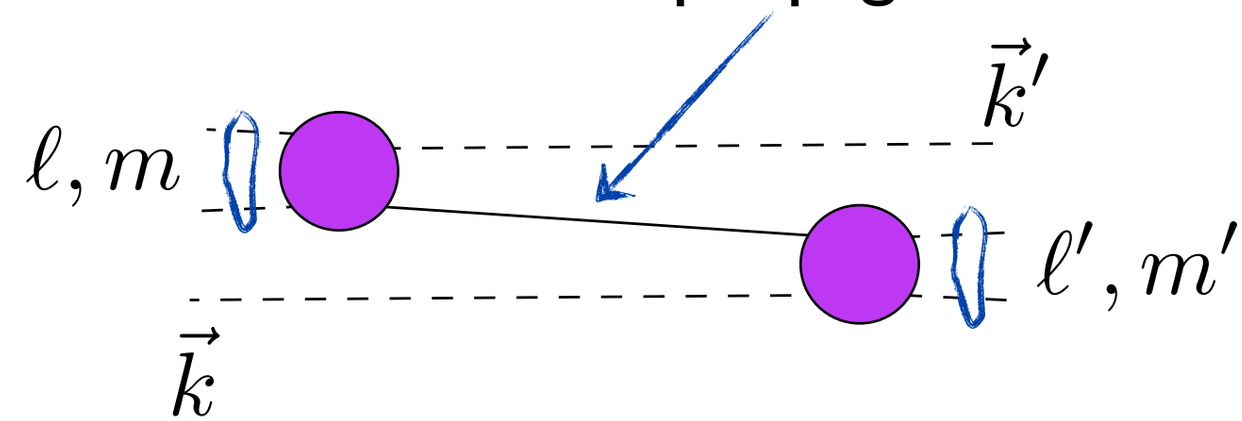
Between $\mathcal{A}$ factors we have first contribution to three-to-three scattering

$i\widetilde{\mathcal{K}}^{(2,\mathrm{unsym})}_{3\to 3;k',\ell',m';k,\ell,m} \equiv$ 

Main Lesson Number 3: On-shell divergences

Certain external moment put the intermediate propagator on-shell

$$i\widetilde{\mathcal{K}}^{(2,\mathrm{unsym})}_{3\to3;k',\ell',m';k,\ell,m} \equiv$$



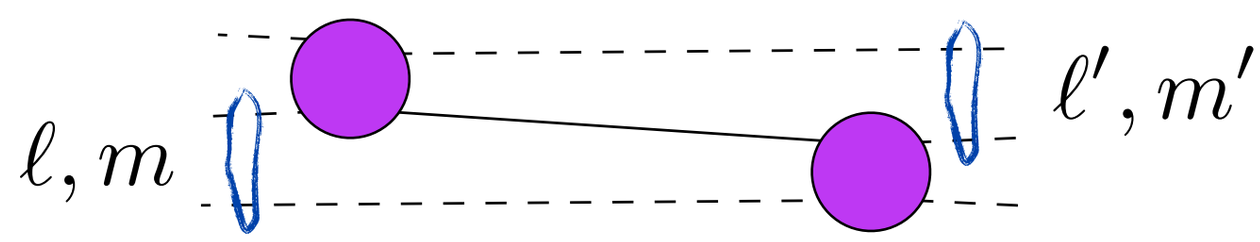
This implies that this diagram, and indeed also the full

$i\widetilde{\mathcal{K}}_{3\to3}$ **has physical singularities above threshold**

nothing to do with bound states

This is a problem because K-matrix is symmetric in external momenta

$$i\widetilde{\mathcal{K}}_{3\to3;k',\ell',m';k,\ell,m} \overset{!}{\supset}$$

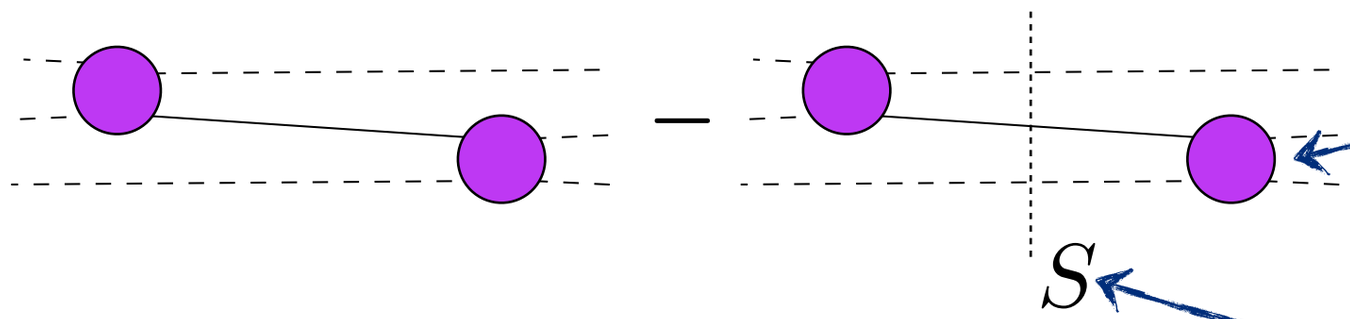


But this would demand decomposing a singular function in $Y_{\ell,m}$

The decomposition is not valid!

Resolution: Introduce

$$i\widetilde{\mathcal{K}}^{(2,\mathrm{unsym})}_{df,3\to3} \equiv i\widetilde{\mathcal{K}}^{(2,\mathrm{unsym})}_{3\to3} - i\widetilde{\mathcal{K}}_{2\to2} S i\widetilde{\mathcal{K}}_{2\to2}$$



on-shell

represents simple kinematic pole factor

$i\widetilde{\mathcal{K}}_{df,3\to3}$ is finite:

Can decompose in harmonics and truncate expansion at low energies

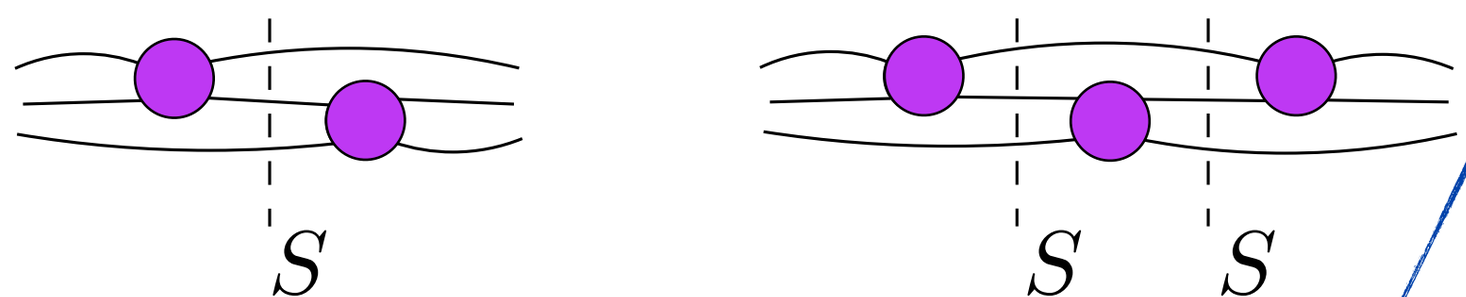
The approach of separating out singularities like this was first suggested over 40 years ago (Rubin et al. *PR 146-6* (1966))

It makes sense to recover singularity-free quantity from finite-volume spectrum.
Then add singular terms back in.

This pattern of separating out singularities persists to all orders

Define

$$i\widetilde{\mathcal{K}}_{df,3\to3} \equiv i\widetilde{\mathcal{K}}_{3\to3} - \left[i\widetilde{\mathcal{K}}_{2\to2} S i\widetilde{\mathcal{K}}_{2\to2} + \int i\widetilde{\mathcal{K}}_{2\to2} S i\widetilde{\mathcal{K}}_{2\to2} S i\widetilde{\mathcal{K}}_{2\to2} + \cdots \right]$$



only on-shell amplitudes here

infinite series built with factors of $S i\widetilde{\mathcal{K}}_{2\to2}$

Definition arises from analyzing all two-to-two diagrams

$$i\widetilde{\mathcal{K}}_{df,3\to3;k',\ell',m';k,\ell,m}$$

is the natural observable to extract from the finite-volume spectrum

Review Lessons

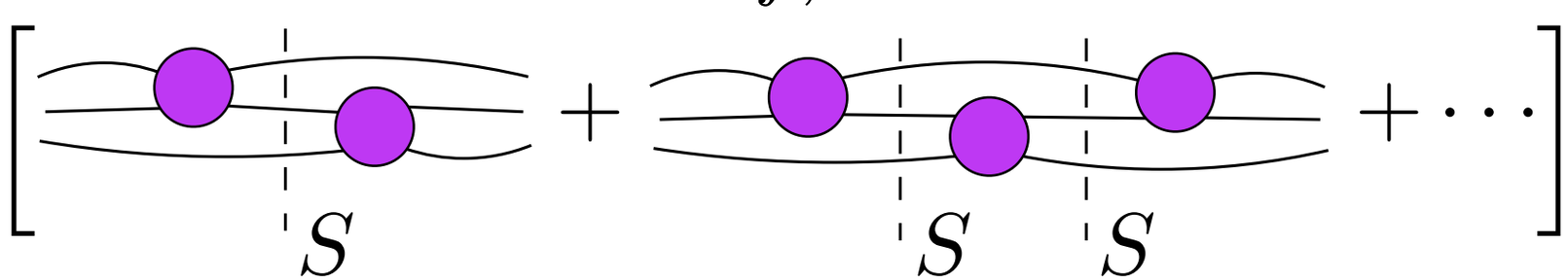
1. Need modified principal value to remove cusp effects

2. In the three particle case, all matrices act on product space
[finite-volume momentum]x[angular momentum]
In other words, they have indices $\vec{k}, \ell, m$

needed to describe three particles

3. Singularities in $i\widetilde{\mathcal{K}}_{3\to 3}$ invalidate decomposition in $Y_{\ell,m}$
Resolution is to introduce $i\widetilde{\mathcal{K}}_{df,3\to 3}$

$i\widetilde{\mathcal{K}}_{df,3\to 3} \equiv i\widetilde{\mathcal{K}}_{3\to 3} -$



This object arises naturally in finite-volume analysis.

Intro- and Two-Particle Material

What can we extract from LQCD?

We are trying to evaluate a difficult integral numerically

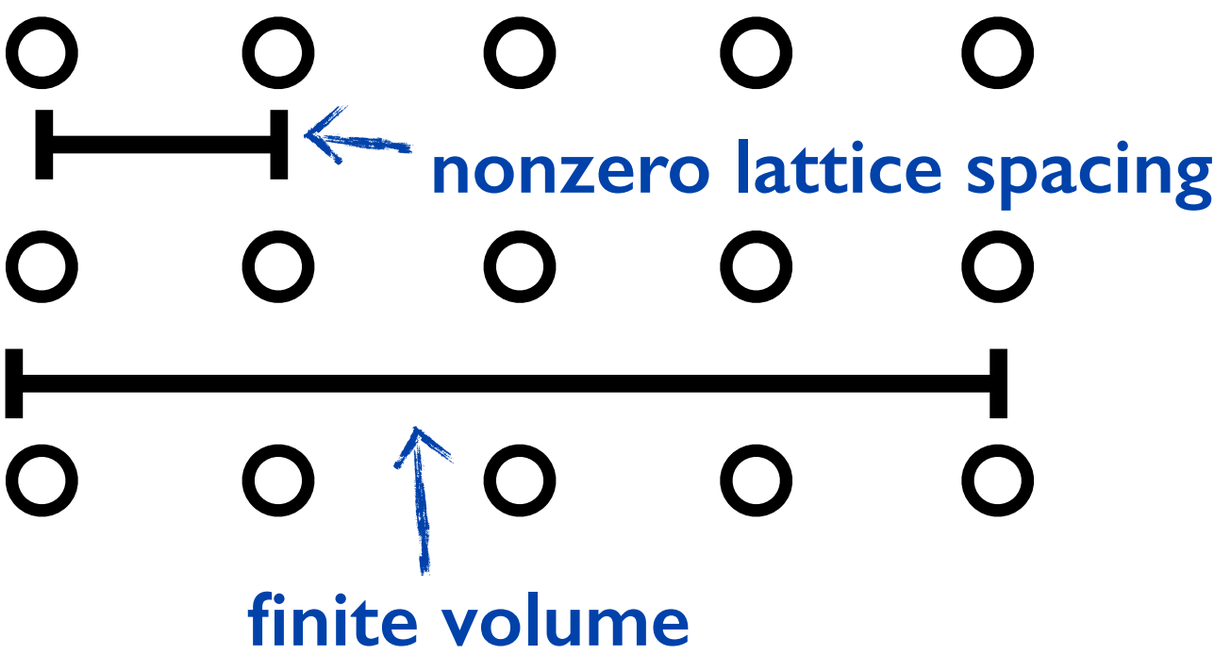
$$\langle T\phi_1 \cdots \phi_n \rangle = \int \mathcal{D}\phi \, e^{iS} \, \phi_1 \cdots \phi_n$$

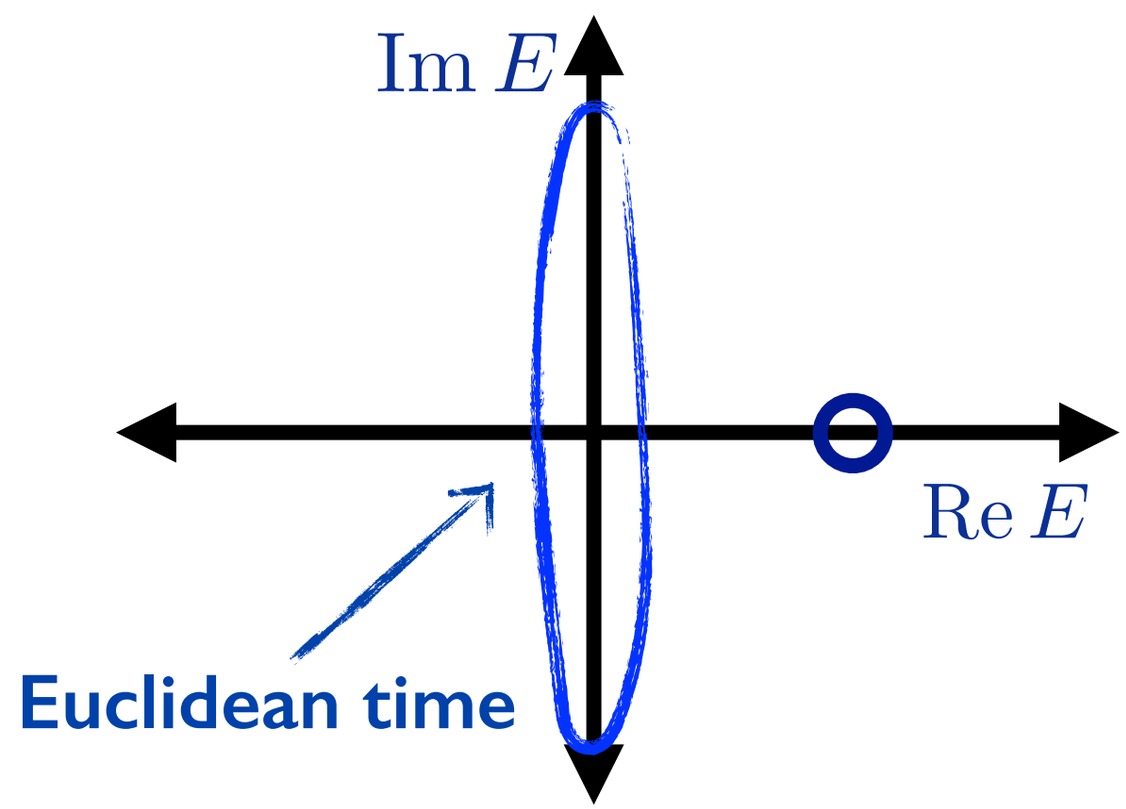
What can we extract from LQCD?

We are trying to evaluate a difficult integral numerically

$$\langle T\phi_1 \cdots \phi_n \rangle_{\text{Euc, latt, fv}} = \int \prod_i^N d\phi_i \, e^{-S} \, \phi_1 \cdots \phi_n$$

To do so we have to make three compromises





What can we extract from LQCD?

Not possible to directly calculate

$\langle \pi\pi | \pi\pi \rangle$

$\langle \pi\pi\pi | \pi\pi\pi \rangle$

$\langle K\pi\pi | \mathcal{J} | B \rangle$

$\langle \pi\pi | \mathcal{H} | K \rangle$

$\langle \pi\pi | \mathcal{J} | \pi \rangle$

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$\langle \pi\pi | \mathcal{H} | K \rangle$

$\langle \pi\pi | \mathcal{J} | \pi \rangle$

$\langle K\pi | \mathcal{J} | B \rangle$

multi-particle in- and outstates

What can we extract from LQCD?

Not possible to directly calculate

$\langle \pi\pi | \pi\pi \rangle$ $\langle \pi\pi\pi | \pi\pi\pi \rangle$

$\langle \pi\pi | \mathcal{H} | K \rangle$ $\langle \pi\pi | \mathcal{J} | \pi \rangle$ $\langle K\pi\pi | \mathcal{J} | B \rangle$ $\langle K\pi | \mathcal{J} | B \rangle$

multi-particle in- and outstates

$\langle \pi\pi | \pi\pi \rangle =$ Amputate and put on-shell $\langle 0 | \tilde{\pi}(p')\tilde{\pi}(k') \; \tilde{\pi}(p)\tilde{\pi}(k) | 0 \rangle$

$\langle \pi\pi | \mathcal{H} | K \rangle =$ Amputate and put on-shell $\langle 0 | \tilde{\pi}(p')\tilde{\pi}(k') \; \mathcal{H}(x) \; \tilde{K}(P) | 0 \rangle$

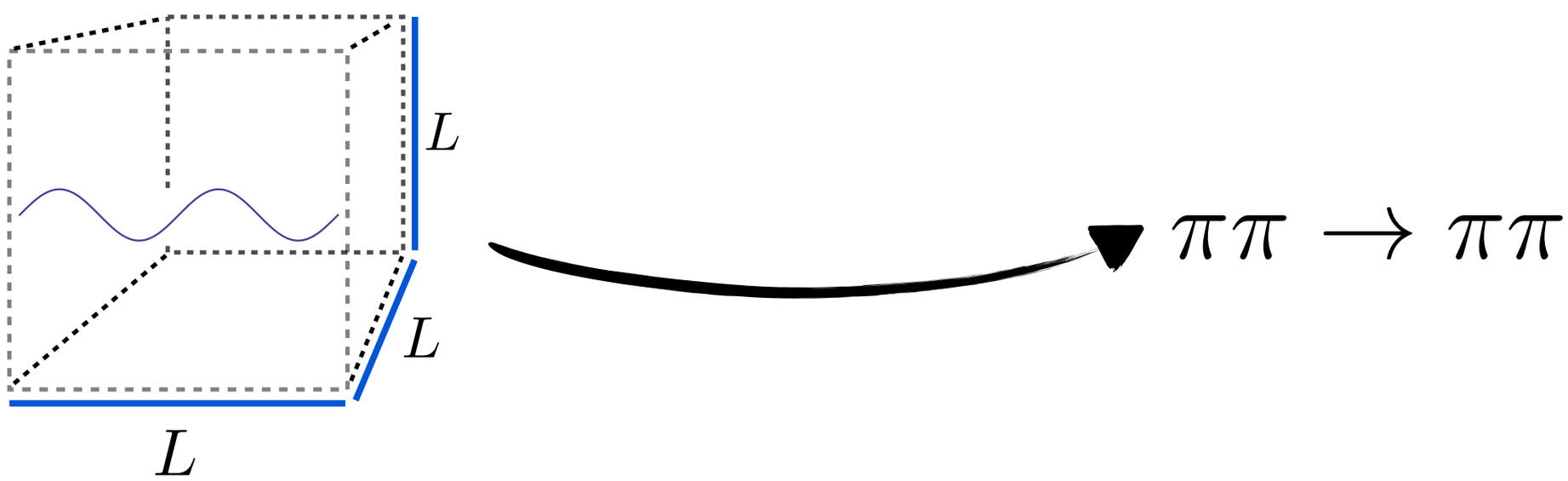
Requires Minkowski momenta and infinite-volume

In 1991 **M. Lüscher** found a method to circumvent this issue and extract $\pi\pi \to \pi\pi$ scattering from LQCD.

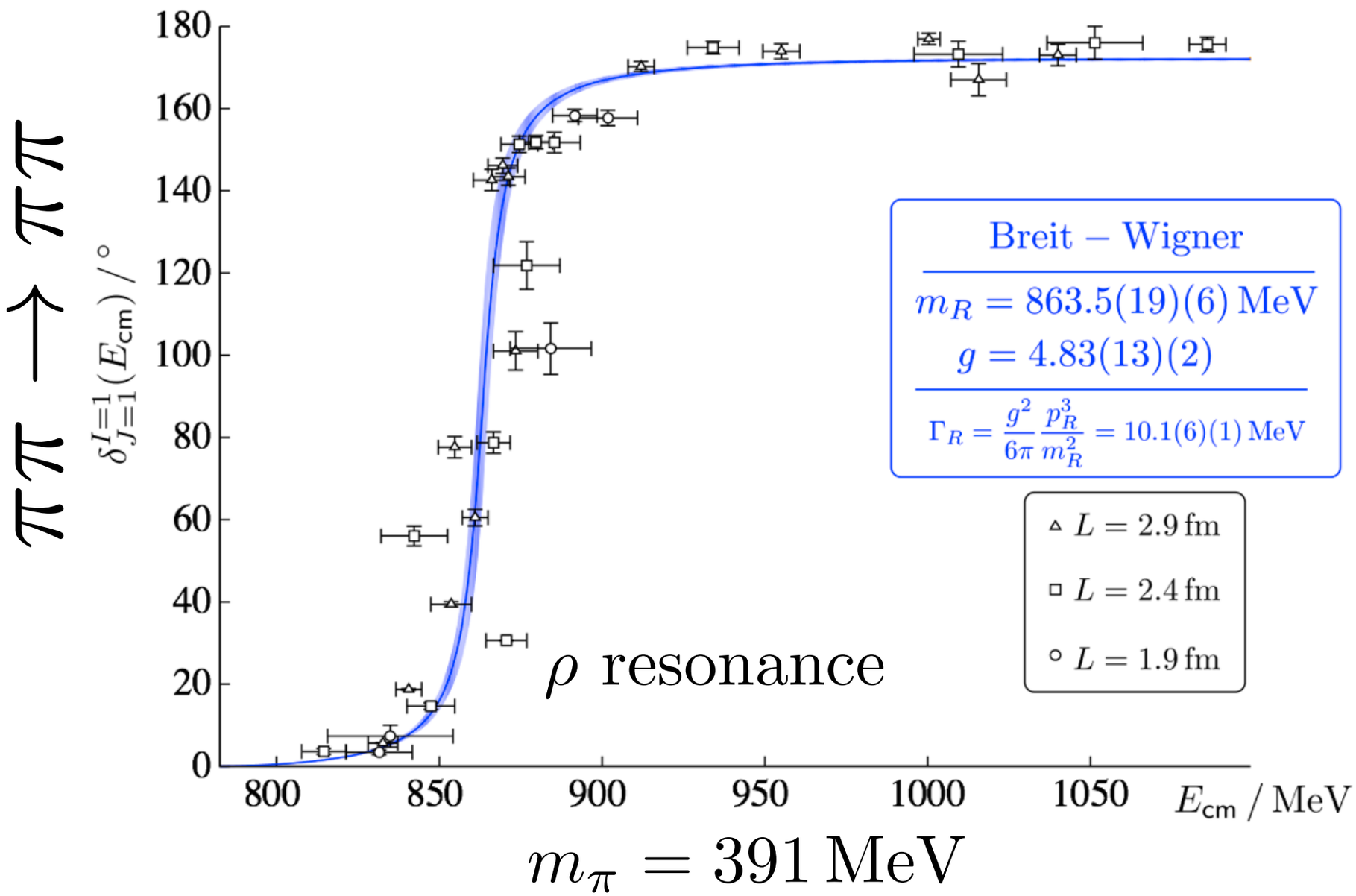
Lüscher, M. *Nucl. Phys* B354, 531-578 (1991)

His key insight was to **use finite-volume as a tool**.

He gave a mapping between **finite-volume spectrum** and **elastic pion scattering amplitude**.



Lüscher's method has led to a large body of work extracting phase shifts from Lattice QCD.



from Dudek, Edwards, Thomas in *Phys.Rev.* D87 (2013) 034505

However, there is **no general method** for extracting scattering amplitudes involving **more than two hadrons**.

As a result LQCD cannot investigate...

However, there is **no general method** for extracting scattering amplitudes involving **more than two hadrons**.

As a result LQCD cannot investigate...

resonances which decay into more than two hadrons

$$\omega(782) \to \pi\pi\pi \qquad N(1440) \to N\pi\pi$$

three-body forces

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

However, there is **no general method** for extracting scattering amplitudes involving **more than two hadrons**.

As a result LQCD cannot investigate...

weak decays coupled to channels containing more than two hadrons

$K \to \pi\pi\pi$ $\quad$ $D \to \pi\pi$ $\quad$ $D \to K\overline{K}$

(couples to $\pi\pi\pi\pi$)

Need strong scattering to relate lattice weak matrix elements to physical decay amplitudes

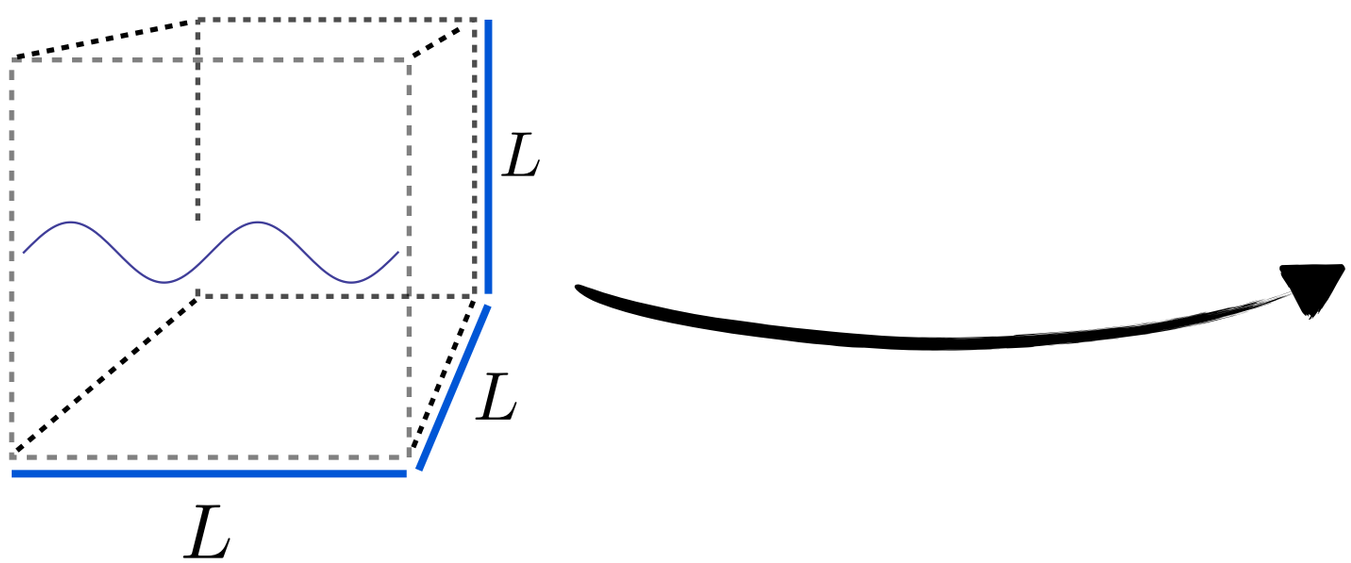
Lellouch, L. & Lüscher, M.
Commun. Math. Phys. 219, 31-44 (2001)

In recent years important progress has been made towards extracting three-particle scattering.

Polejaeva, K. and Rusetsky, A. *Eur. Phys. J.* A48 (2012) 67
Briceno, R. A. and Davoudi, Z. *Phys. Rev.* D87 (2013) 094507

However a relativistic, model-independent method is still unknown.

This is the focus of today's talk.



$$\pi\pi \to \pi\pi$$
$$\pi\pi\pi \to \pi\pi\pi$$

Outline

Detailed set-up

Two particles in a box

Three particles in a box

Conclusion

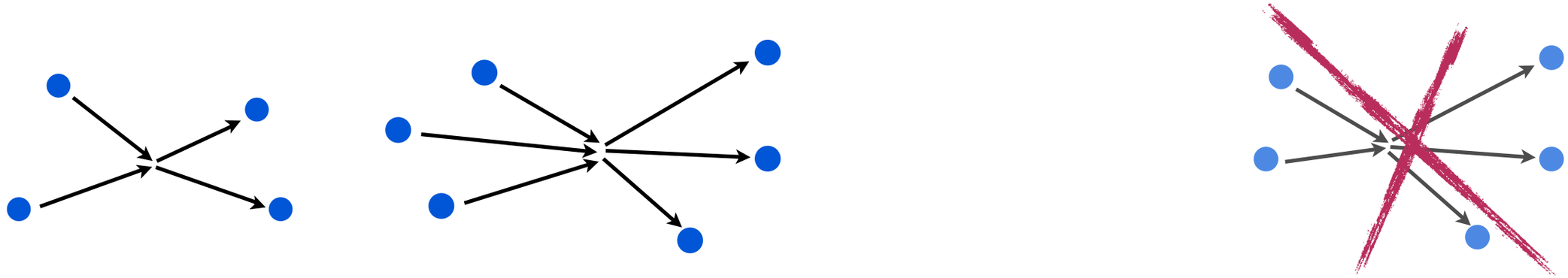
Particle content

Single scalar, mass m

all results for identical scalars

Relativistic field theory

$\mathbb{Z}_2$ **symmetry**

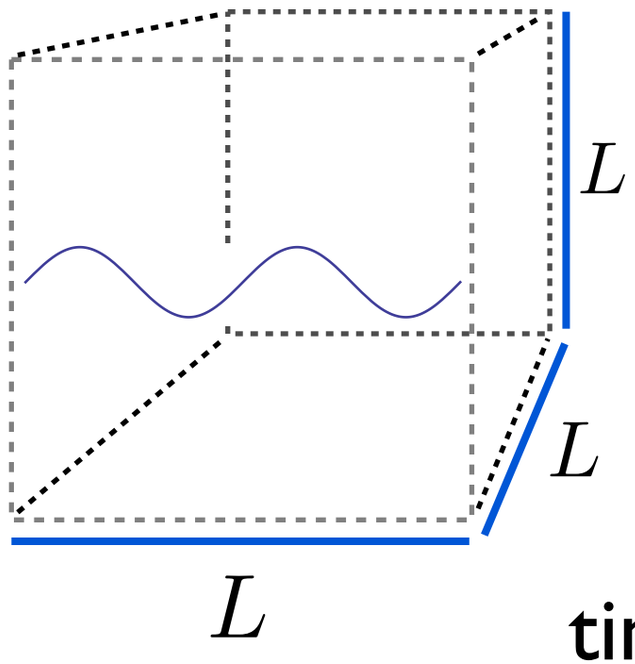


(For pions in QCD this is G-parity)

Include all vertices

with even number of legs

Finite volume



cubic, spatial volume (extent L)

periodic boundary conditions

$$\vec{p} \in (2\pi/L)\mathbb{Z}^3$$

time direction **infinite** and **Minkowski**

Take L large enough to ignore e^{-mL}

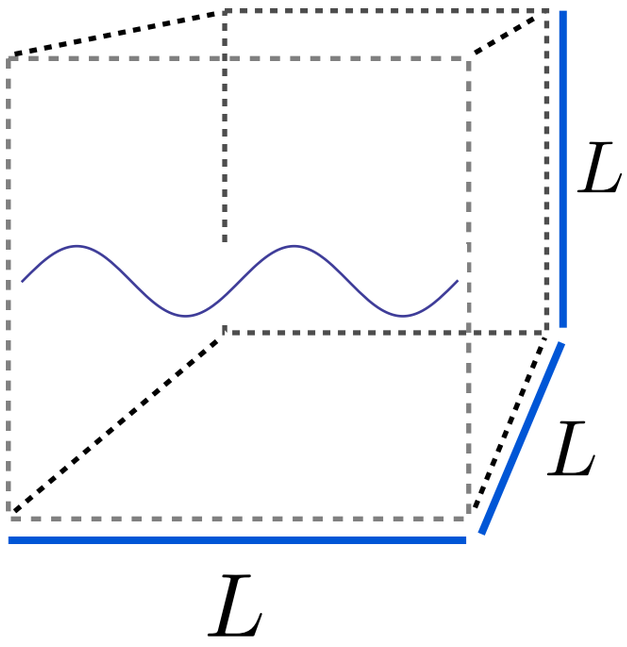
dropped throughout!

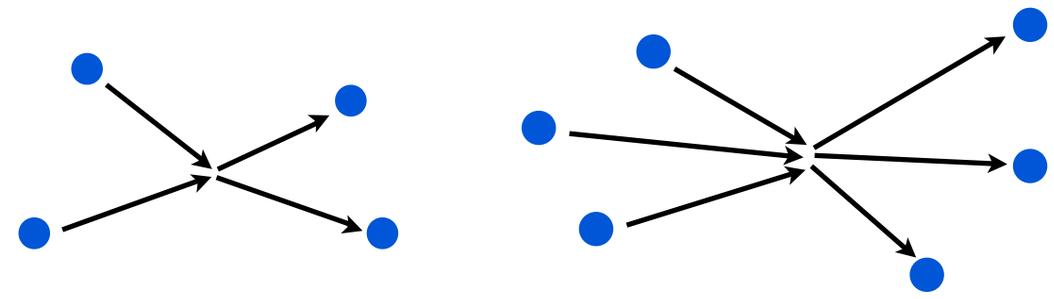
Take space to be continuous

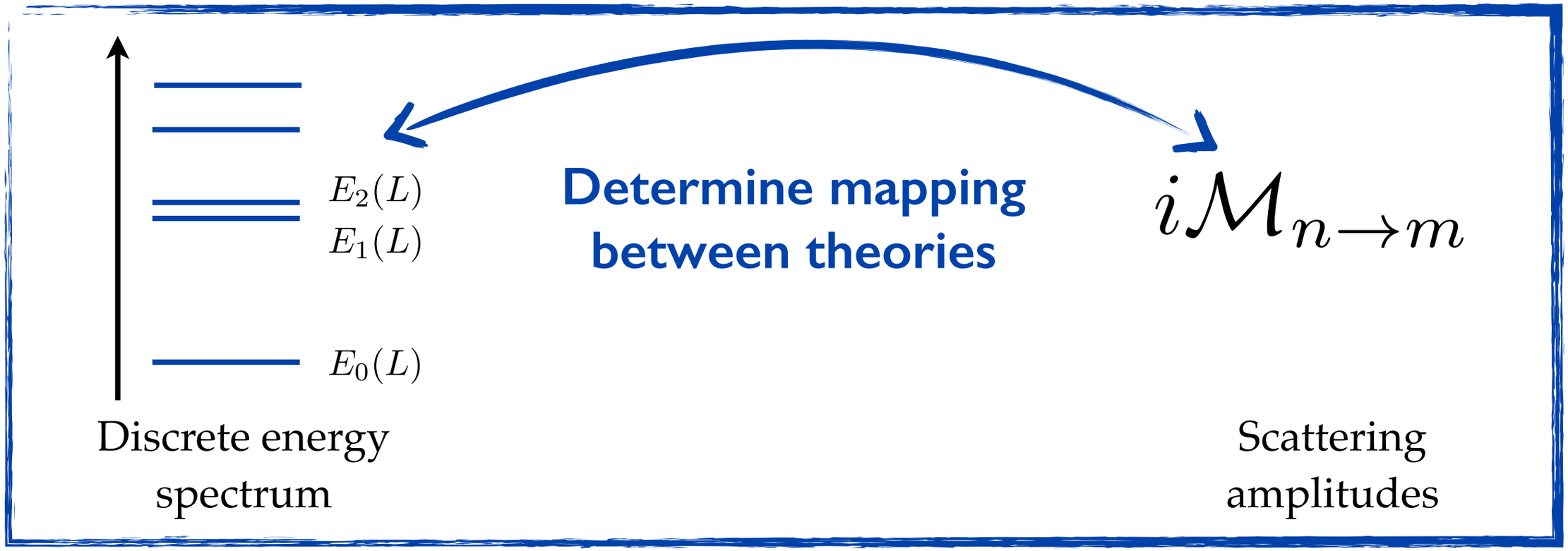
lattice spacing set to zero

Finite volume

Infinite volume







Determine relation using finite-volume correlator

$$C_L(E,\vec{P}) \equiv \int_L d^4x\, e^{i(Ex^0 - \vec{P}\cdot\vec{x})} \langle 0|\mathrm{T}\sigma(x)\sigma^\dagger(0)|0\rangle$$

Determine relation using finite-volume correlator

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energy E, momentum $\vec{P} = (2\pi/L)\vec{n}_P$

CM energy $E^{*2} \equiv E^2 - \vec{P}^2$

interpolating field

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energy E, momentum $\vec{P} = (2\pi/L)\vec{n}_P$

CM energy $E^{*2} \equiv E^2 - \vec{P}^2$

interpolating field

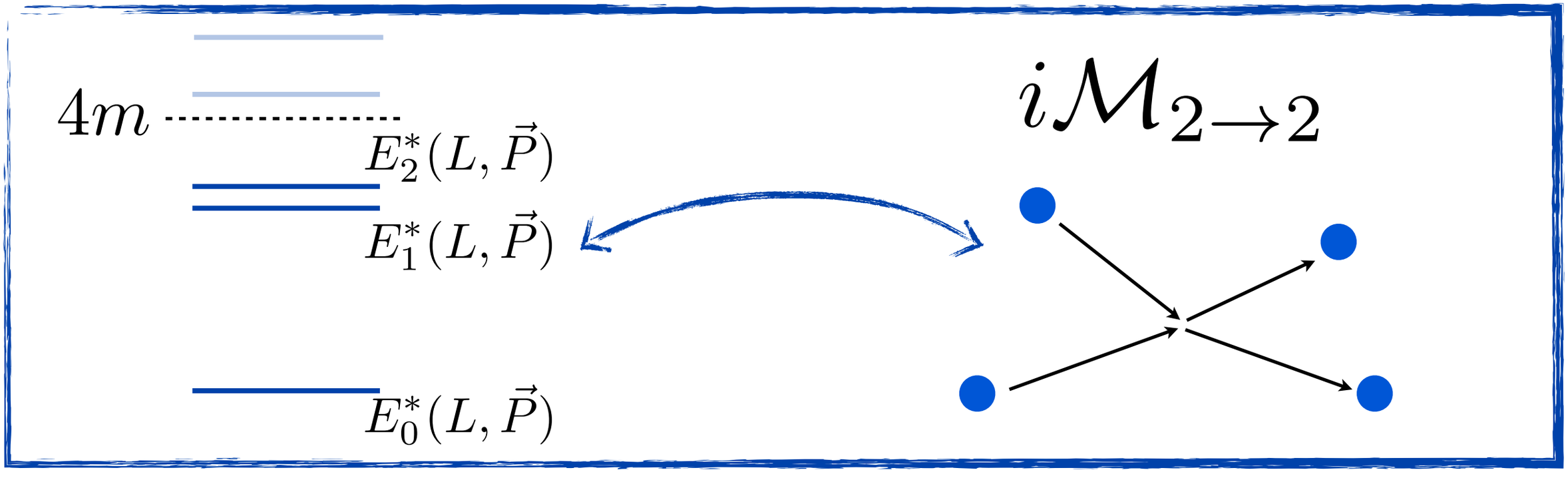
At fixed $L, \vec{P}$, poles in C_L give finite-volume spectrum

We calculate $C_L(E,\vec{P})$ to all orders in perturbation theory and determine condition of divergence.

First, two particles in a box

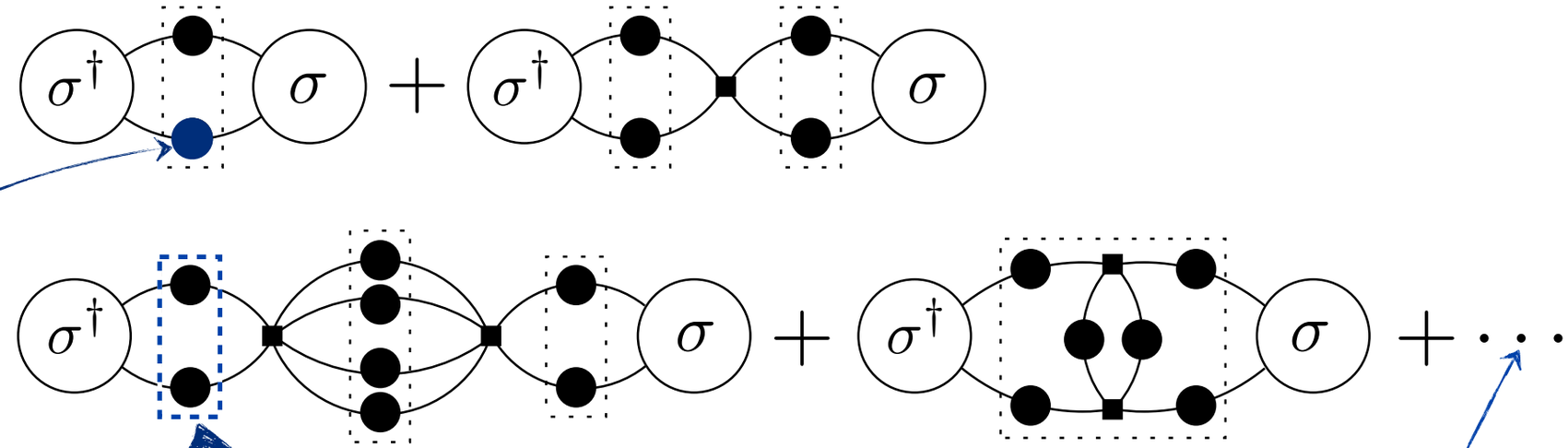
$$C_L(E,\vec{P}) \equiv \int_L d^4x\, e^{i(Ex^0 - \vec{P}\cdot\vec{x})} \langle 0|\mathrm{T}\sigma(x)\sigma^\dagger(0)|0\rangle$$

Require $E^* < 4m$ **even-particle quantum numbers**



Derivation from Kim, Sachrajda and Sharpe. *Nucl. Phys.* B727, 218-243 (2005)

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



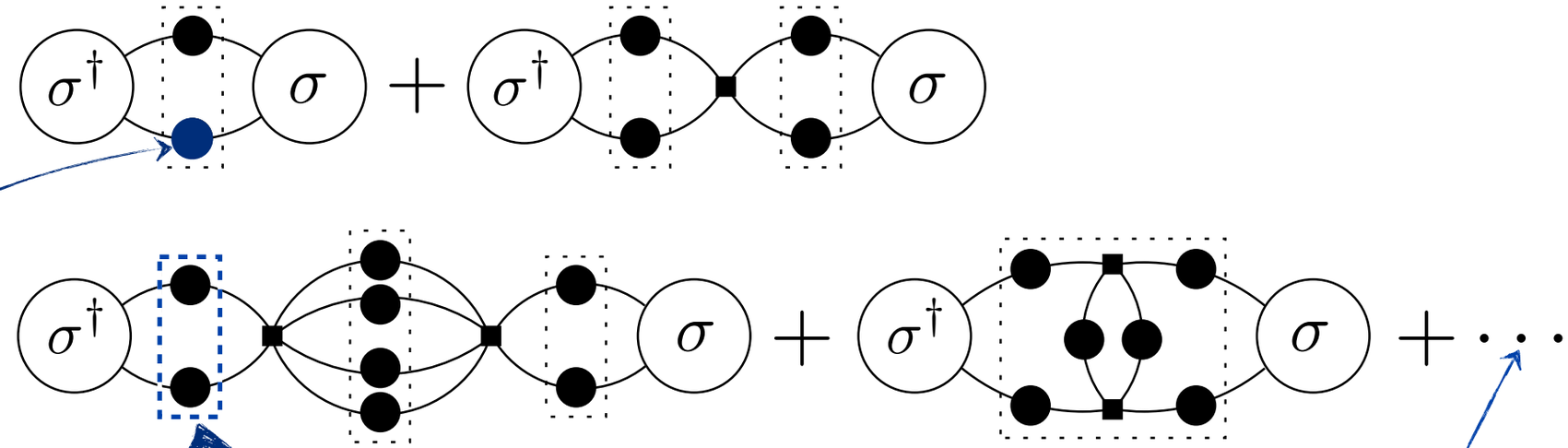
fully dressed propagators

infinite set of terms
no assumed suppression

spatial loop momenta are summed

$$\frac{1}{L^3} \sum_{\vec{k}\in(2\pi/L)\mathbb{Z}^3} \int \frac{dk^0}{2\pi}$$

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



fully dressed propagators

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spatial loop momenta are summed

$$\frac{1}{L^3}\sum_{\vec{k}\in(2\pi/L)\mathbb{Z}^3}\int\frac{dk^0}{2\pi}$$

Key observation:

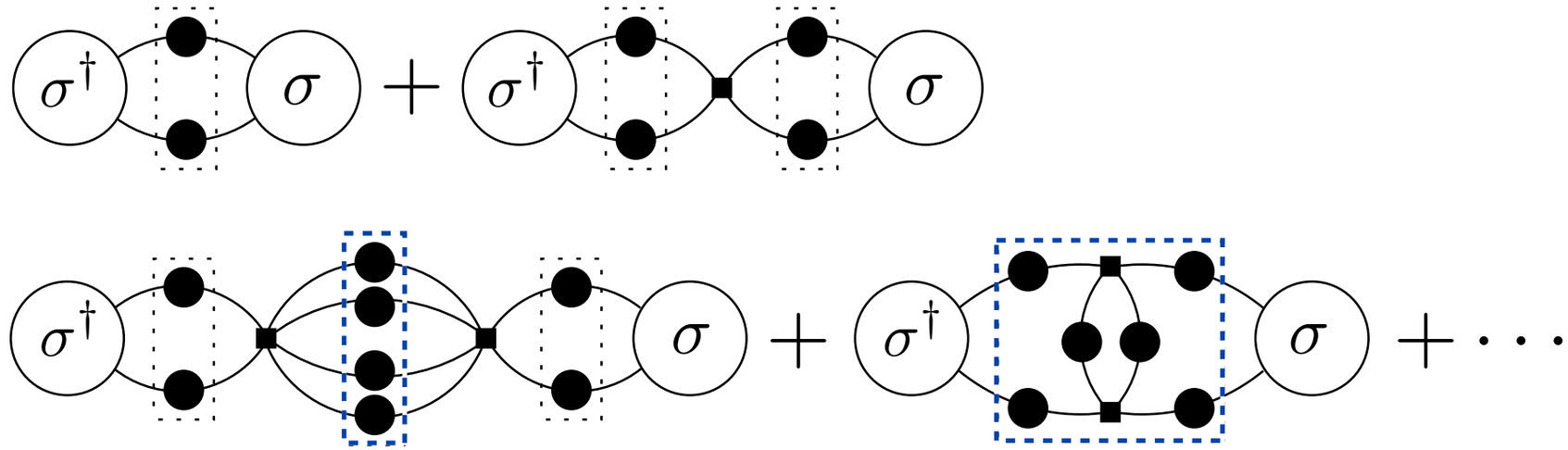
If particles in summed loops cannot all go on shell, then replace

$$\frac{1}{L^3}\sum_{\vec{k}} \longrightarrow \int\frac{d^3k}{(2\pi)^3}$$

difference is order

$$e^{-mL}$$

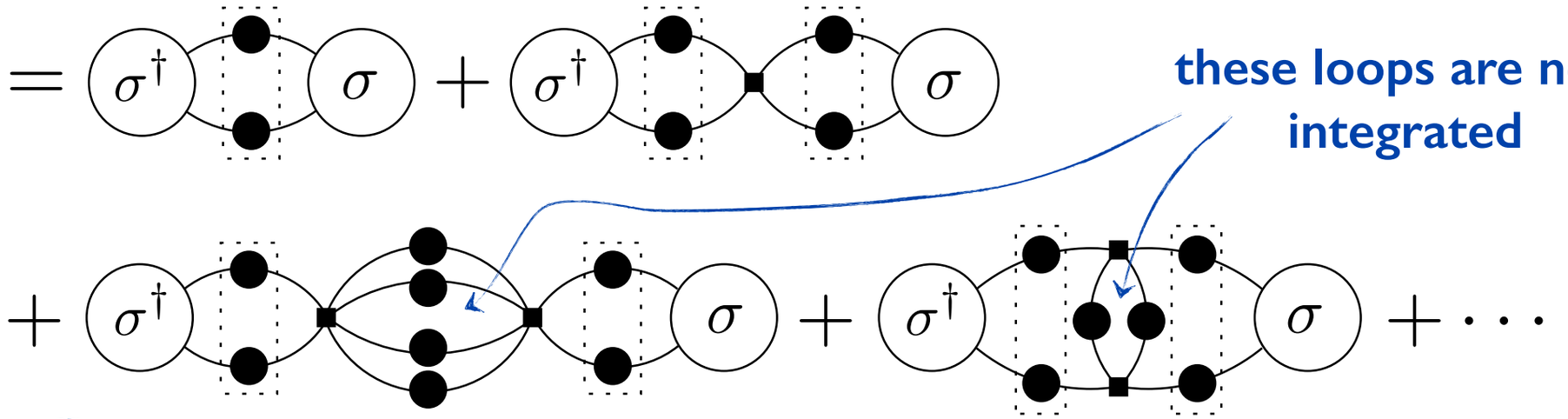
$C_L(E, \vec{P}) \equiv$



$$\frac{1}{L^3}\sum_{\vec{k}} \longrightarrow \int_{\vec{k}} \equiv \int \frac{d^3k}{(2\pi)^3}$$

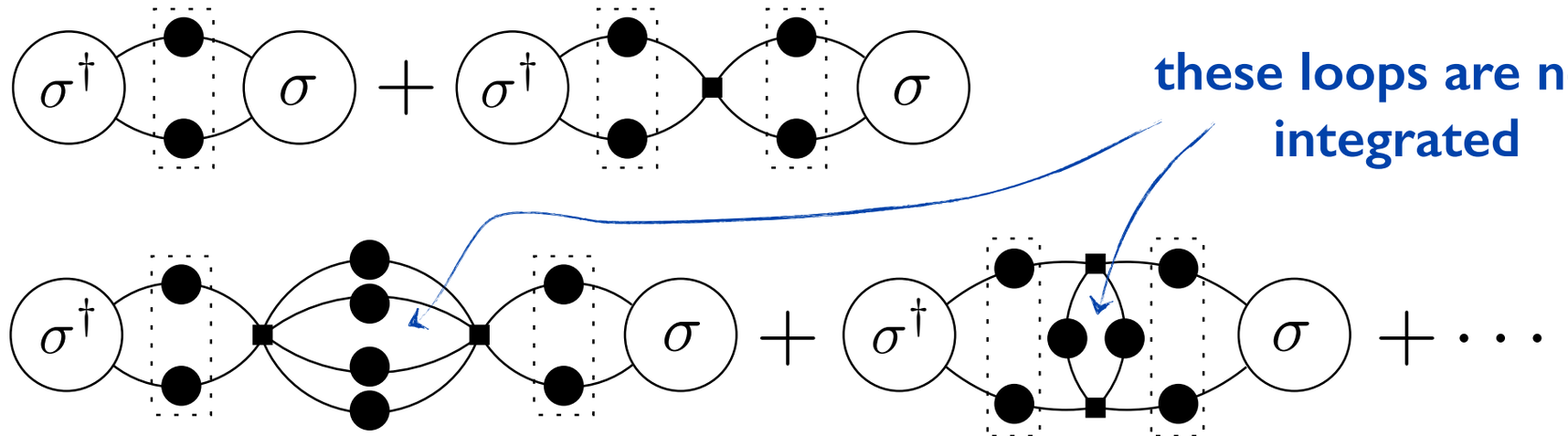
Since $E^* < 4m$, **only two** particles with total momentum $(E, \vec{P})$ **can go on-shell**

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



these loops are now integrated

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



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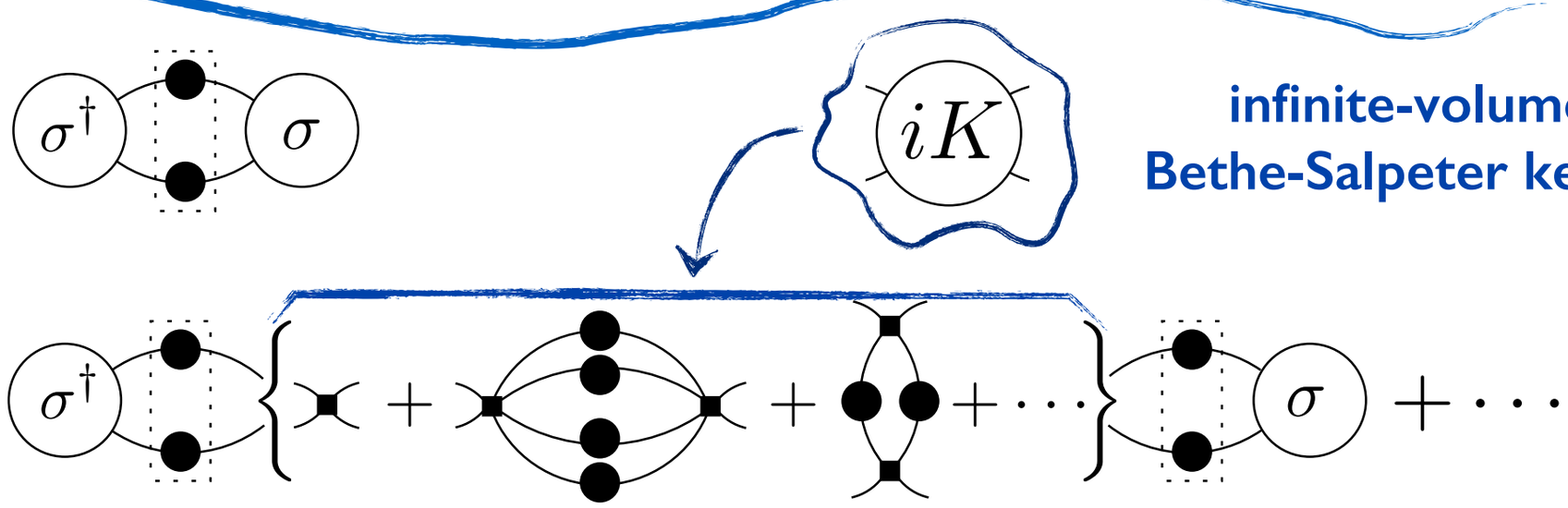
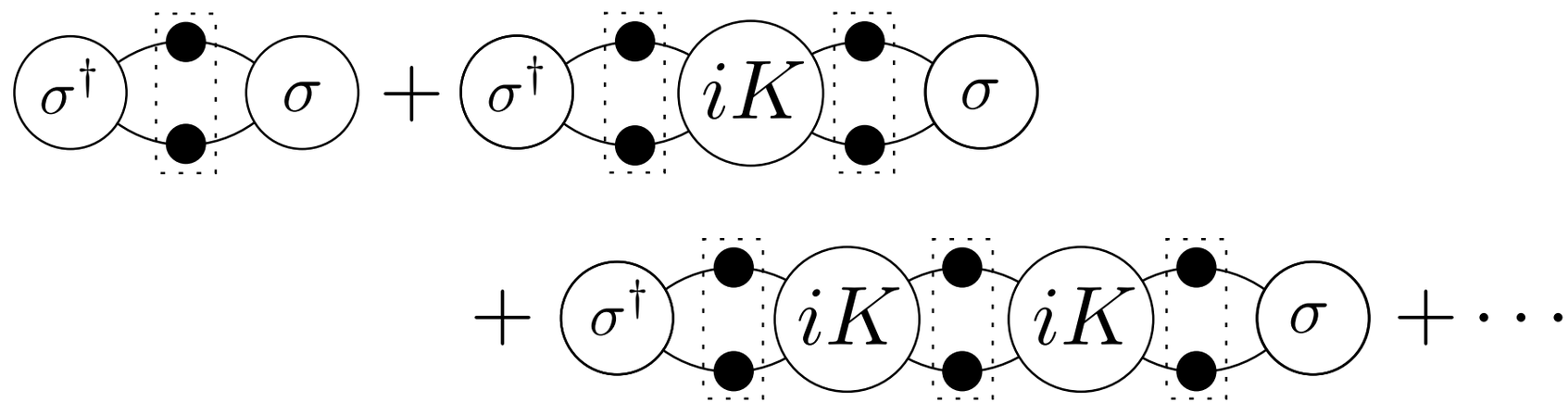
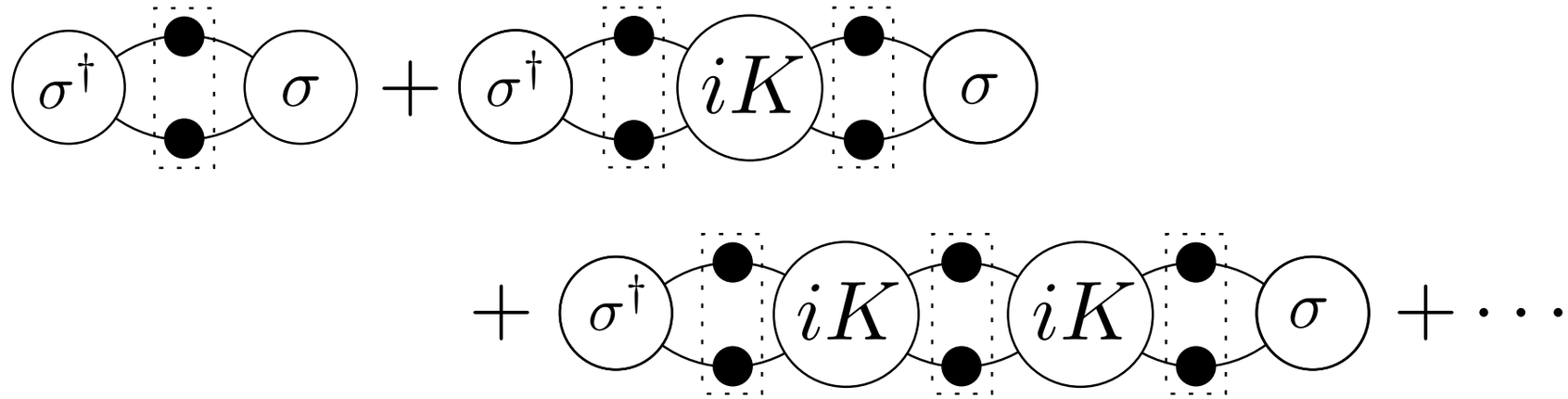


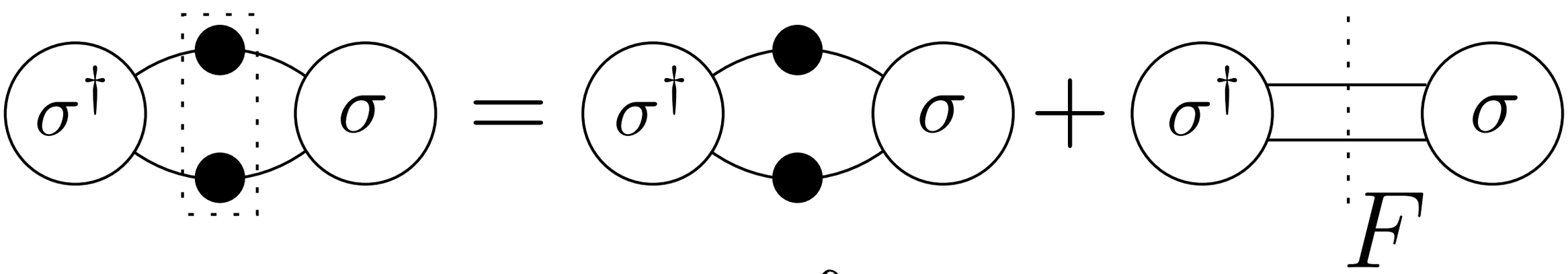
infinite-volume Bethe-Salpeter kernel

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



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

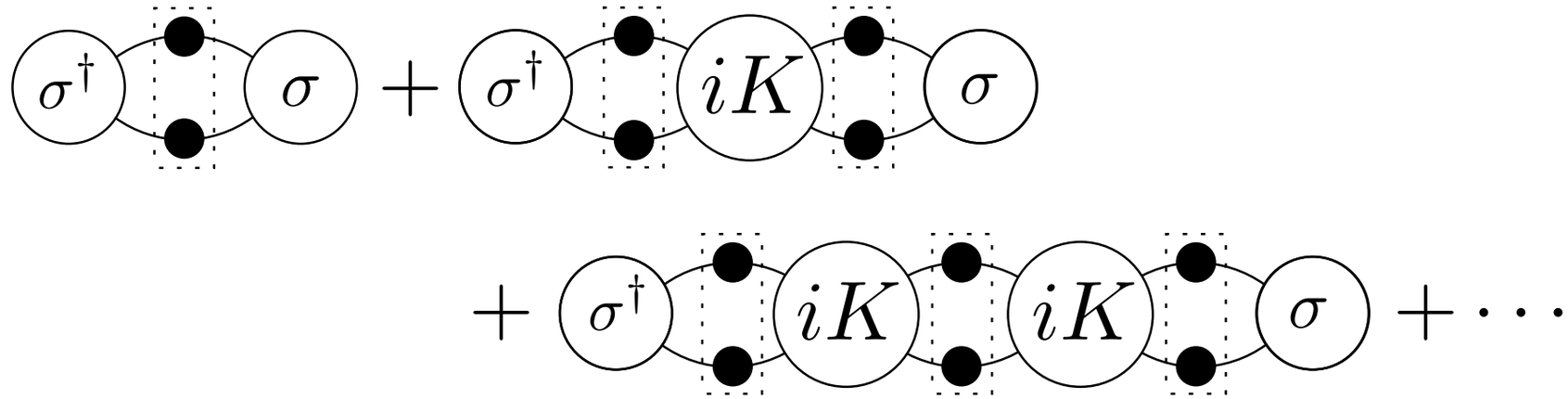
Next we introduce an important identity



$$\frac{1}{L^3}\sum_{\vec{k}} \qquad \int_{\vec{k}}$$

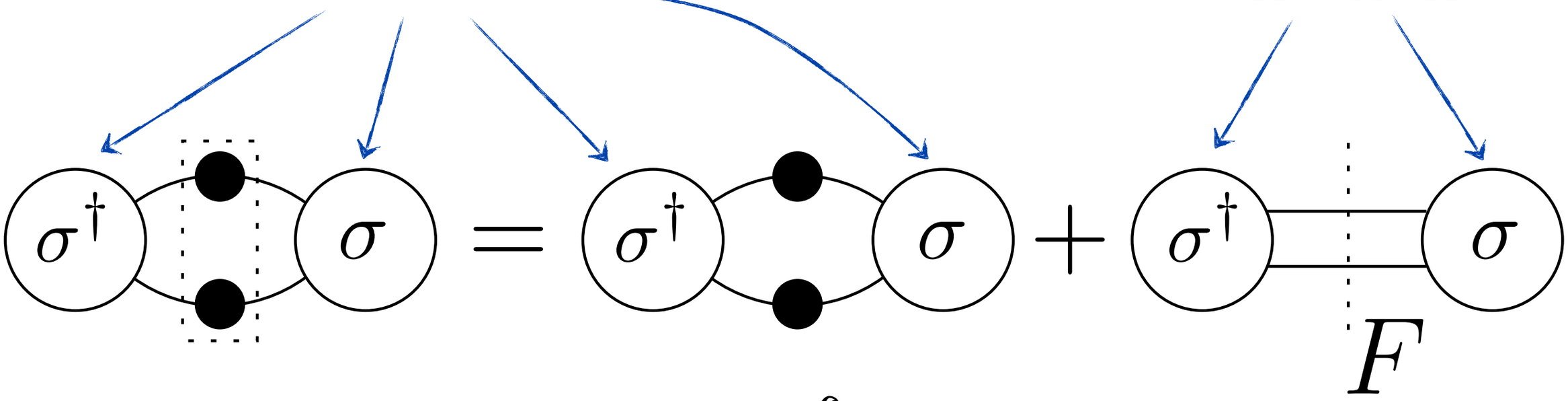
contains all power-law corrections

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



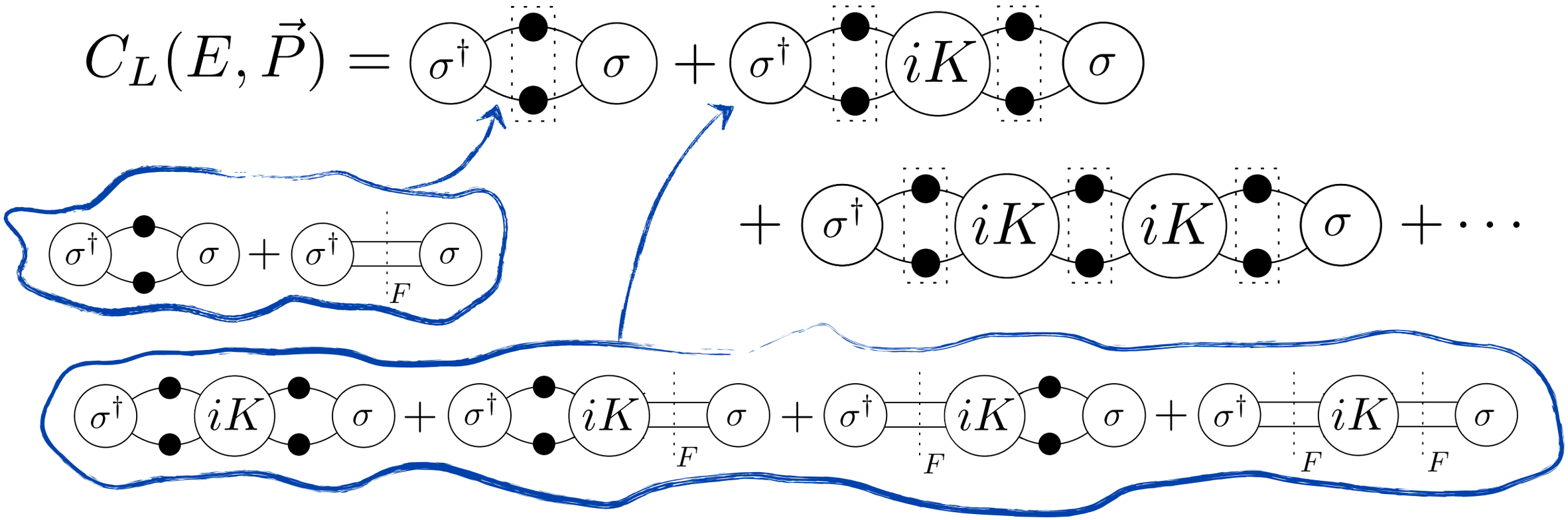
Next we introduce an important identity

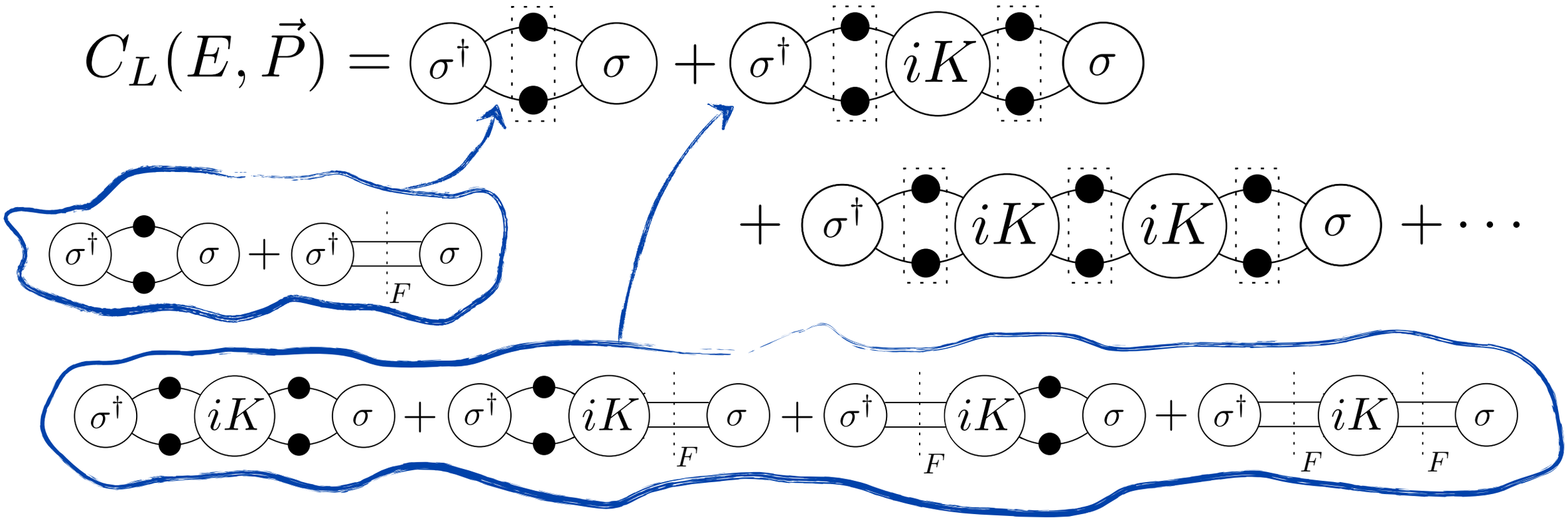
off-shell **on-shell**



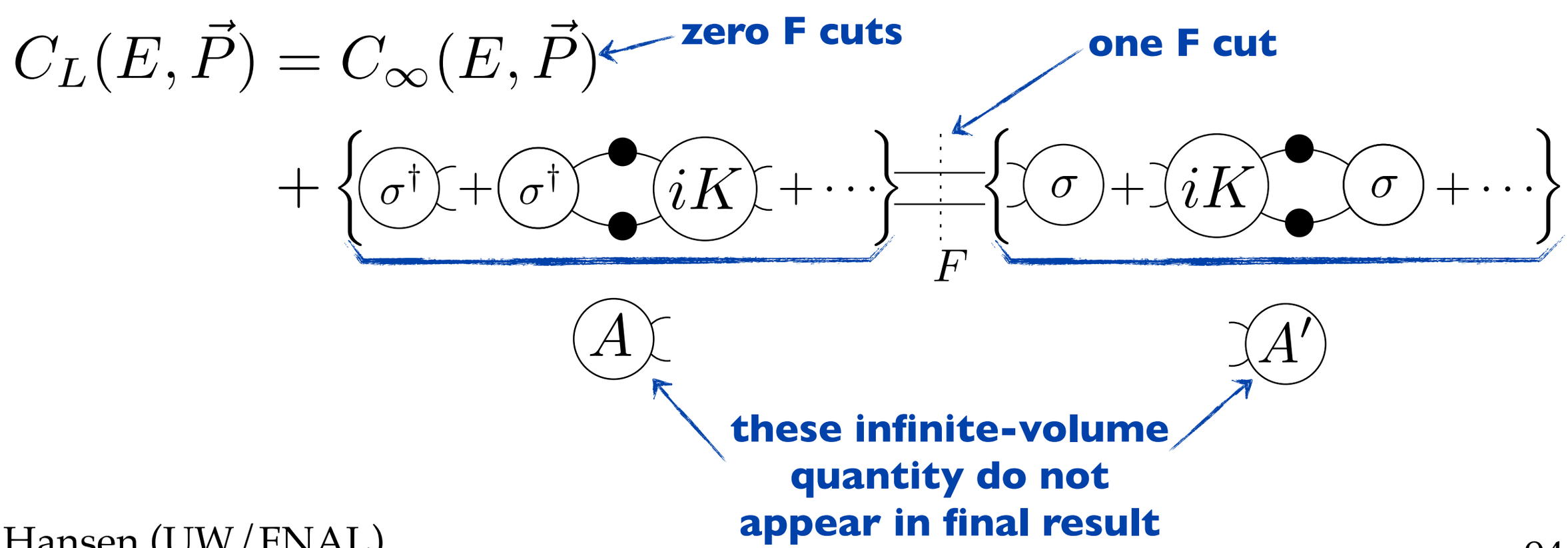
$$\frac{1}{L^3}\sum_{\vec{k}} \qquad \int_{\vec{k}}$$

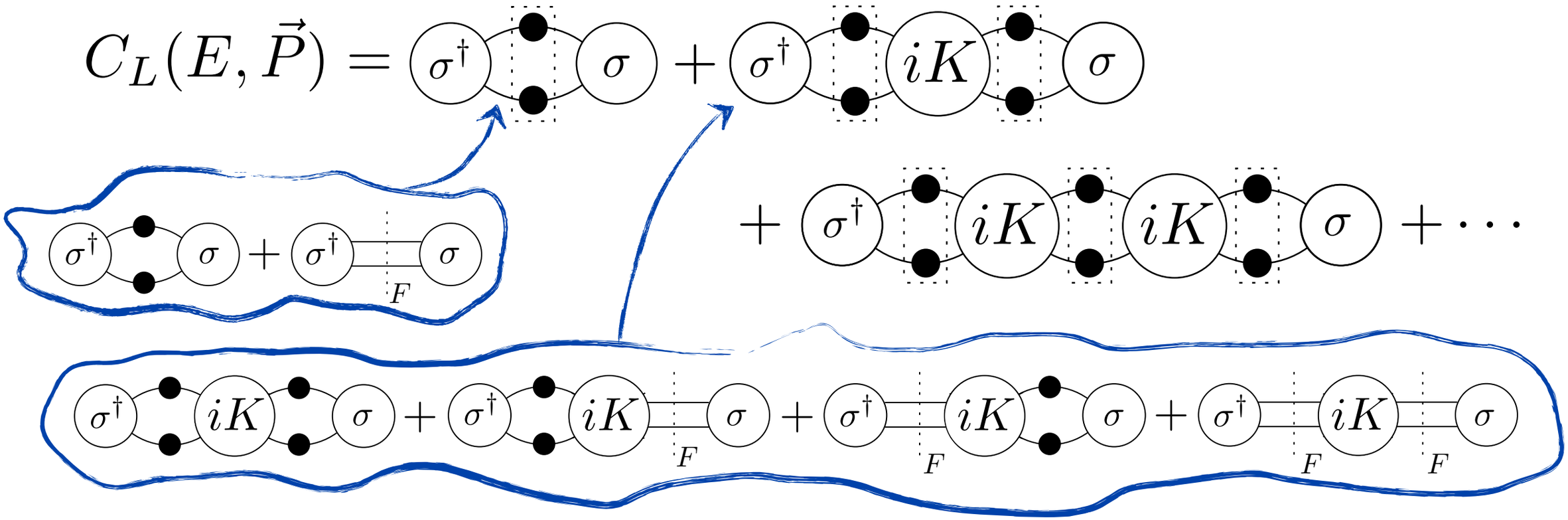
contains all power-law corrections


$C_L(E,\vec{P}) =$
$\sigma^\dagger$
σ
iK
F
$+ \cdots$

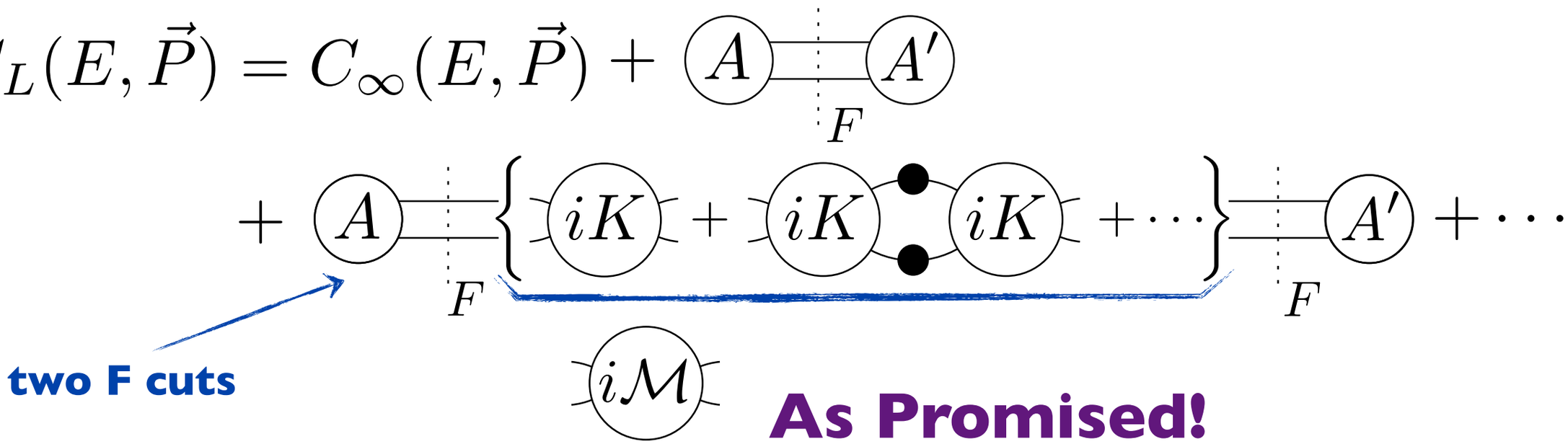


Now regroup by number of F cuts



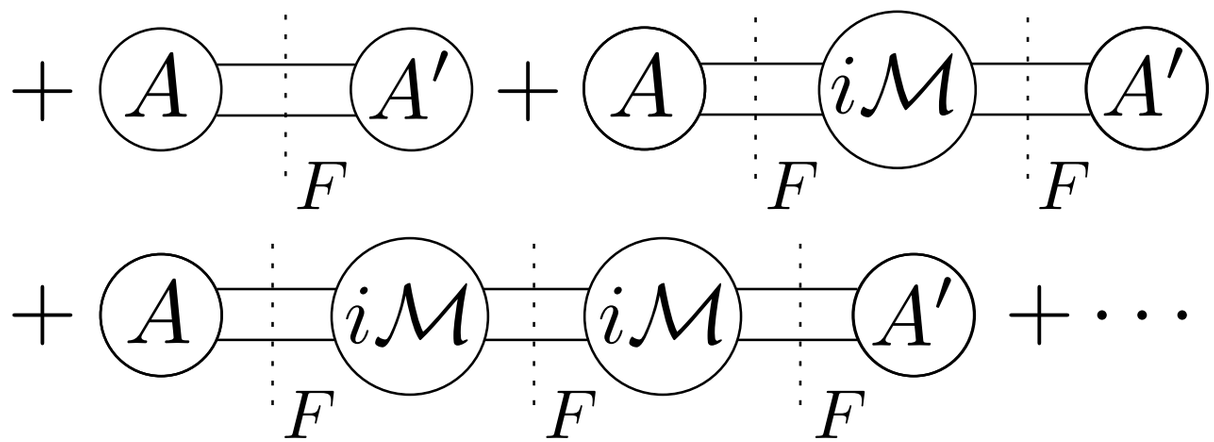


Now regroup by number of F cuts



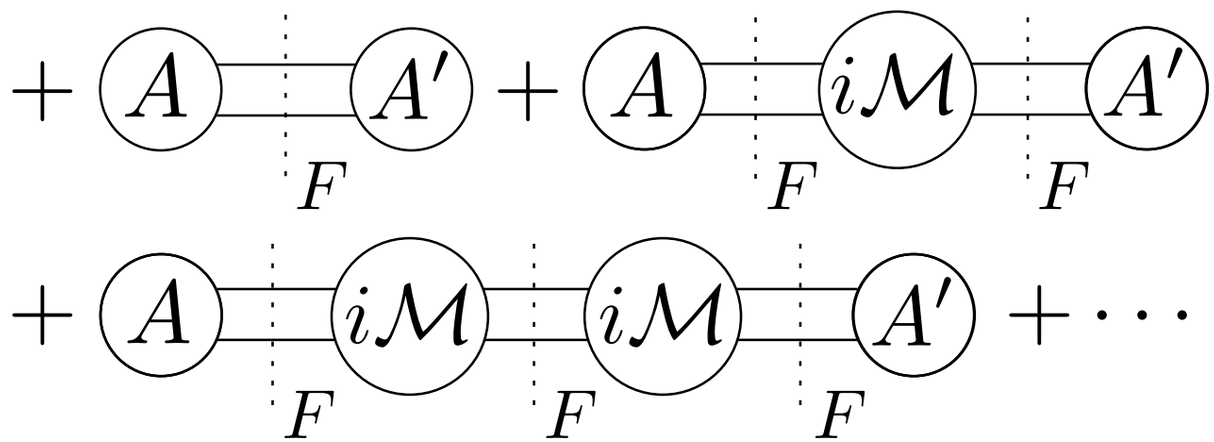
As Promised!
infinite-volume on-shell two-to-two scattering amplitude

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



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

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



$$+ \cdots$$

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

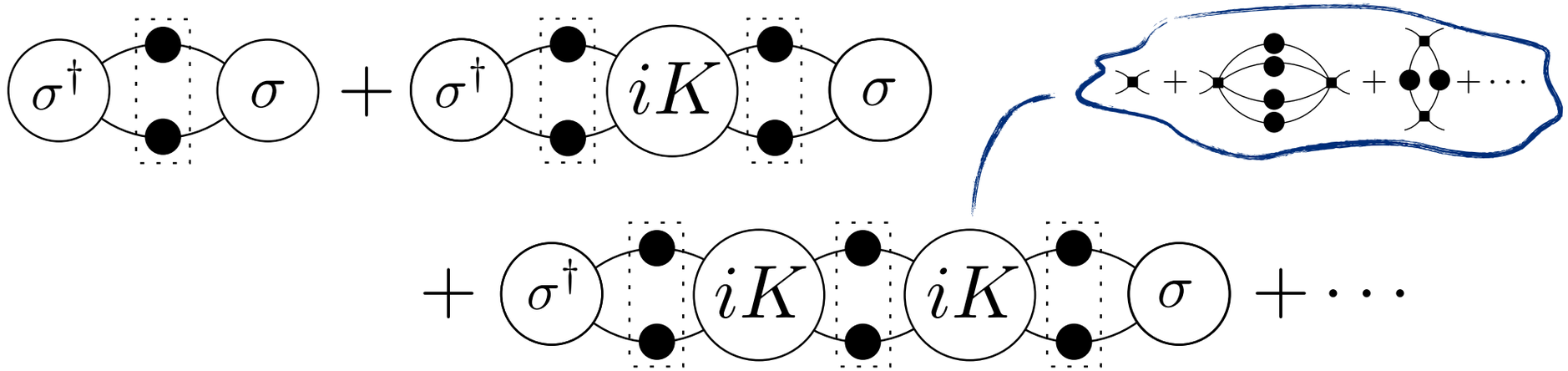
$$C_L(E,\vec{P}) = C_\infty(E,\vec{P}) + A' iF \frac{1}{1 - i\mathcal{M}_{2\to 2} iF} A$$

no poles **no poles** **no poles**

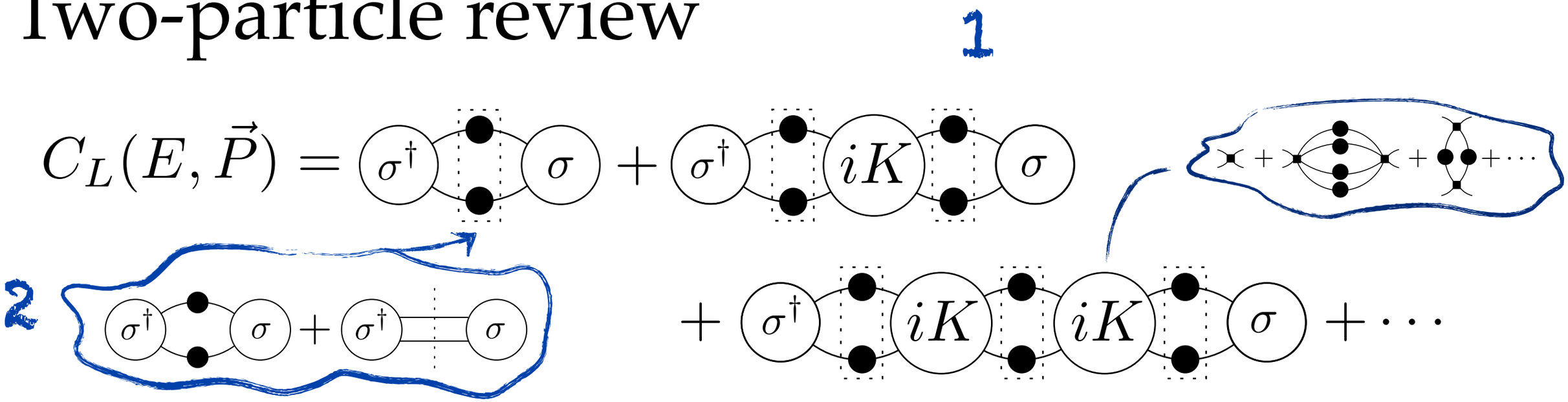
$C_L(E,\vec{P})$ **diverges whenever** $iF \dfrac{1}{1 - i\mathcal{M}_{2\to 2} iF}$ **diverges**

Two-particle review

1

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

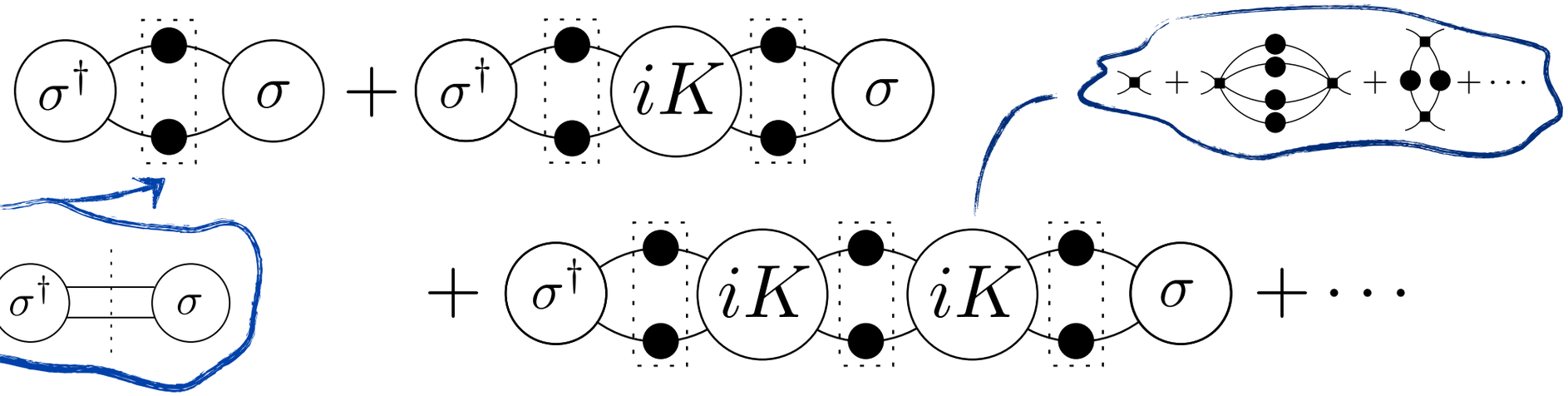
Two-particle review



Two-particle review

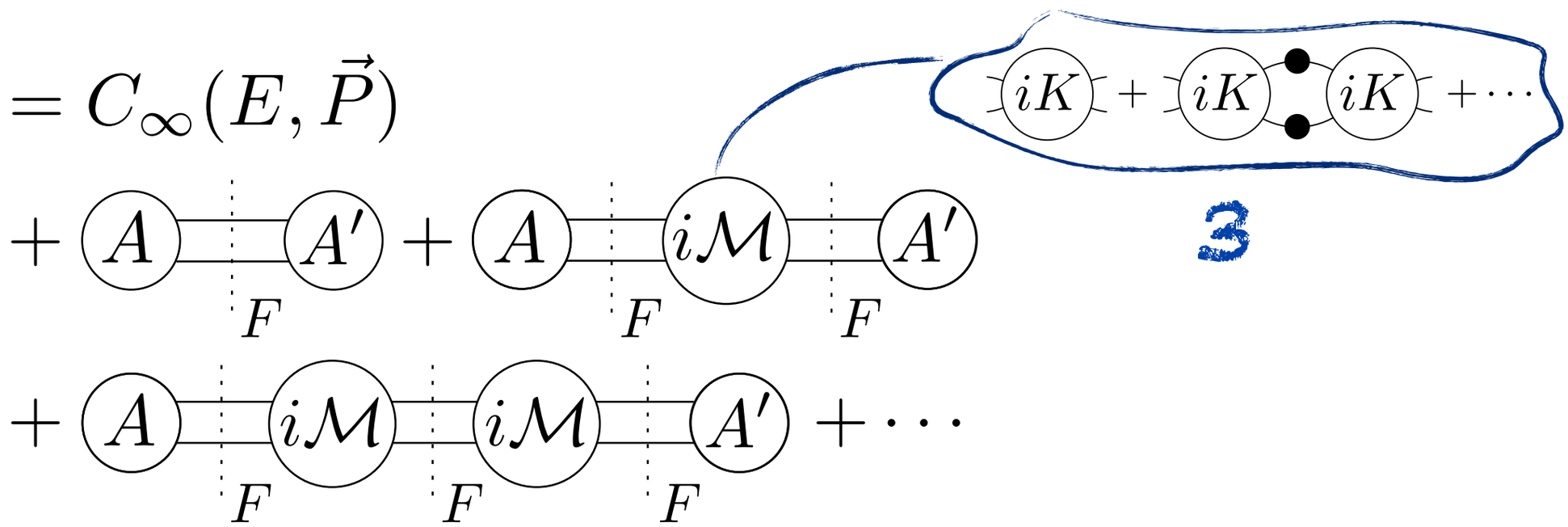
1

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



2

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

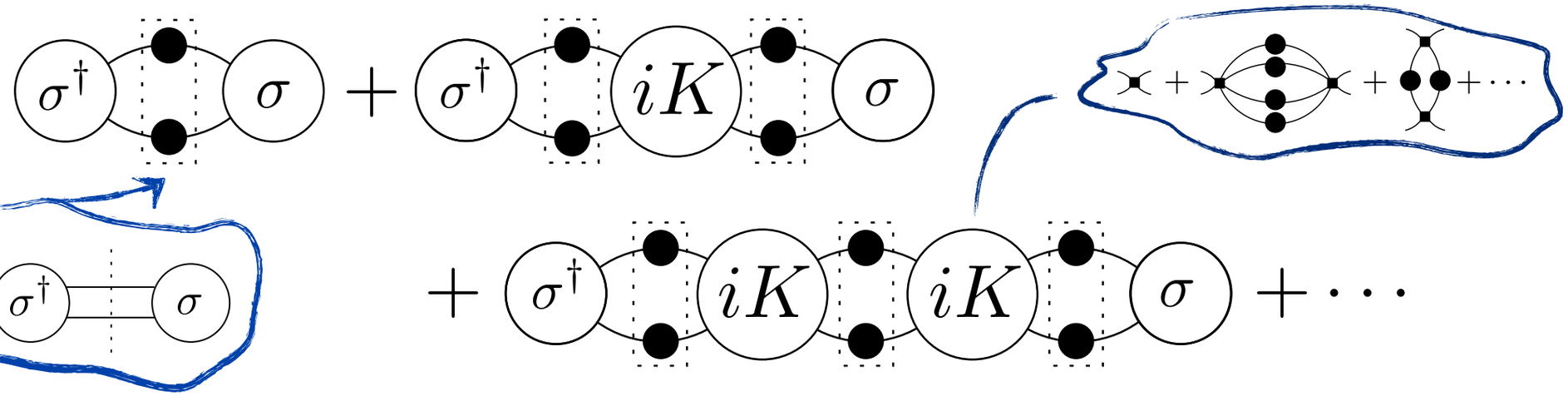


3

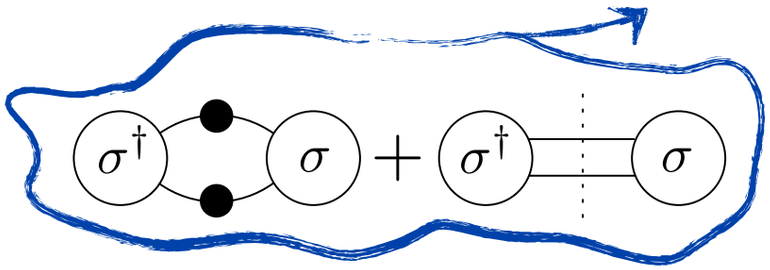
Two-particle review

1

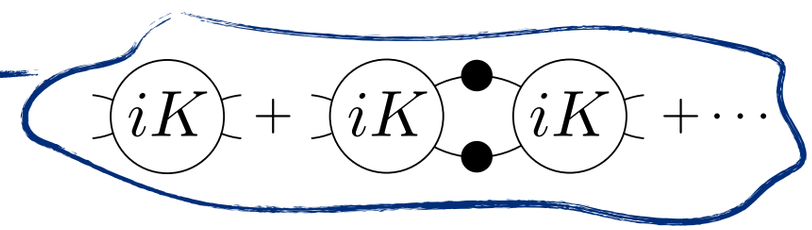
$$C_L(E,\vec{P}) =$$



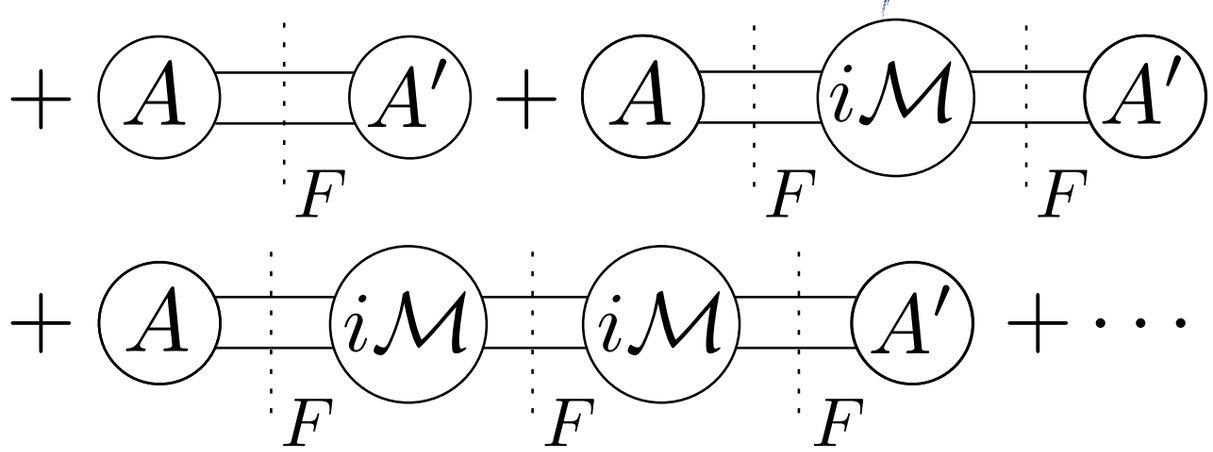
2



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



3



4

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

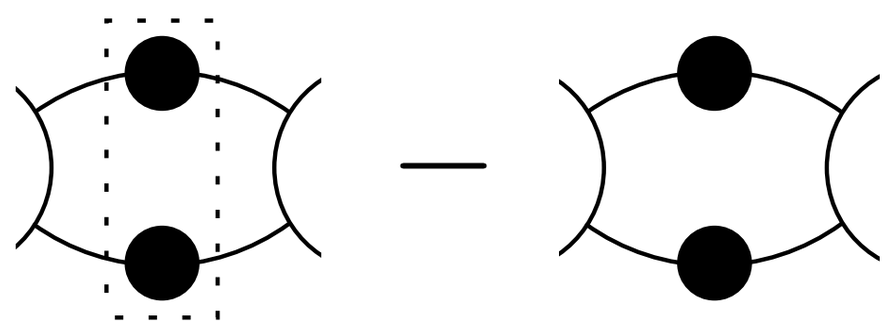
Two-particle result

At fixed $(L, \vec{P})$, finite-volume spectrum is all solutions to

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

diagonal matrix in angular momentum space

kinematic (related to Lüscher Zeta function)

$F \equiv$ 

Two-particle result

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

...is it useful?

At low energies, s-wave dominates

$$[\mathcal{M}^s_{2\to 2}(E^*_n)]^{-1} = -F^s(E_n, \vec{P}, L)$$

$$F^s(E, \vec{P}, L) \equiv \frac{1}{2}\left[\frac{1}{L^3}\sum_{\vec{k}} - \int \frac{d^3k}{(2\pi)^3}\right] \frac{1}{2\omega_k 2\omega_{P-k}(E - \omega_k - \omega_{P-k} + i\epsilon)}$$

Two-particle result

Note also, equation is real

$$[\mathcal{M}^s_{2\to 2}(E^*_n)]^{-1} = -F^s(E_n, \vec{P}, L)$$

$$\boxed{p_n \cot\delta^s(p_n) - i\cancel{p}_n = -16\pi E^*_n \,\mathrm{Re}F^s - i\cancel{p}_n}$$

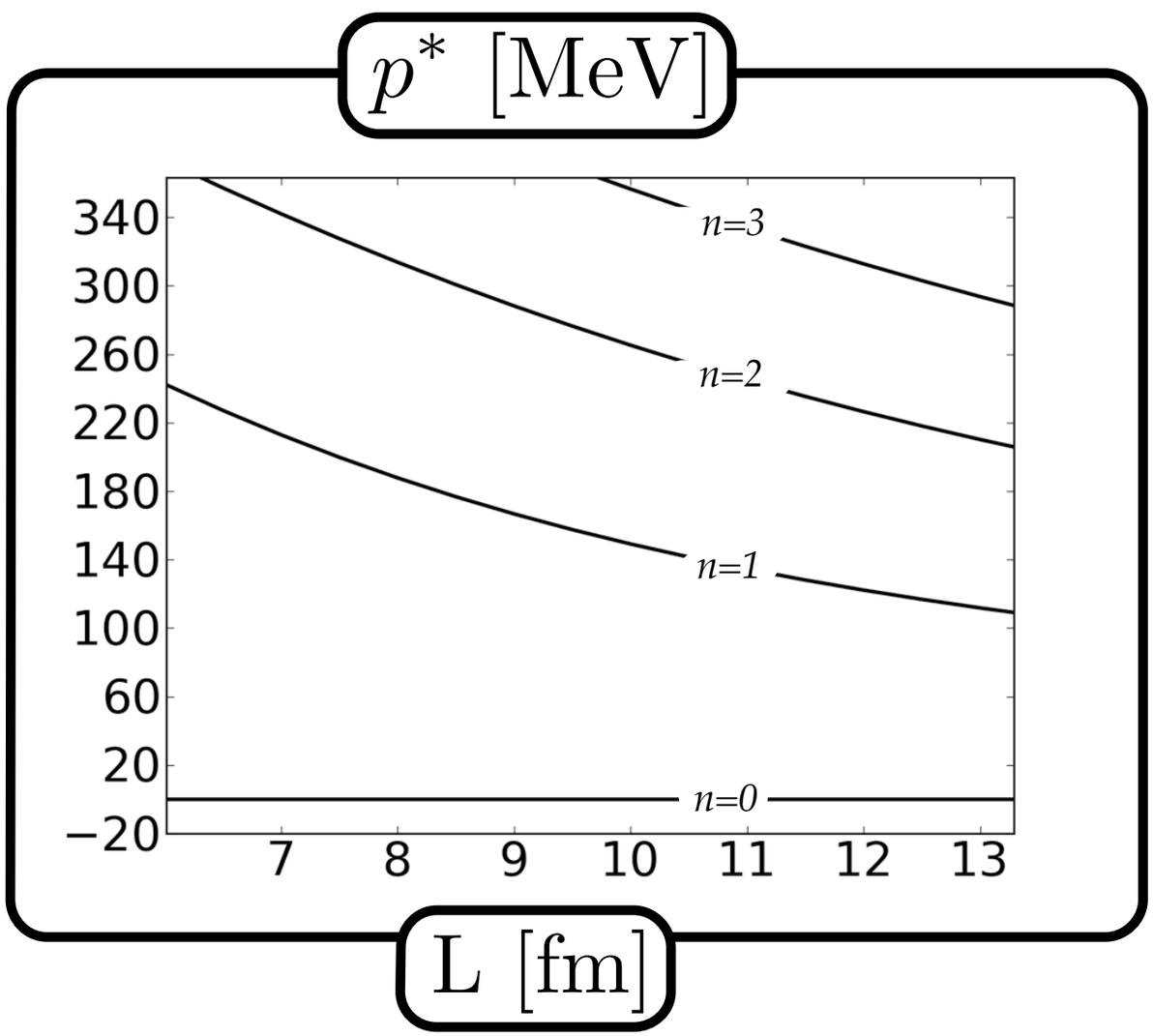
This can also be seen by **replacing i-epsilon with principal value** everywhere in derivation.

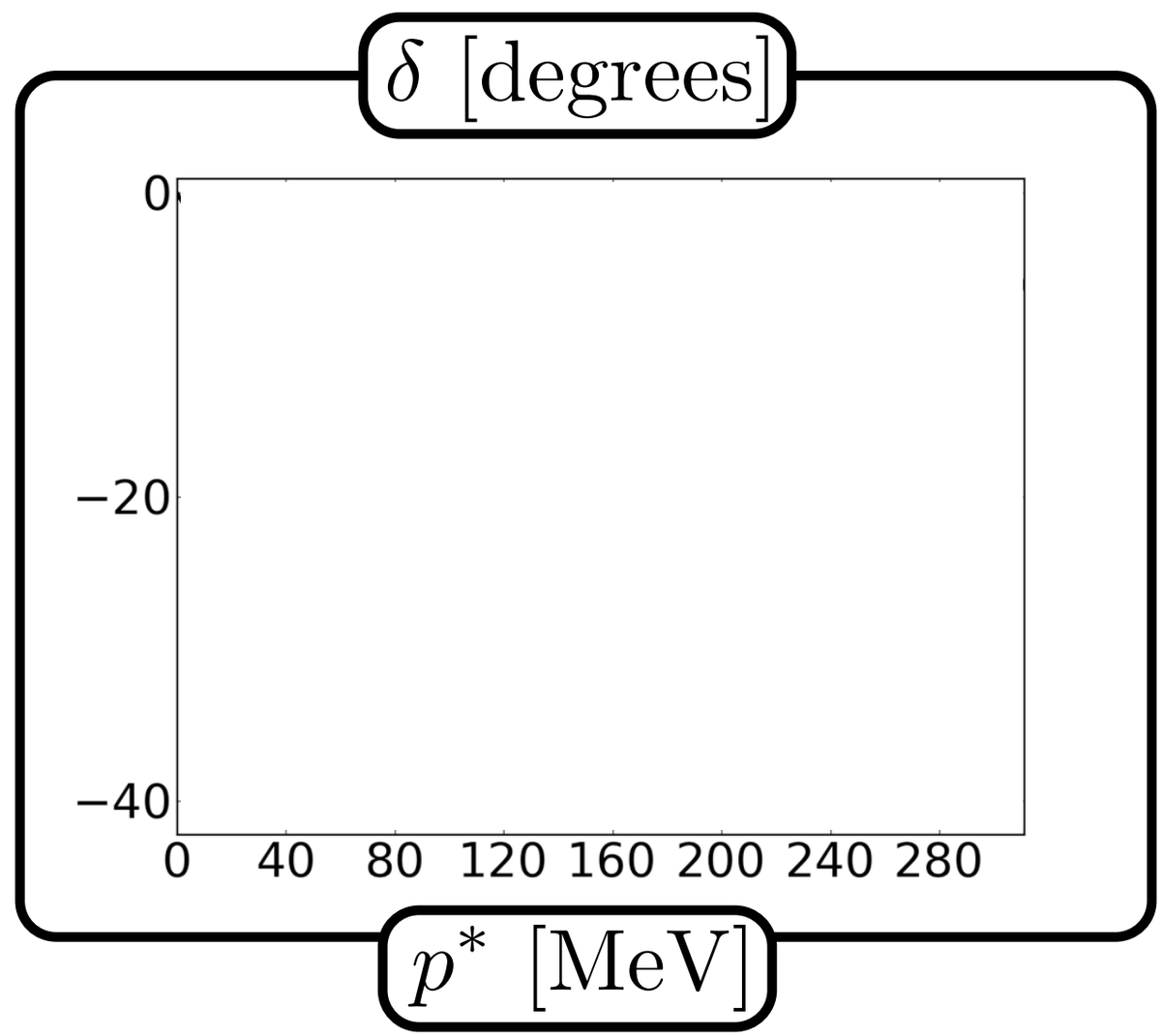
$$\mathcal{M}_{2\to 2} \longrightarrow \mathcal{K}_{2\to 2} \qquad\qquad F \longrightarrow \mathrm{Re}\, F$$

Important for three-particle case

$$p_n \cot \delta(p_n) = -16\pi E_n^* \mathrm{Re} F$$

$$\mathcal{M}^s_{2\to 2}(E) = \frac{16\pi E}{p \cot \delta(p) - ip}$$





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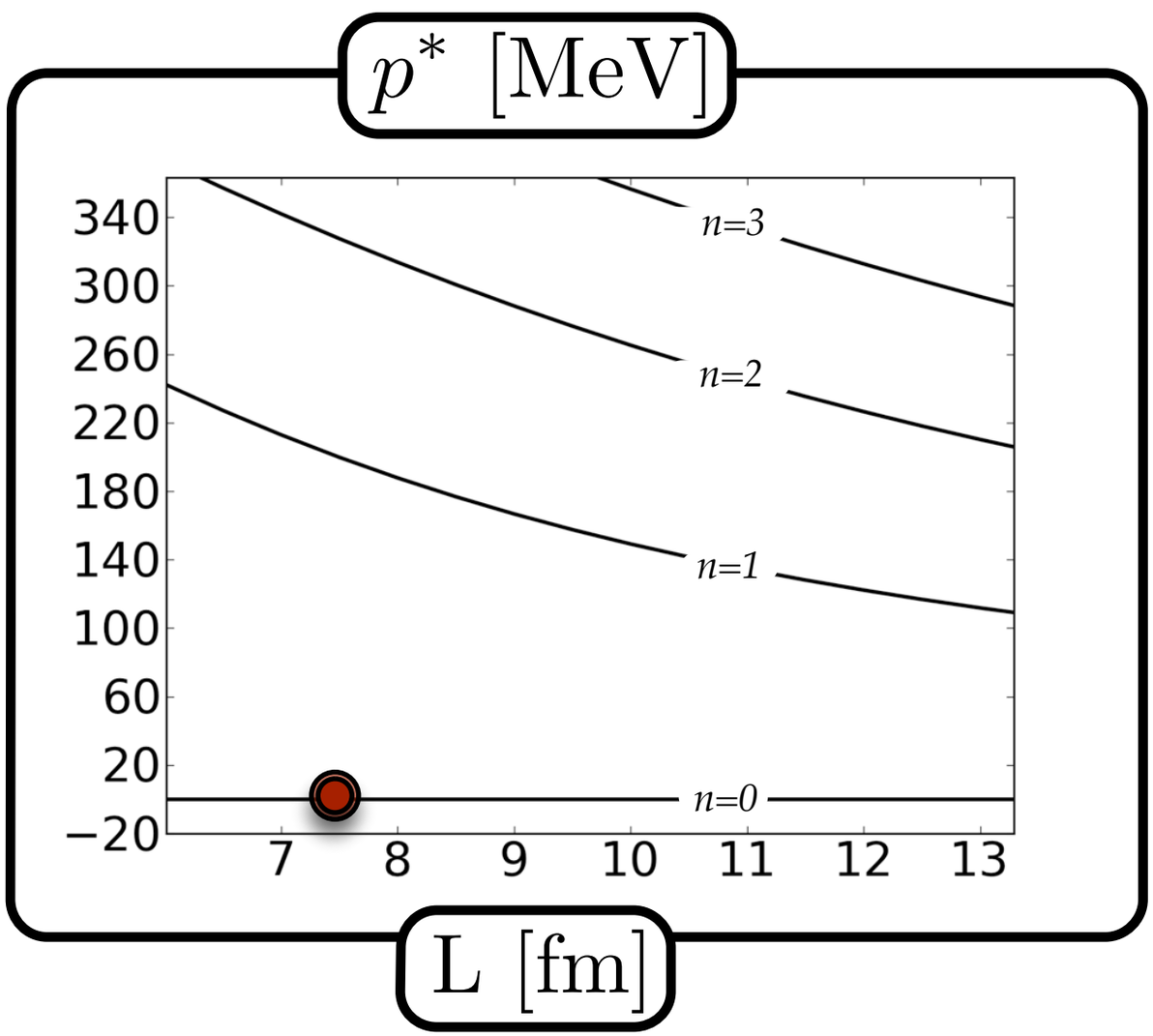
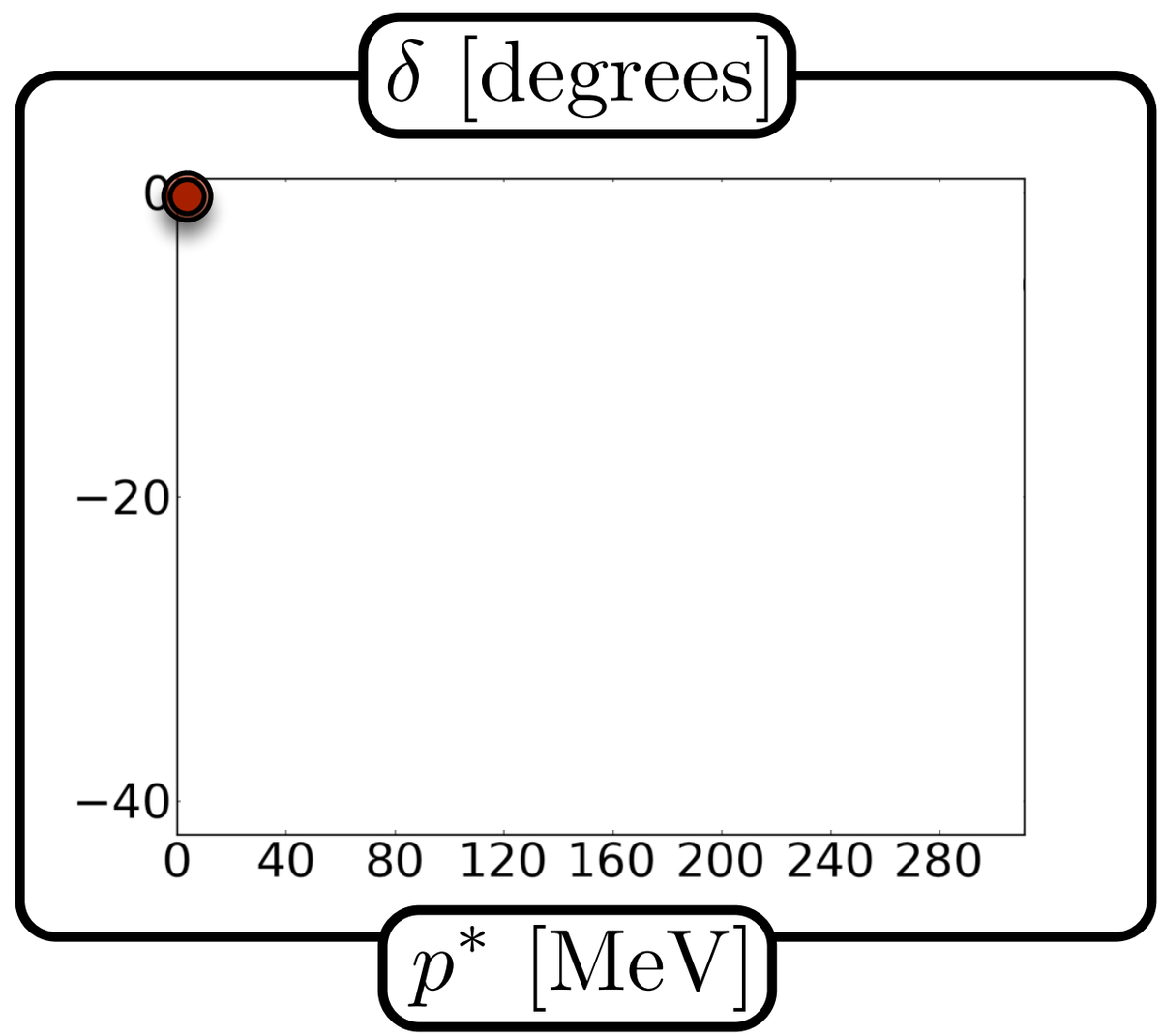
$$\mathcal{M}^s_{2\to 2}(E) = \frac{16\pi E}{p \cot \delta(p) - ip}$$





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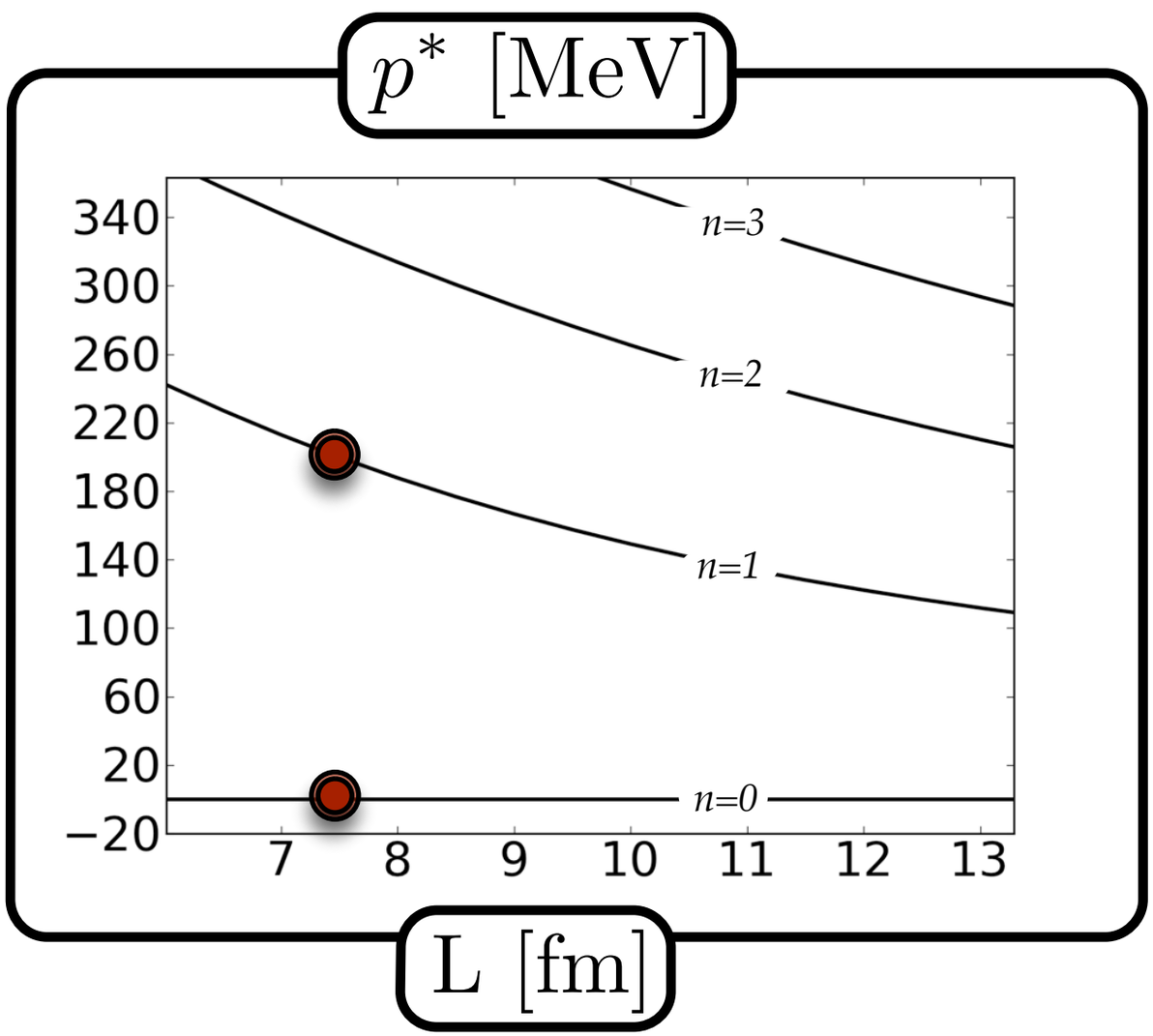

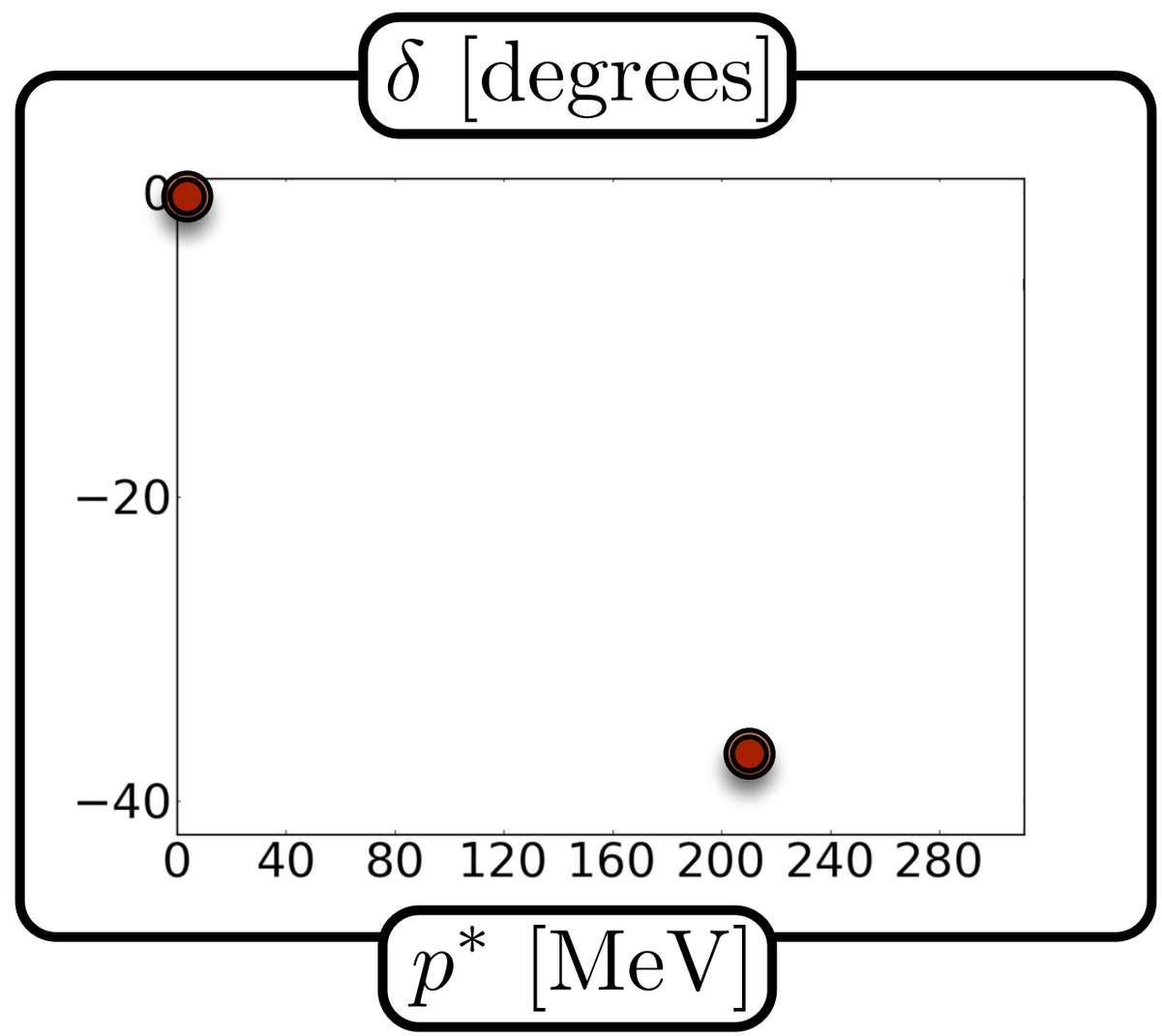

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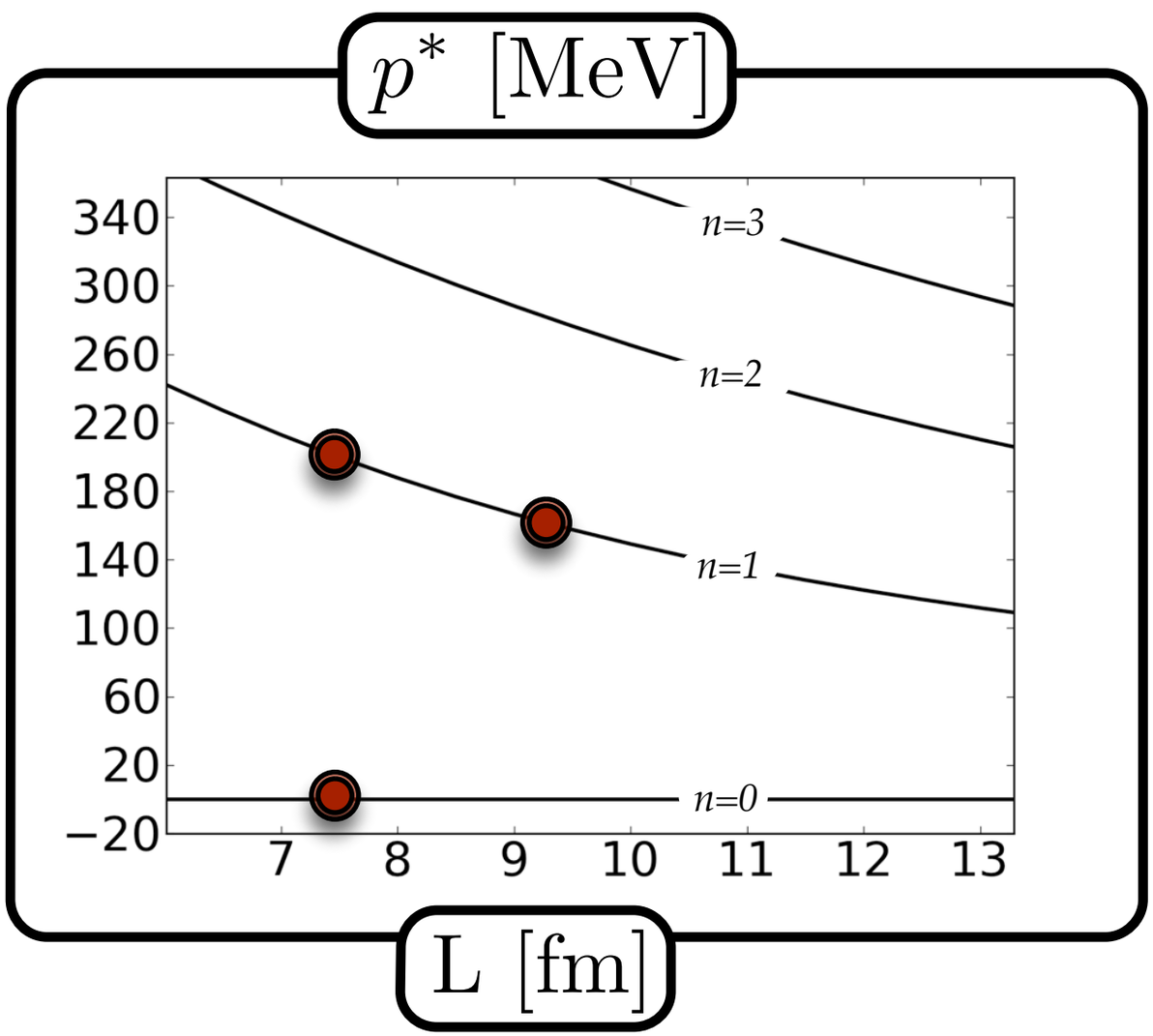

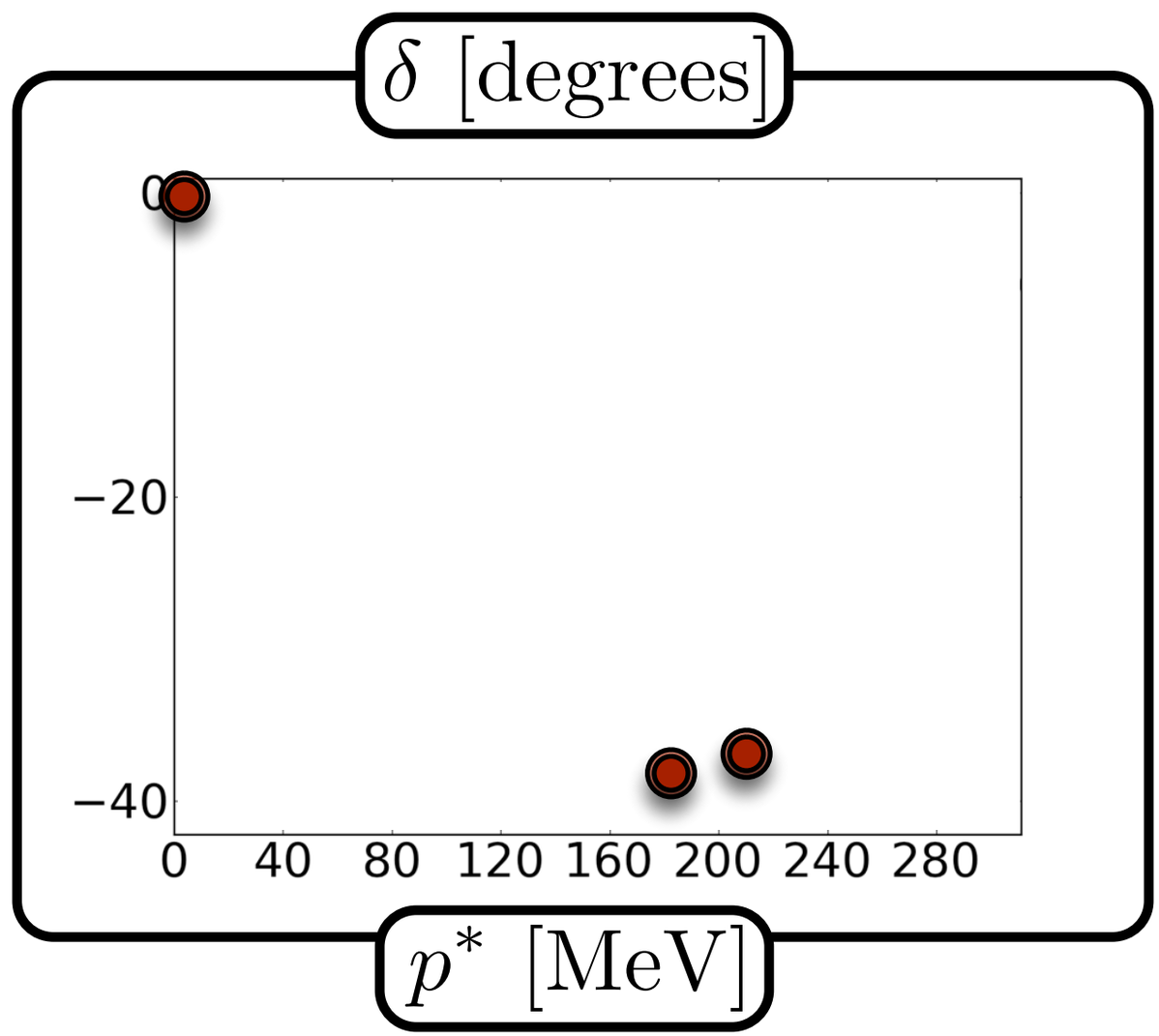

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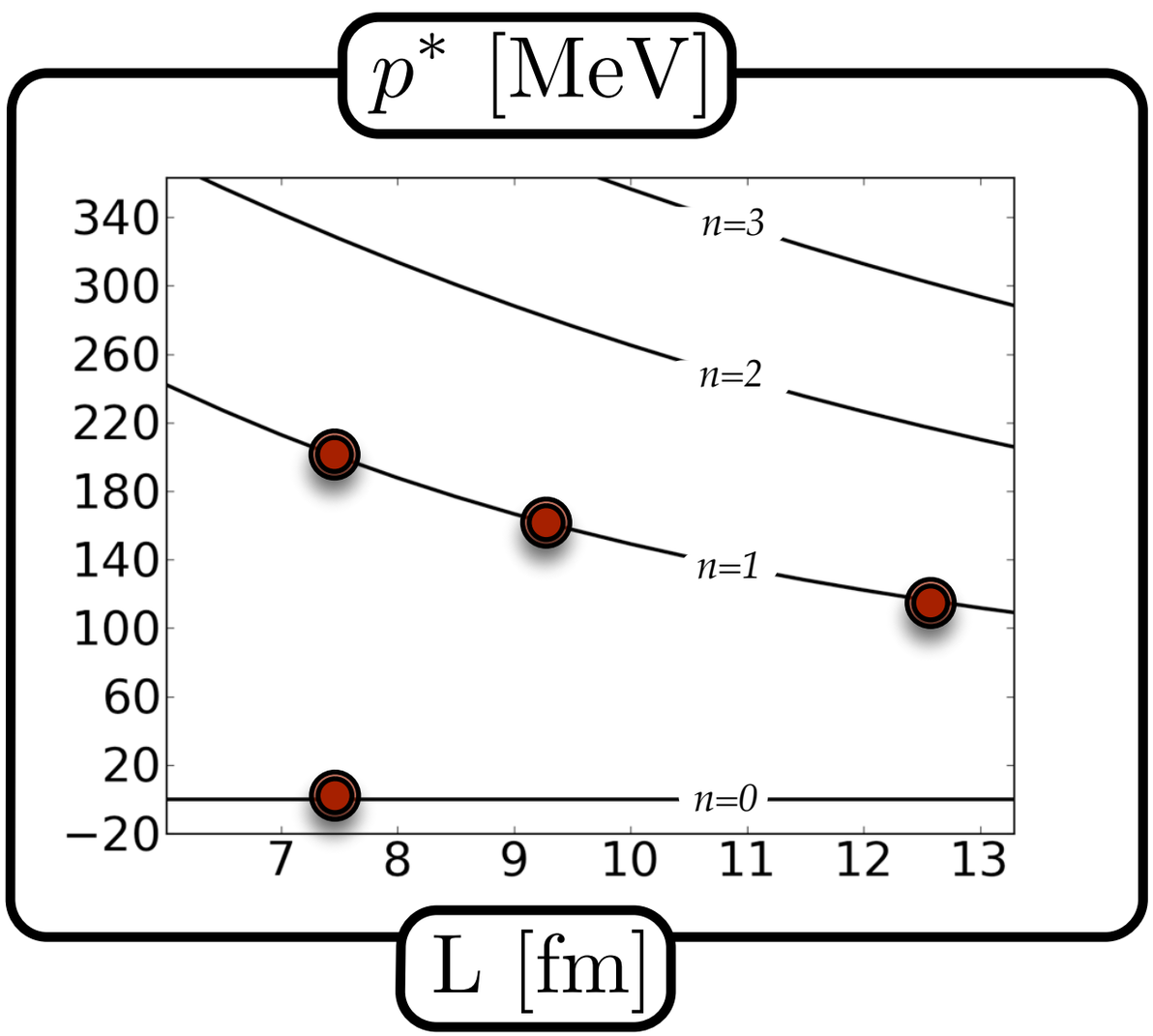

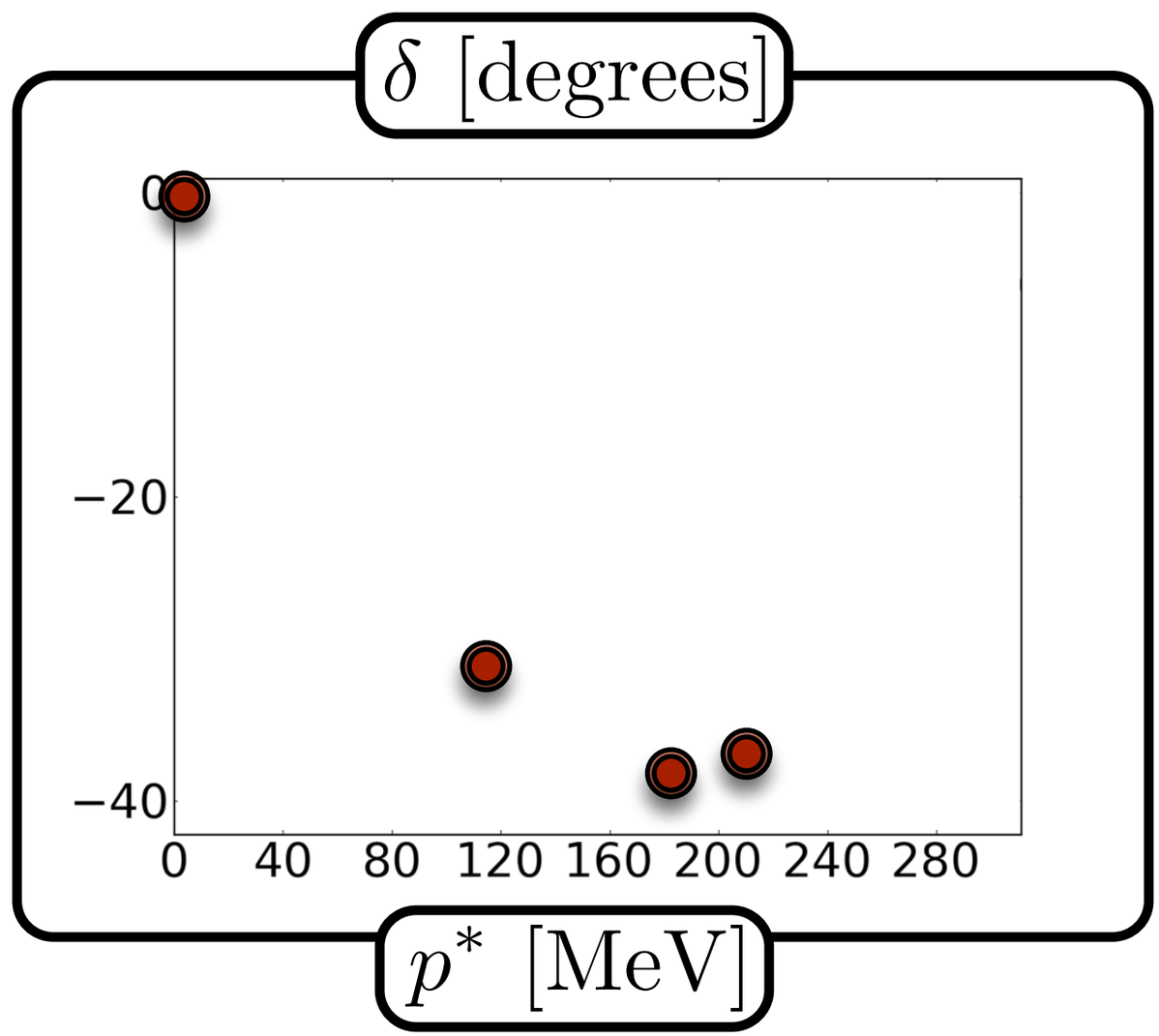

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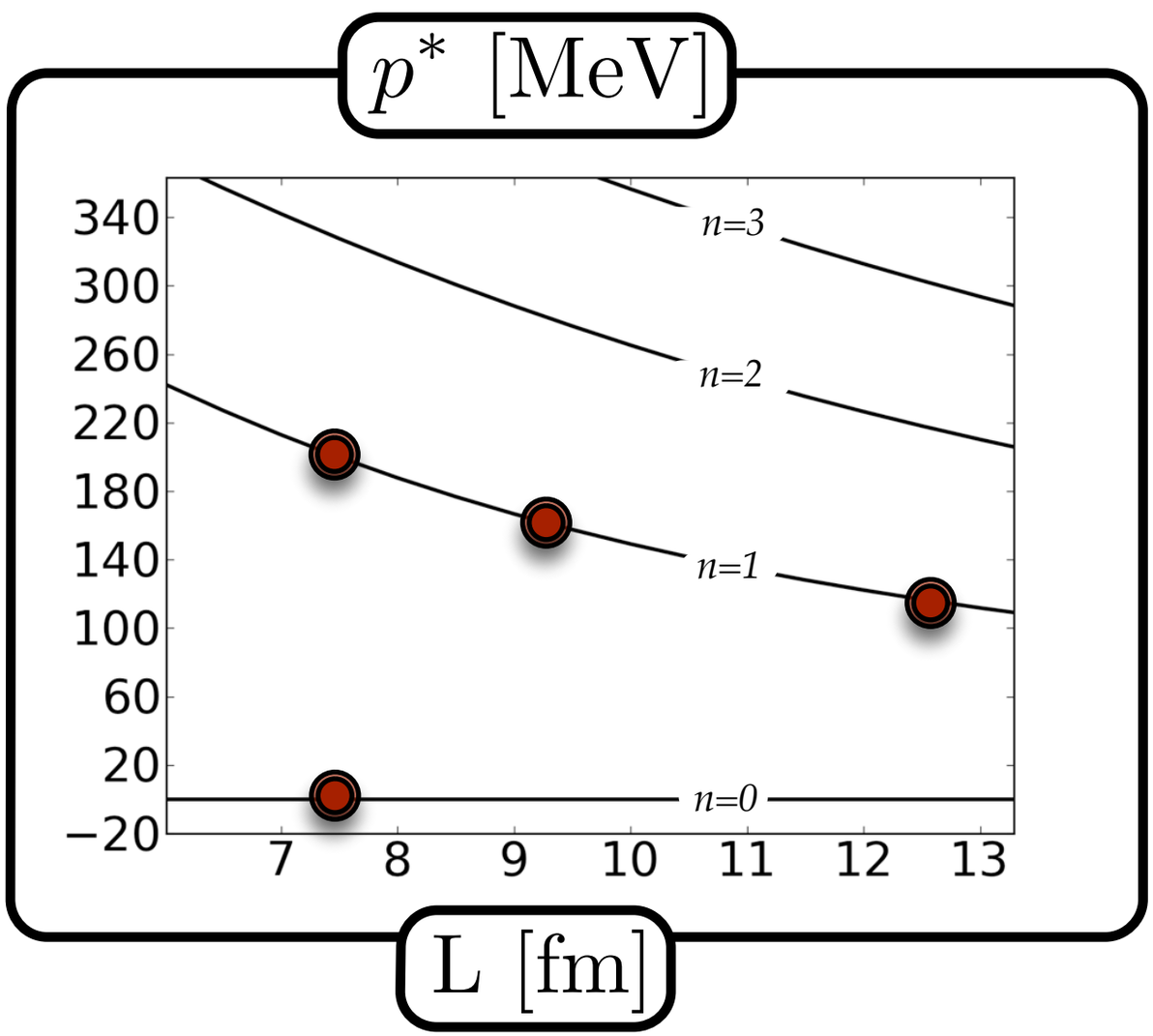
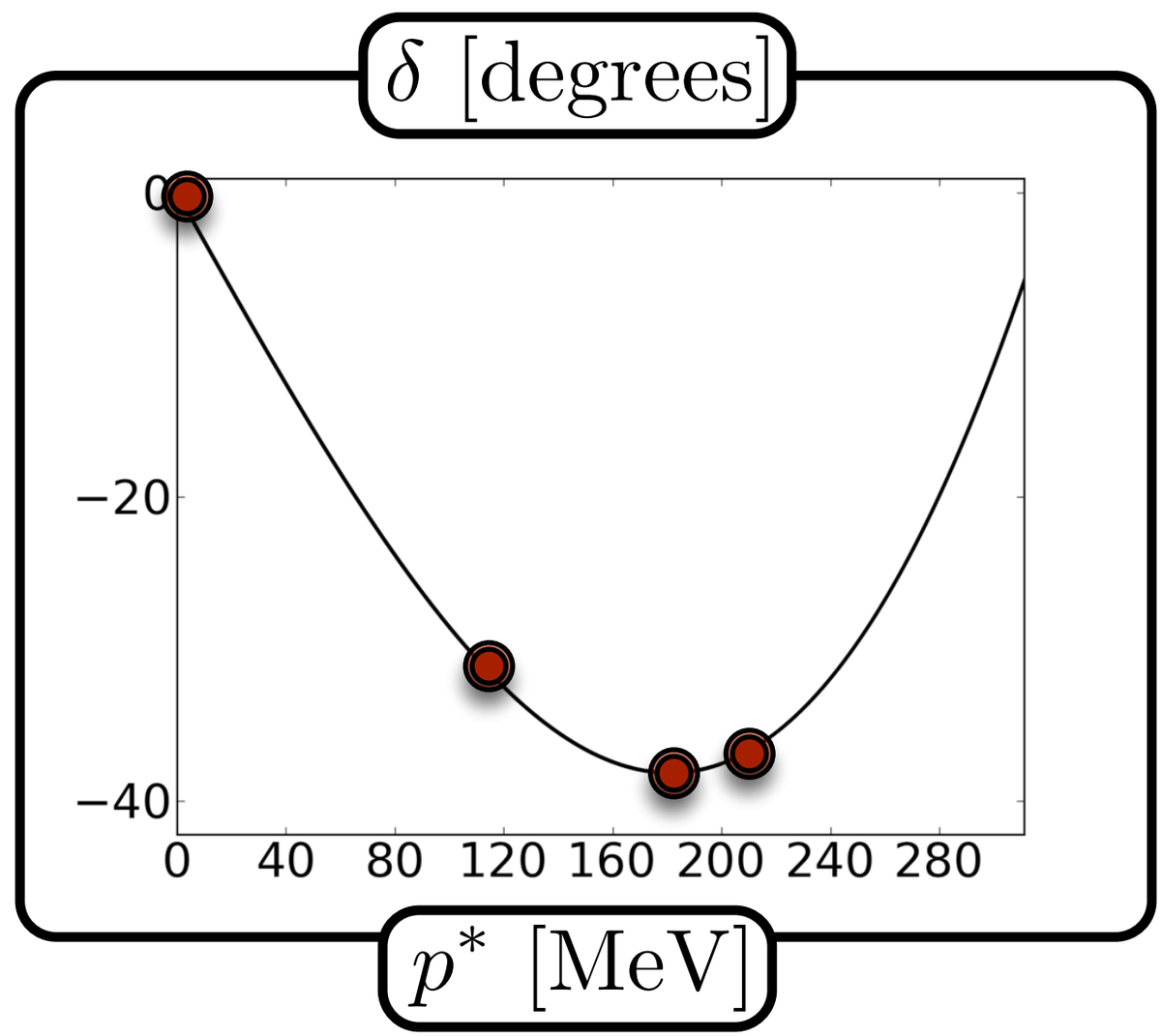
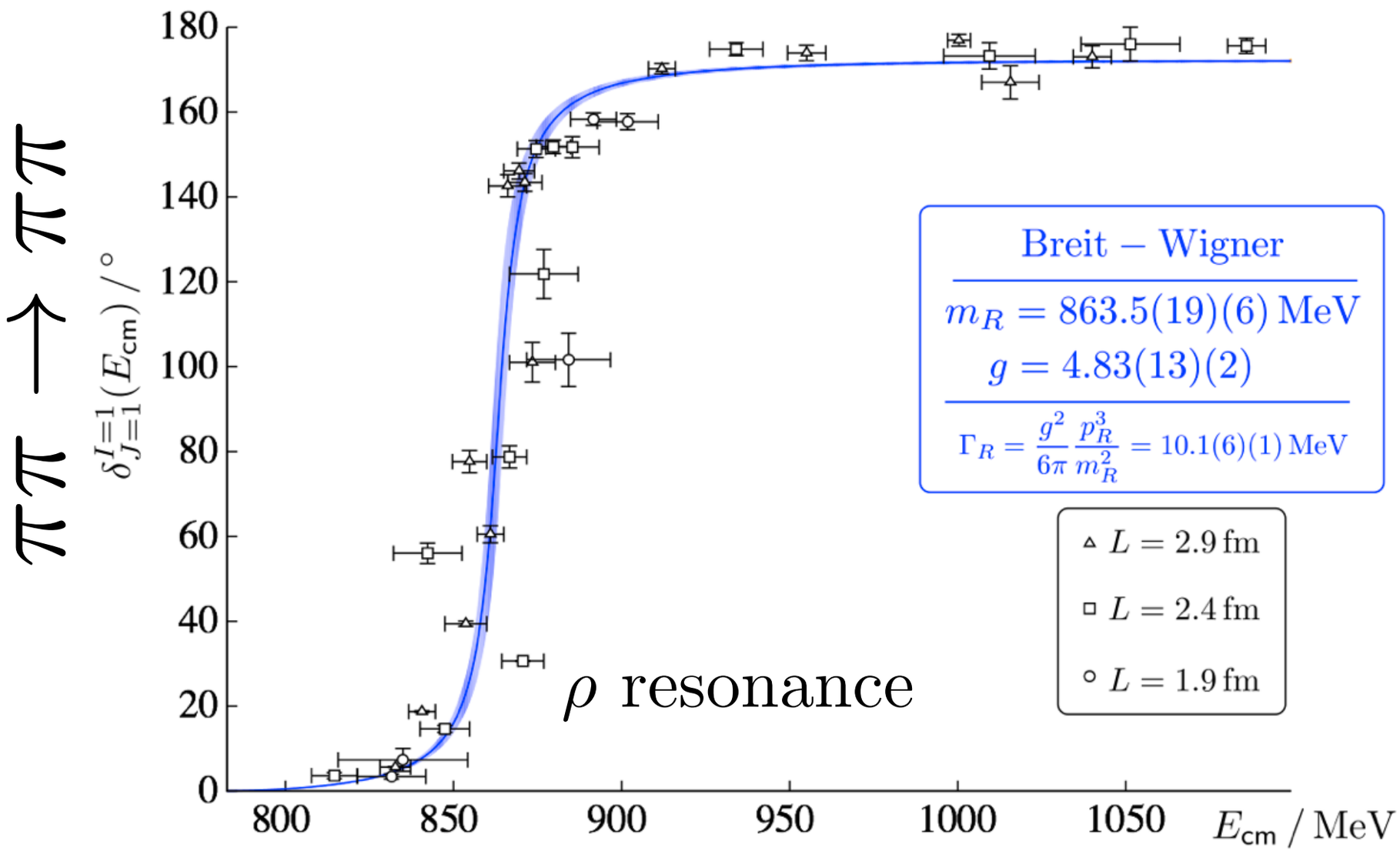




$$p_n \cot \delta_{J=1}(p_n) = -16\pi E_n^* \,\mathrm{Re}\, F_{10;10}(E_n, \vec{P}, L)$$



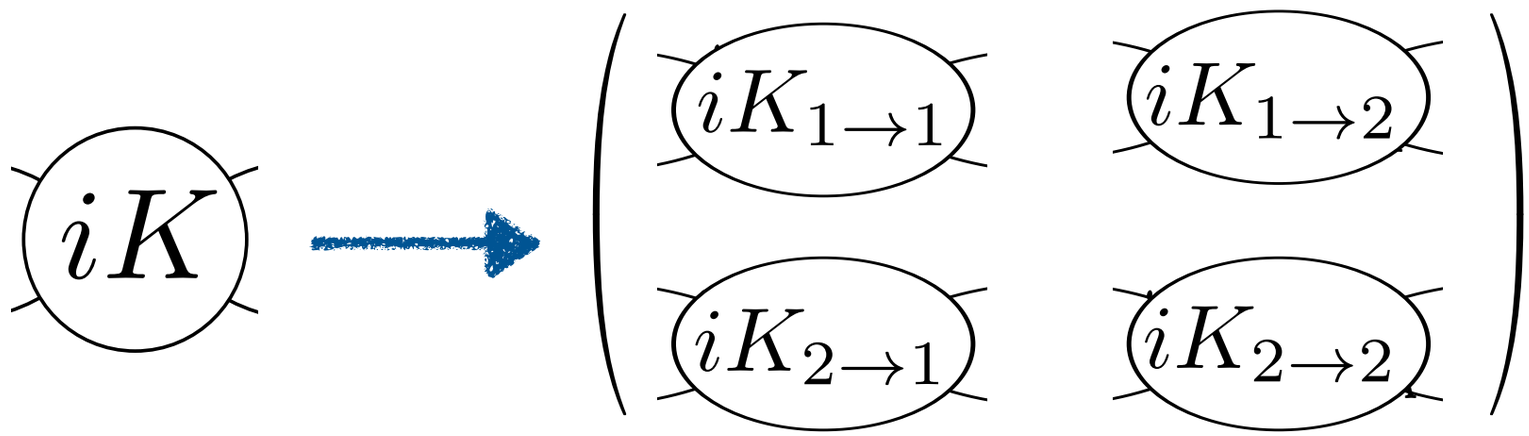
$m_\pi = 391$ MeV

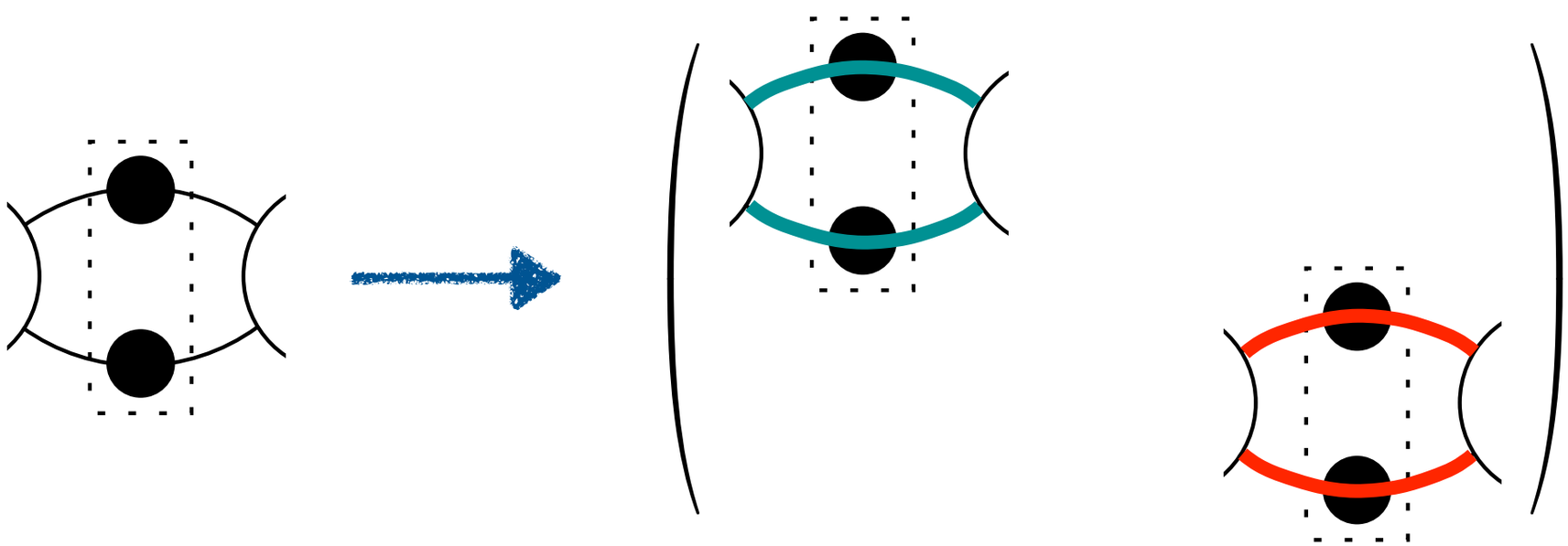
from Dudek, Edwards, Thomas in *Phys.Rev*. D87 (2013) 034505

Scattering of multiple two-particle channels

$$\pi\pi \to \overline{K}K \qquad \pi K \to \eta K$$

Make following replacements





Scattering of multiple two-particle channels

$$\pi\pi \to \overline{K}K \qquad \pi K \to \eta K$$

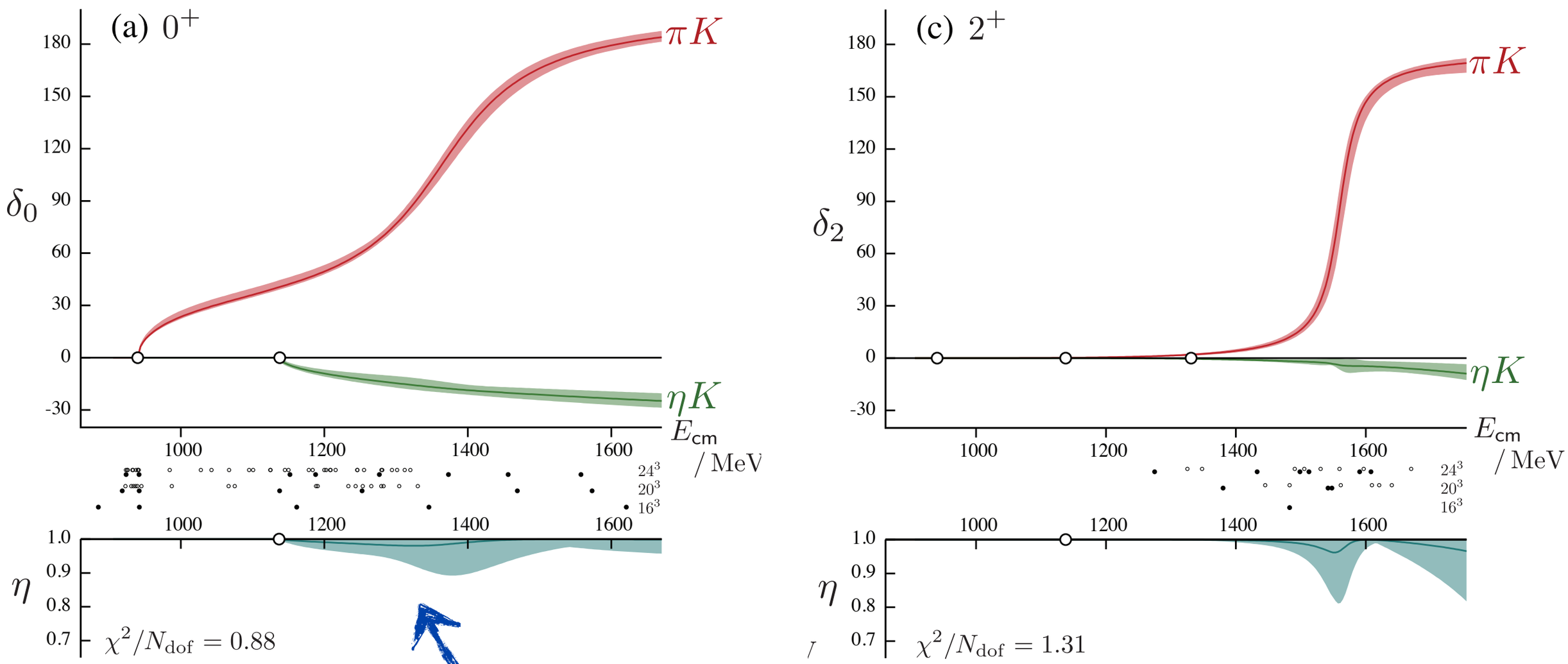
One finds

$$\det\left[1 - \begin{pmatrix} i\mathcal{M}_{1\to1} & i\mathcal{M}_{1\to2} \\ i\mathcal{M}_{2\to1} & i\mathcal{M}_{2\to2} \end{pmatrix} \begin{pmatrix} iF_1 & 0 \\ 0 & iF_2 \end{pmatrix}\right] = 0$$

M. Lage, U.-G. Meißner, and A. Rusetsky, Phys.Lett., B681, 439 (2009)
V. Bernard, M. Lage, U.-G. Meißner, and A. Rusetsky, JHEP, 1101, 019 (2011)
M. Döring, U.-G. Meißner, E. Oset, and A. Rusetsky, Eur.Phys.J., A47, 139 (2011)
MTH, S. R. Sharpe, *Phys.Rev. D86* (2012) 016007
R. A. Briceño, Z. Davoudi, *Phys.Rev. D88* (2013) 094507

Already implemented in LQCD calculation

$$\pi K \to \eta K$$



$$\mathcal{M}(\pi K \to \eta K) \sim \sqrt{1-\eta^2}$$

from Dudek, Edwards, Thomas, Wilson in arXiv:1406:4158