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

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MTH, Stephen R. Sharpe
to appear

In 2012 LHCb and CDF reported surprisingly high CP asymmetry in

$$D^0 \to \pi^+\pi^- \qquad\qquad D^0 \to K^+K^-$$

(this has recently reduced to naive SM expectations)

LHCb, *PRL* 108, 111602 (2012) CDF, *PRL* 109, 111801 (2012)

LHCb, *PLB* 723 (2013) 33-43

Numerical Lattice QCD is the only systematic method for calculating non-perturbative matrix elements. So it is natural to ask whether it can be applied here.

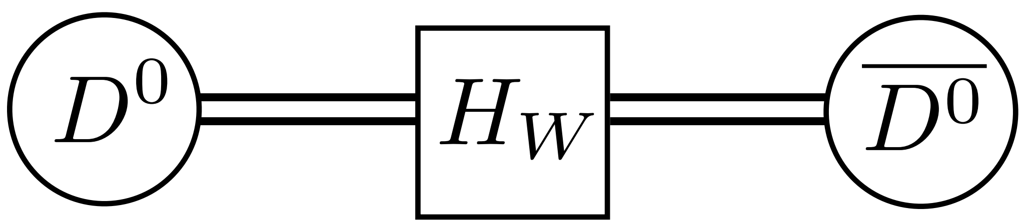
It turns out that the theoretical **tools** for extracting D decays from Lattice QCD **do not yet exist**.

We were motivated to develop the required formalism.

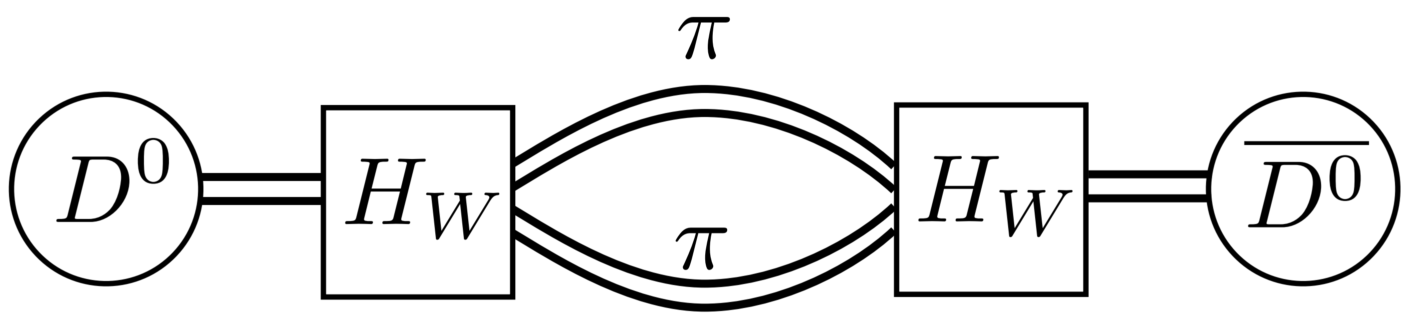
Extracting D decays is also relevant for neutral D meson mixing.

$$D^0 \longleftrightarrow \overline{D^0}$$

More precisely, mixing splits into short and long distance contributions:



short distance



long distance

The formalism for extracting D decays is also needed for extracting the long distance contribution.

Why is this difficult?

Lattice QCD can be used to obtain Euclidean correlators numerically:

$$\langle 0|\pi(x_1)\pi(x_2)H_W(x_3)D(x_4)|0\rangle$$

$$\langle 0|K(x_1)K(x_2)H_W(x_3)D(x_4)|0\rangle$$

However, it is **not possible to analytically continue** these numerical functions from Euclidean to Minkowski time.

In addition taking limits on Euclidean correlators directly will not give the decay amplitude.

Maiani, L. & Testa, M. *PLB* 245, 585-590 (1990)

One needs a more clever approach.

Indeed such a clever approach was worked out by M. Lüscher and L. Lellouch for

$$K \to \pi\pi$$

First M. Lüscher found a method to determine $\pi\pi \to \pi\pi$ from lattice simulations.

Highly nontrivial since same Euclidean/ Minkowski issue is relevant here.

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

Then M. Lüscher and L. Lellouch used perturbation theory in weak interaction to derive a method for extracting $K \to \pi\pi$ amplitude from Lüscher's $\pi\pi \to \pi\pi$ result

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

Can we generalize Lellouch-Lüscher method to extract

$$D^0 \to \pi^+\pi^- \qquad D^0 \to K^+K^- \;\textbf{?}$$

First step is to generalize $\pi\pi \to \pi\pi$ extraction.
To handle D decays, we must determine how to extract all strongly coupled channels that are open at $M_D \approx 1865\,\mathrm{MeV}$

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

There exists no formalism to extract scattering amplitudes from Lattice QCD for states with more than two hadrons.

So, what is Lüscher's method for extracting $\pi\pi \to \pi\pi$?

Still starts with four pion interpolator,

$$\langle 0|\pi(x_1)\pi(x_2)\pi(x_3)\pi(x_4)|0\rangle$$

But now recall this interpolator is calculated in a finite-volume.

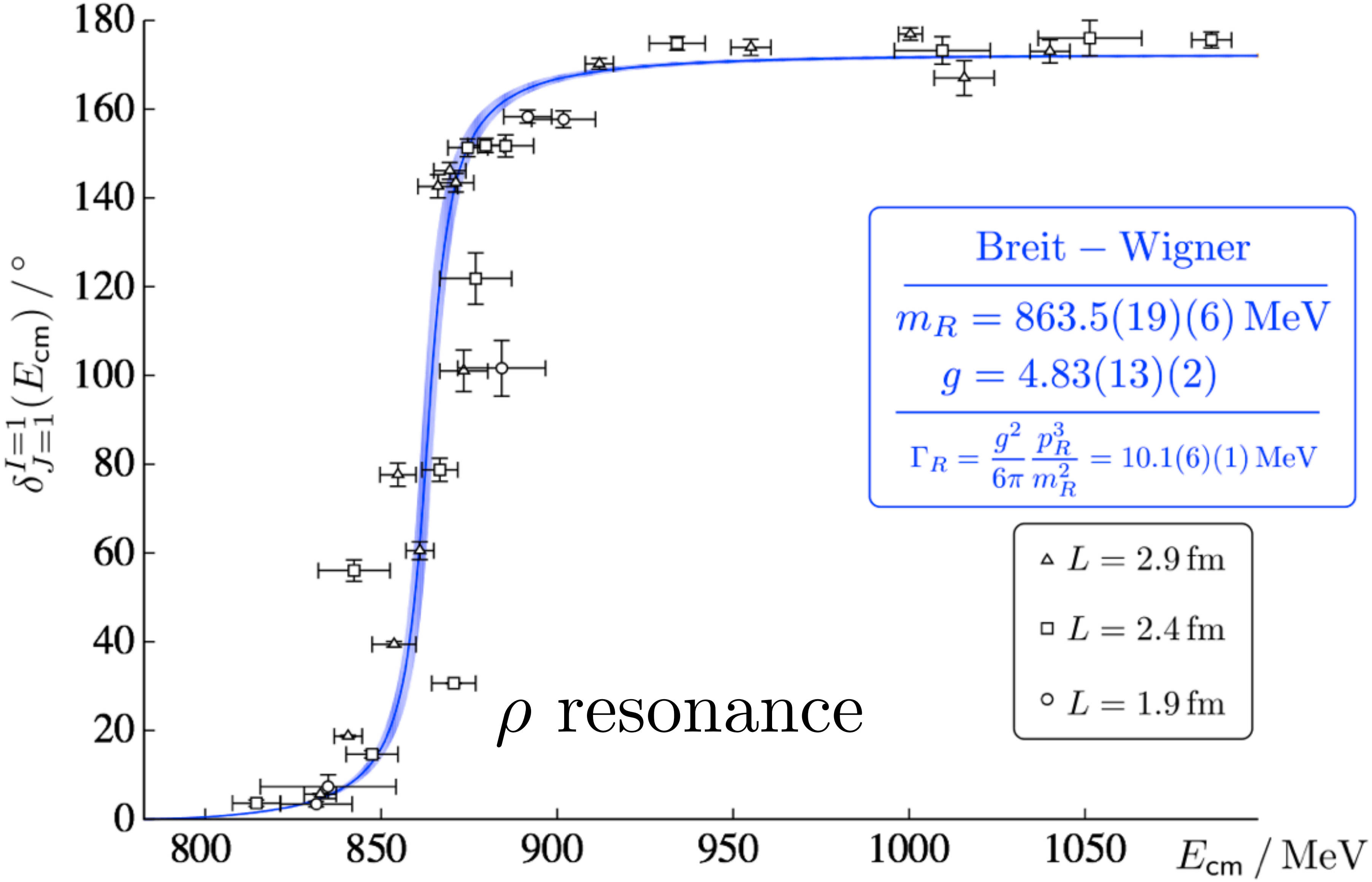
Naively one would seek to remove finite-volume effects.

Instead we embrace finite-volume theory and
use this correlator to determine finite-volume spectrum.

Lüscher found a method for mapping finite-volume spectrum to elastic pion scattering amplitude.

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

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



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

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

In this talk we focus on extracting $\begin{array}{c}\pi\pi \to \pi\pi \\ \pi\pi\pi \to \pi\pi\pi\end{array}$ from Lattice QCD

Lattice QCD

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

This is a necessary first step towards

$D^0 \to \pi^+\pi^- \qquad D^0 \to K^+K^-$

long distance part of $D^0 \longleftrightarrow \overline{D^0}$

More generally it is needed for any decay/scattering with open channels containing more than two hadrons.

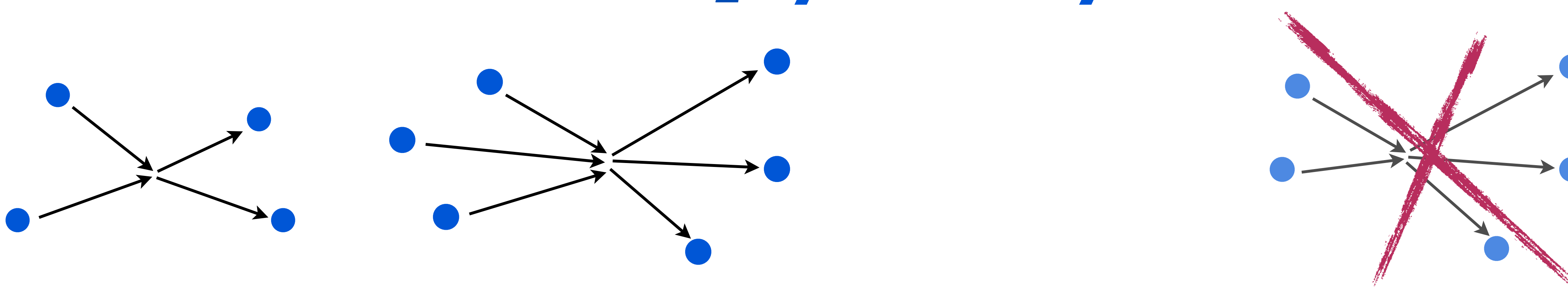
Particle content

Single scalar, mass m

all results for identical scalars

Interactions governed by local, relativistic field theory

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



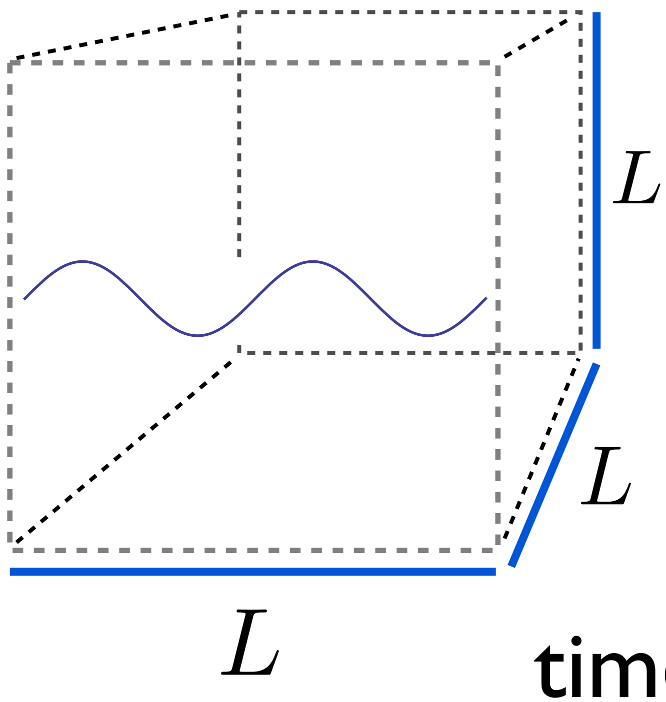
(For pions in QCD this is G-parity)

Theory is otherwise arbitrary...

Include all operators with even number of fields

Make **no assumptions about couplings**

Finite volume



cubic, spatial volume (extent L)

periodic boundary conditions

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

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

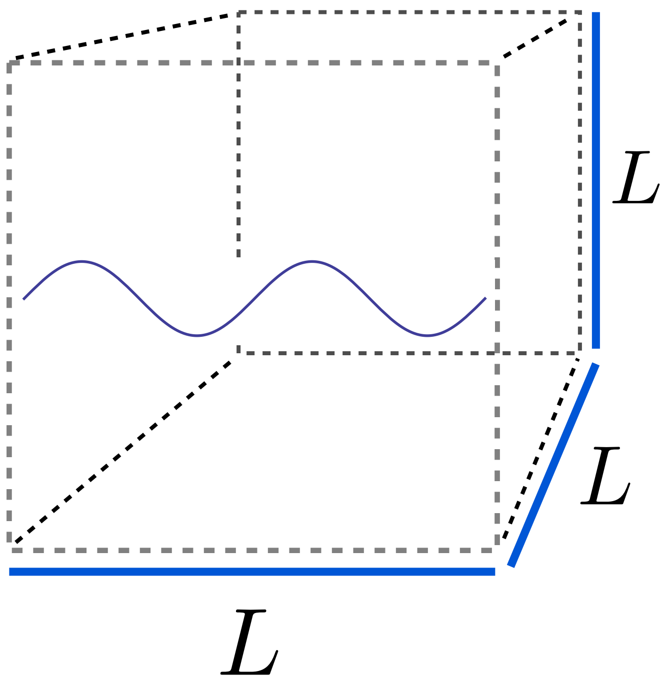
Take L large enough to ignore e^{-mL}

dropped throughout!

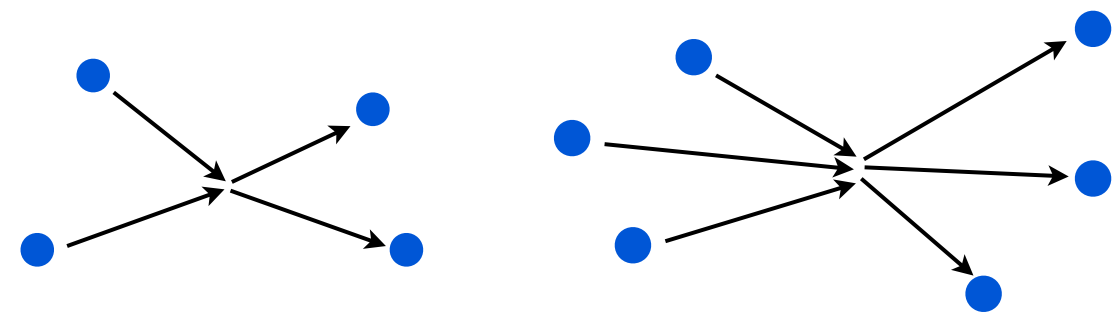
Take space to be continuous

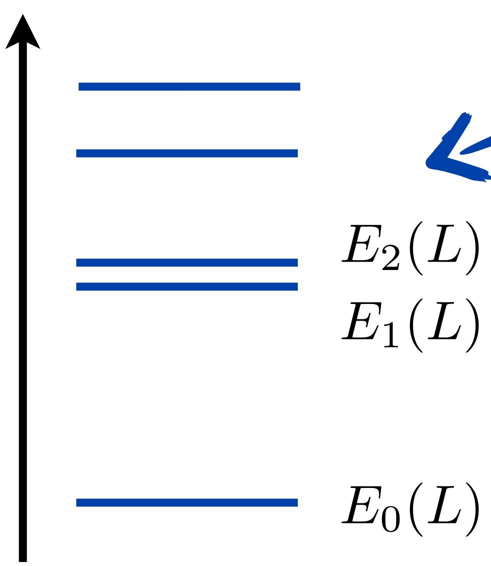
lattice spacing set to zero

Finite volume



Infinite volume





Discrete energy spectrum

Determine mapping between theories

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

Scattering amplitudes

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 $\vec{P} = (2\pi/L)\vec{n}_P$

periodic interpolator
(specify quantum numbers)

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

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nonzero momentum in finite-volume frame

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.

Result depends only on on-shell scattering amplitudes

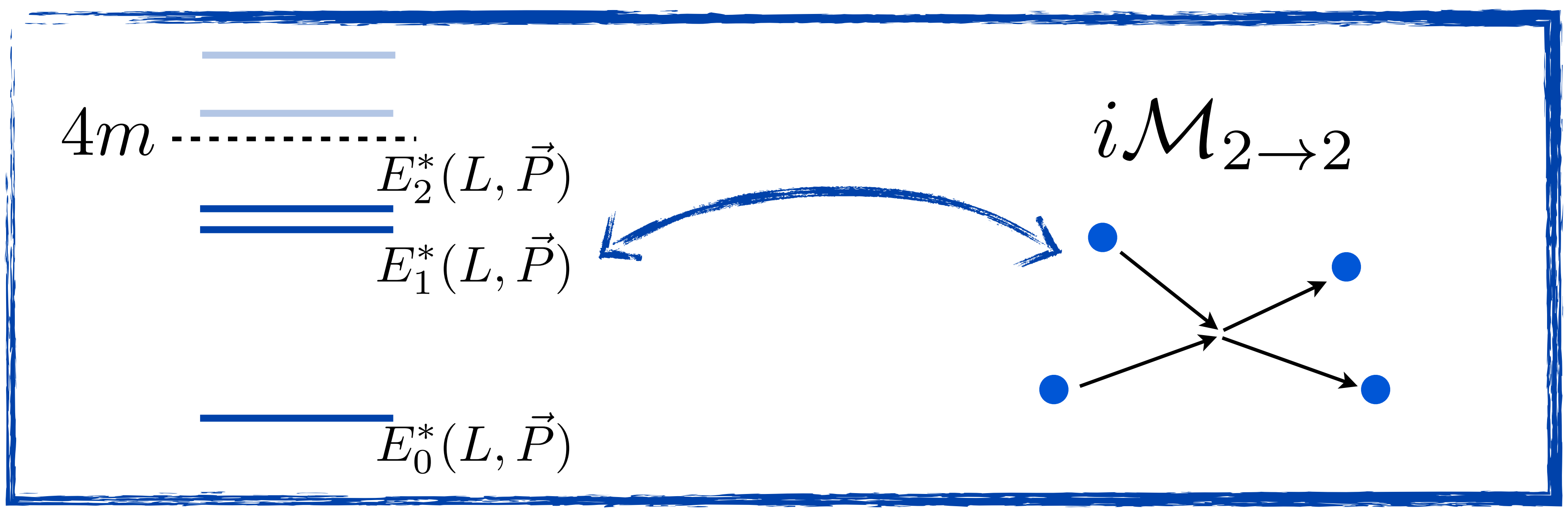
First, two particles in a box

Require $E^* < 4m$

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

give interpolator even-particle quantum numbers

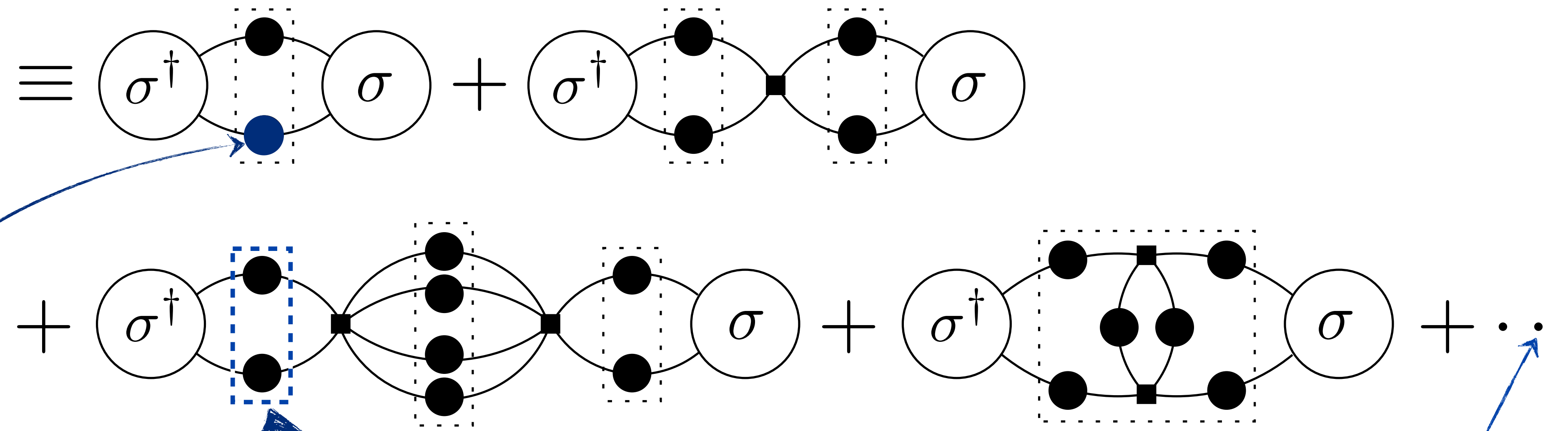
Then only two-to-two scattering enters result



Following derivation is from Kim, Sachrajda and Sharpe.

Nucl. Phys. B727, 218-243 (2005)

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



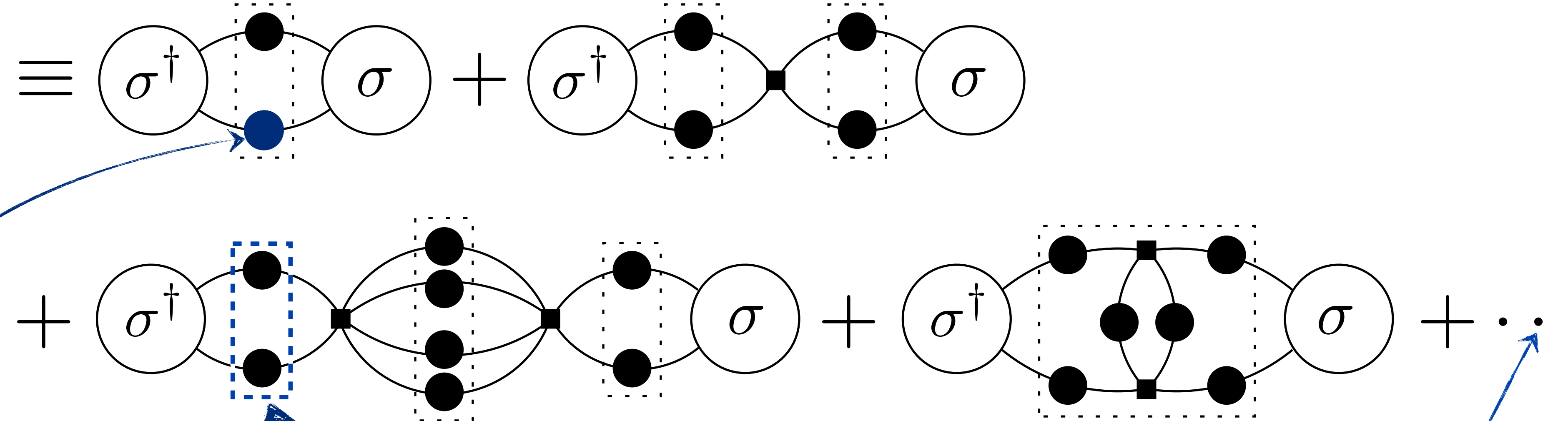
fully dressed propagators

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

infinite set of terms
no assumed suppression

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

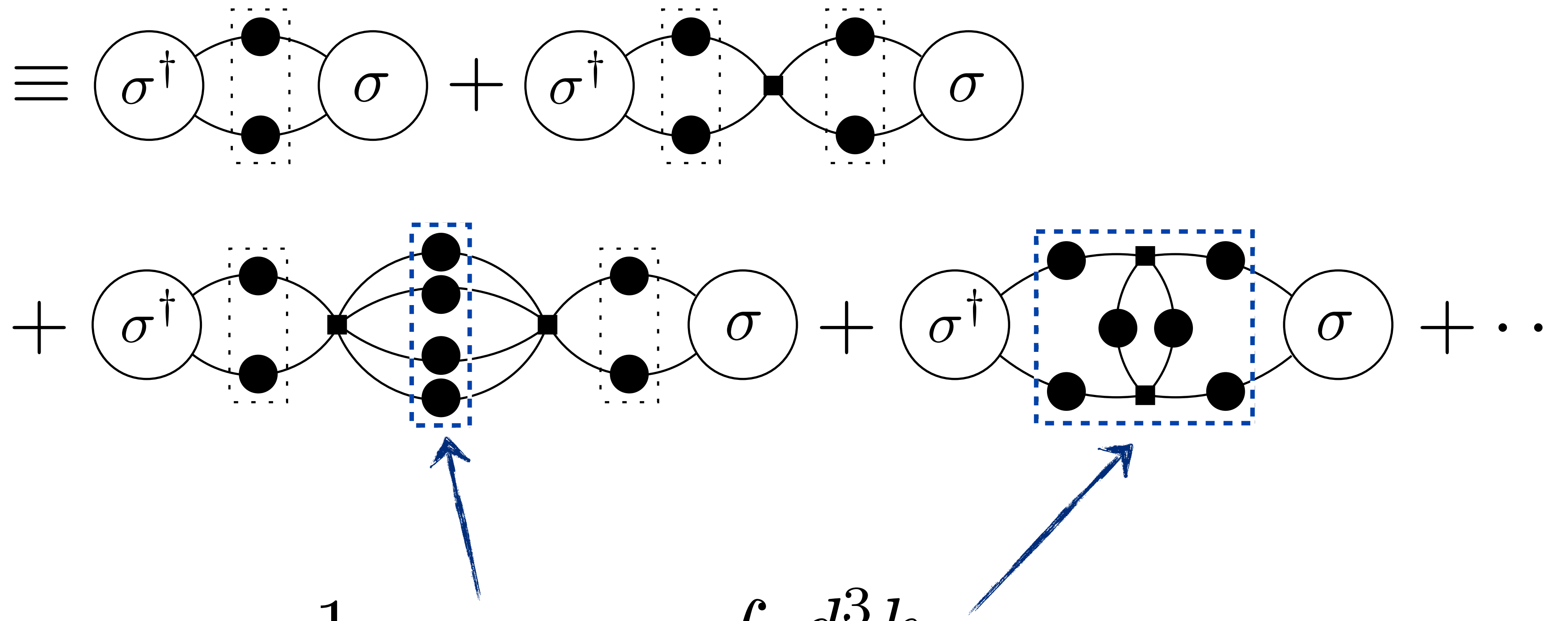
Key observation:

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

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

difference is order e^{-mL}

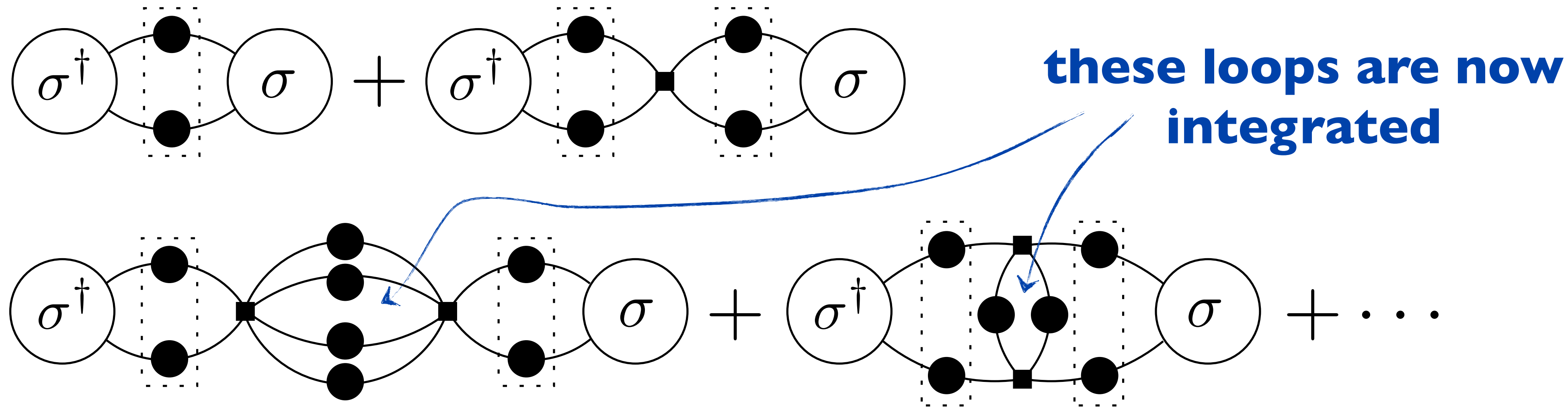
$C_L(E, \vec{P}) \equiv$

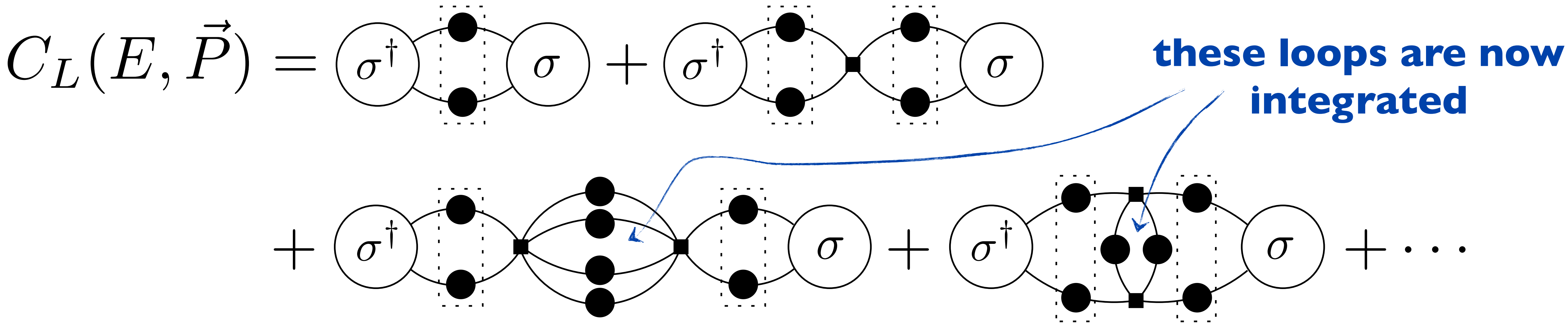


$$\frac{1}{L^3} \sum_{\vec{k}} \longrightarrow \int \frac{d^3 k}{(2\pi)^3}$$

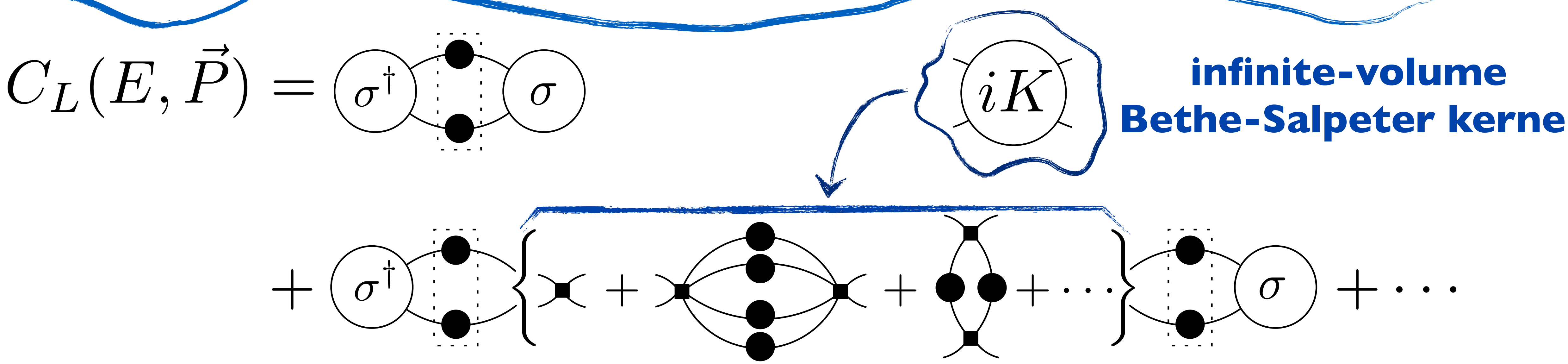
Since $E^* < 4m$, **only two** particles with total momentum $(E, \vec{P})$ **can go on-shell**

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

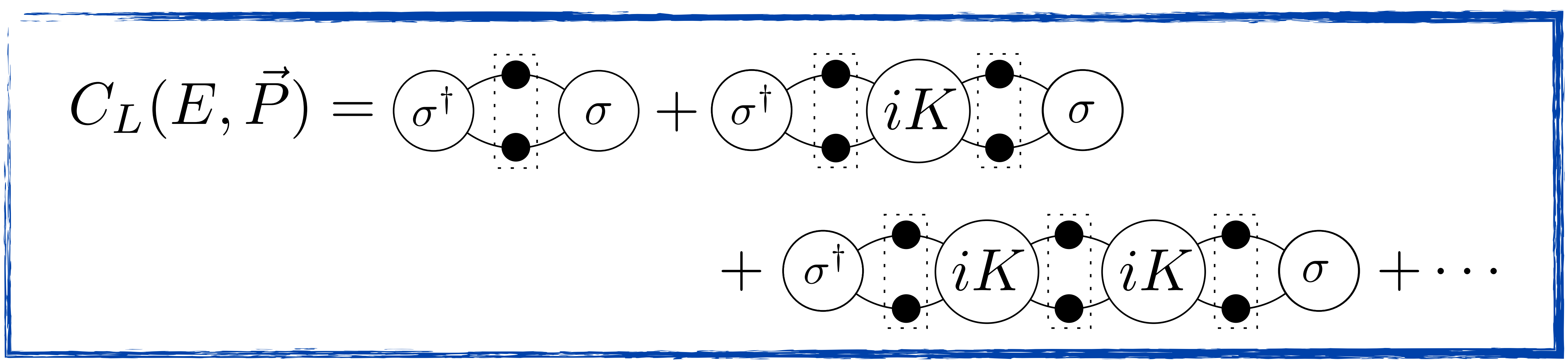




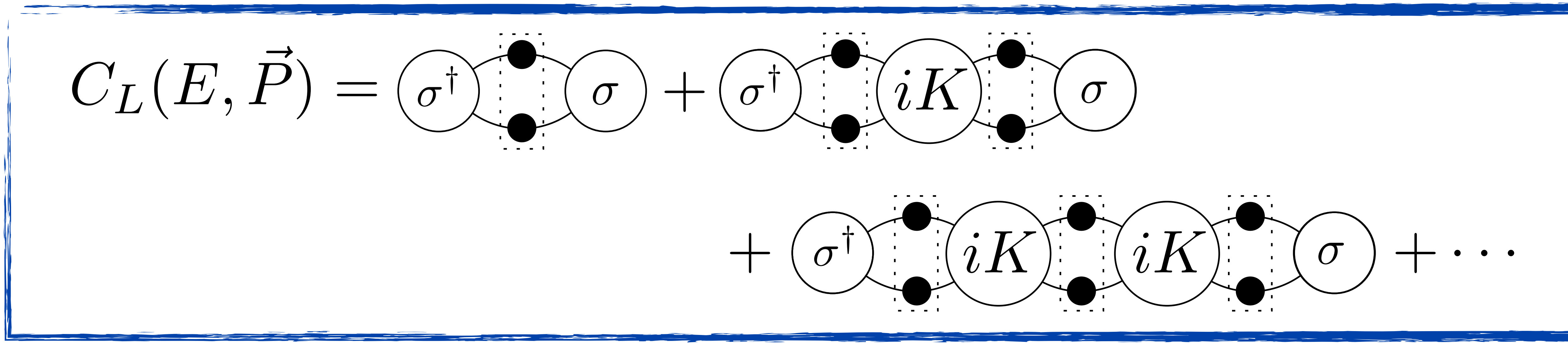
$C_L(E,\vec{P}) =$
these loops are now integrated



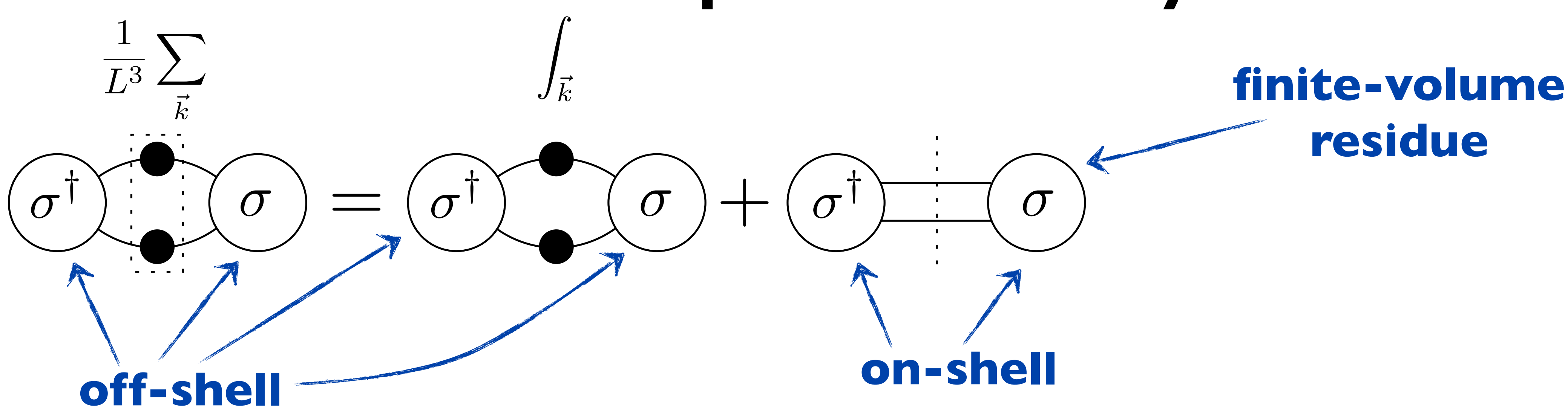
$C_L(E,\vec{P}) =$
iK
infinite-volume Bethe-Salpeter kernel

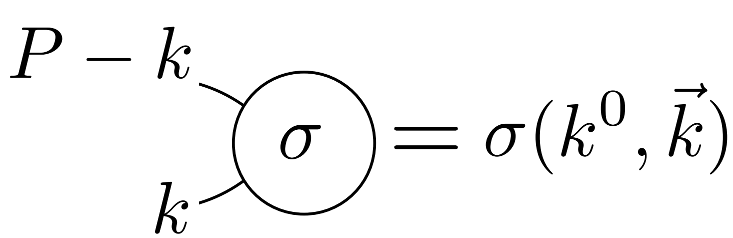


$C_L(E,\vec{P}) =$
iK



Next we introduce an important identity

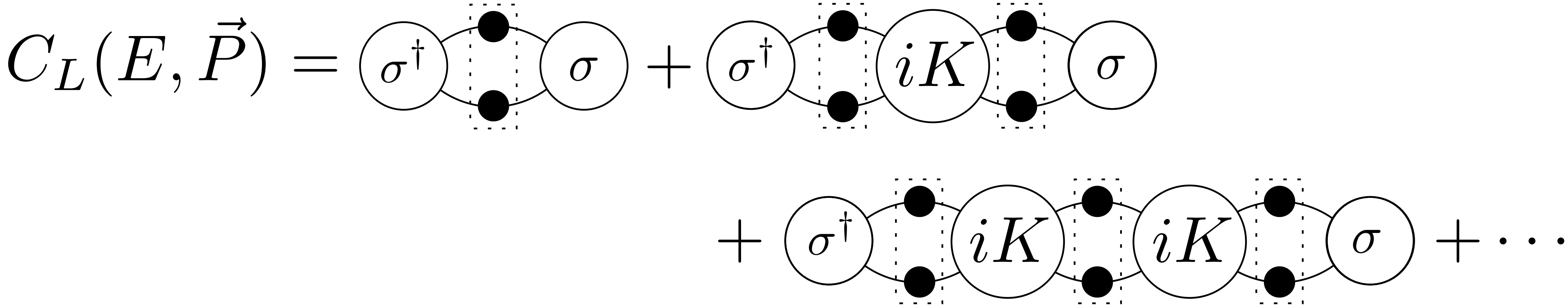




$$\sigma^*(\hat{k}^*) \equiv \sigma(\omega_k,\vec{k})\Big|_{\text{on-shell}}$$

$\hat{k}^*$ parametrizes two on-shell particles with fixed $(E,\vec{P})$

$*$ means CM frame



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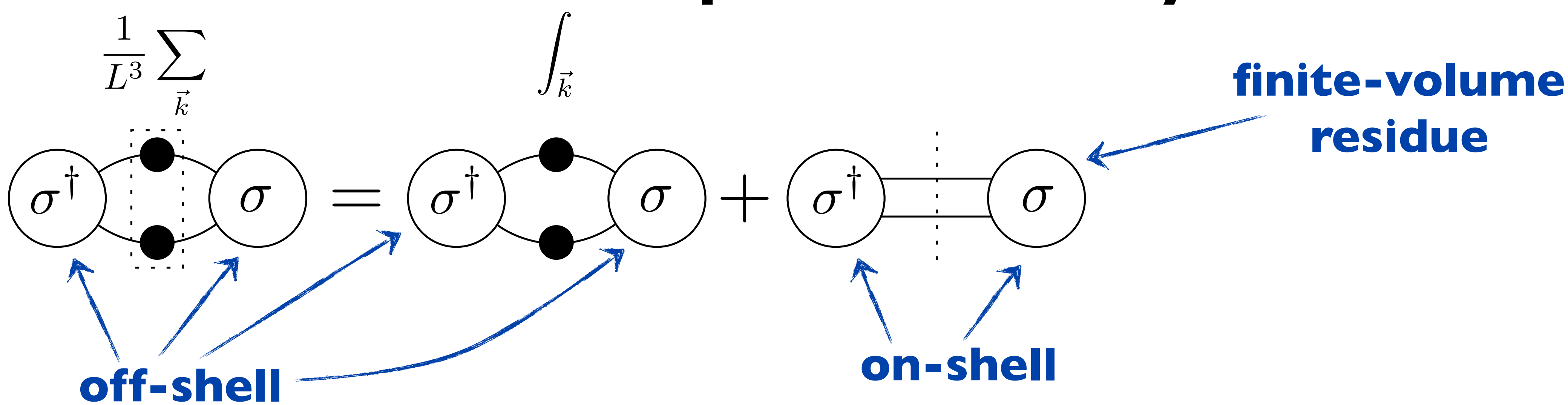
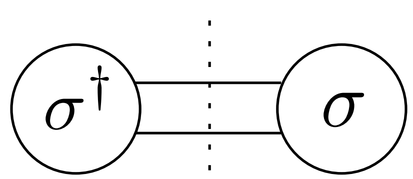


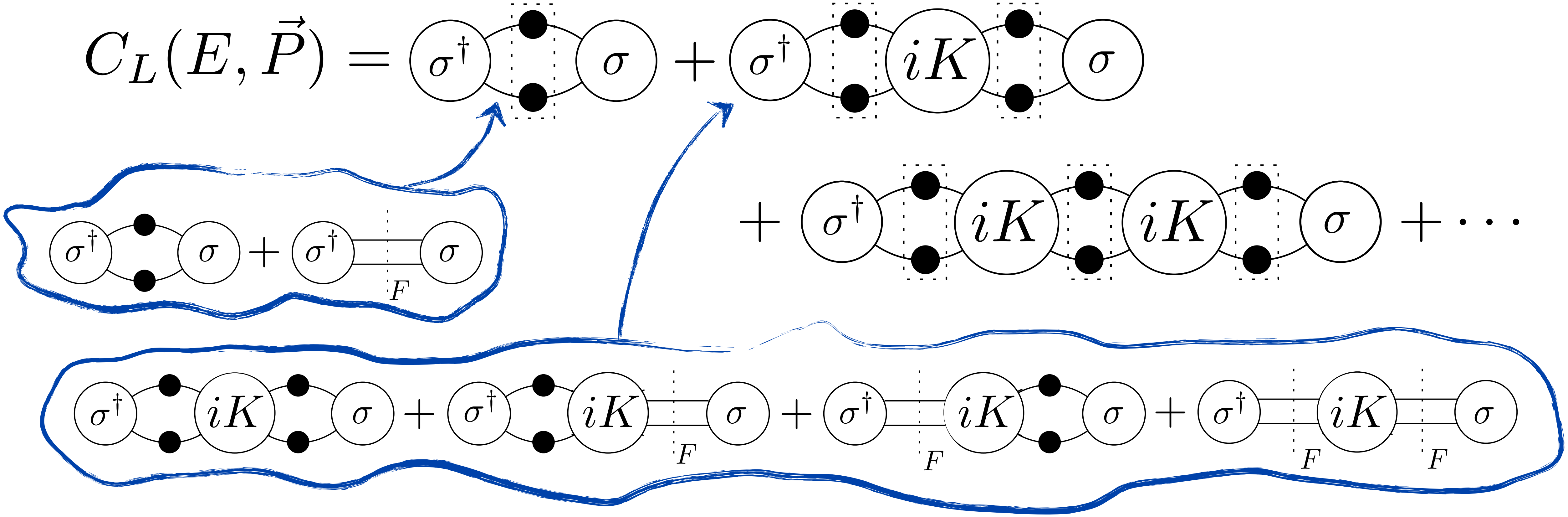


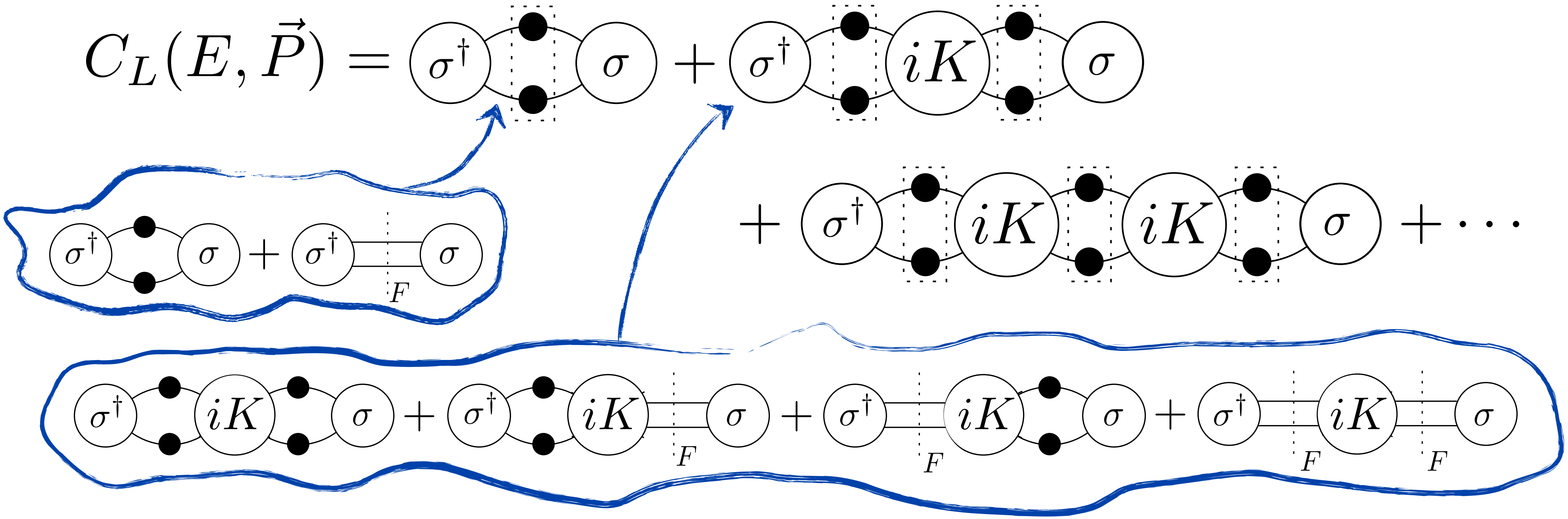
$$= \sigma^*_{\ell',m'} iF_{\ell',m';\ell,m}\sigma^{\dagger *}_{\ell,m} = \sigma^* iF\sigma^{\dagger *}$$

where $\sqrt{4\pi}\,\sigma^*_{\ell,m} Y_{\ell,m}(\hat{k}^*) = \sigma^*(\hat{k}^*)$

and F is a **known** matrix, depending only on **kinematics**

F



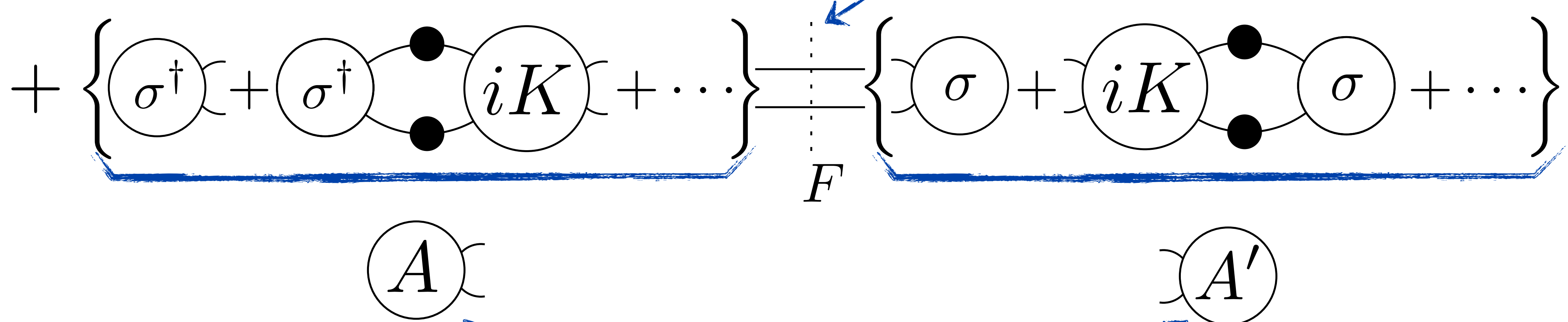


Now regroup by number of F cuts

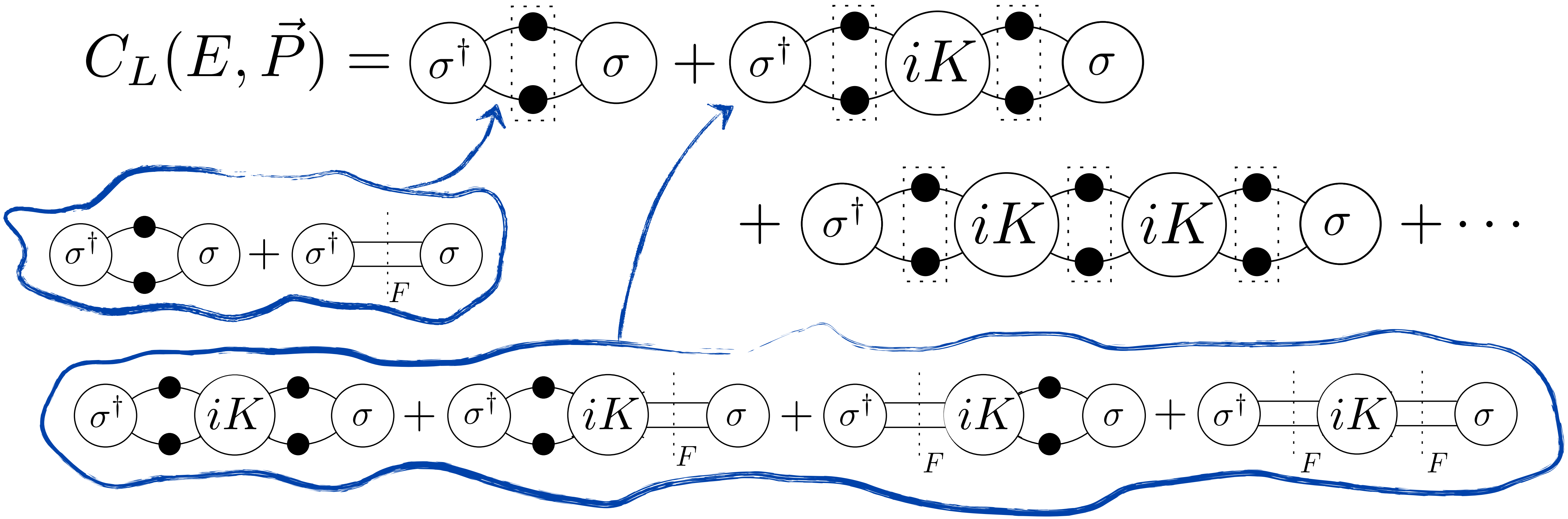
$$C_L(E,\vec{P}) = C_\infty(E,\vec{P})$$

zero F cuts

one F cut



these infinite-volume quantity do not appear in final result



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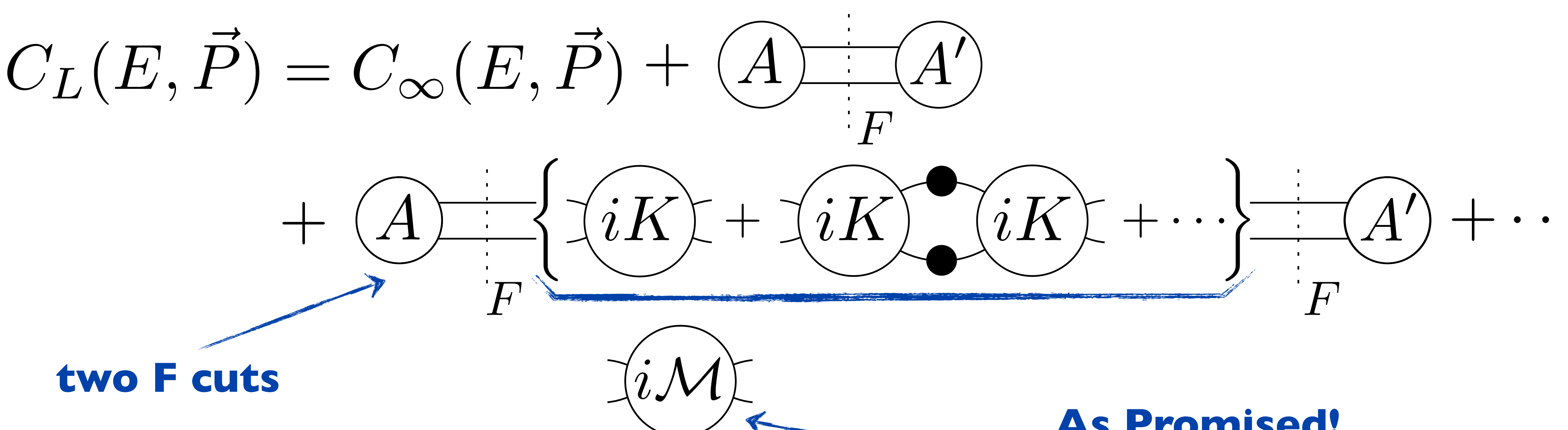
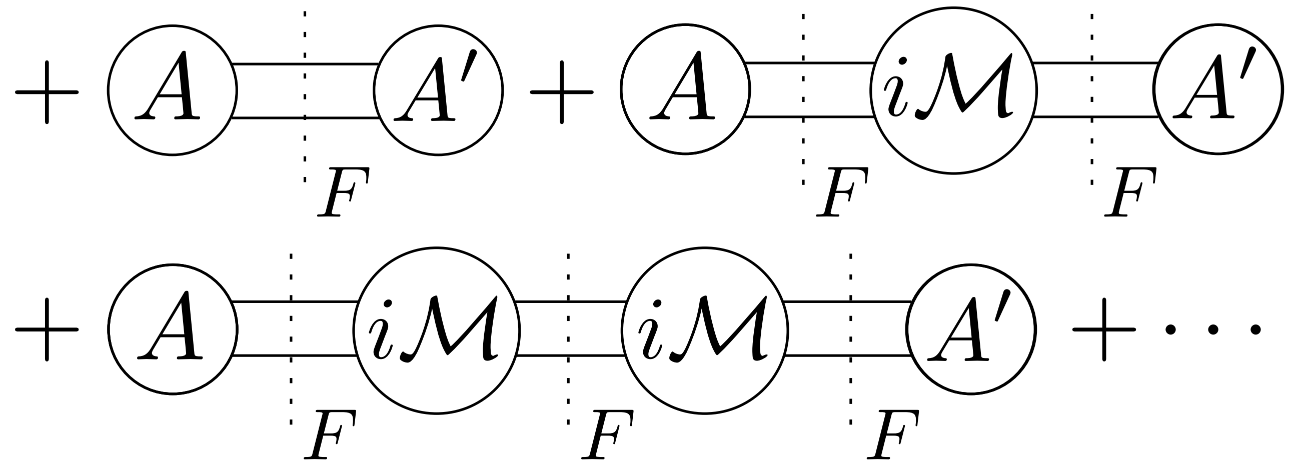


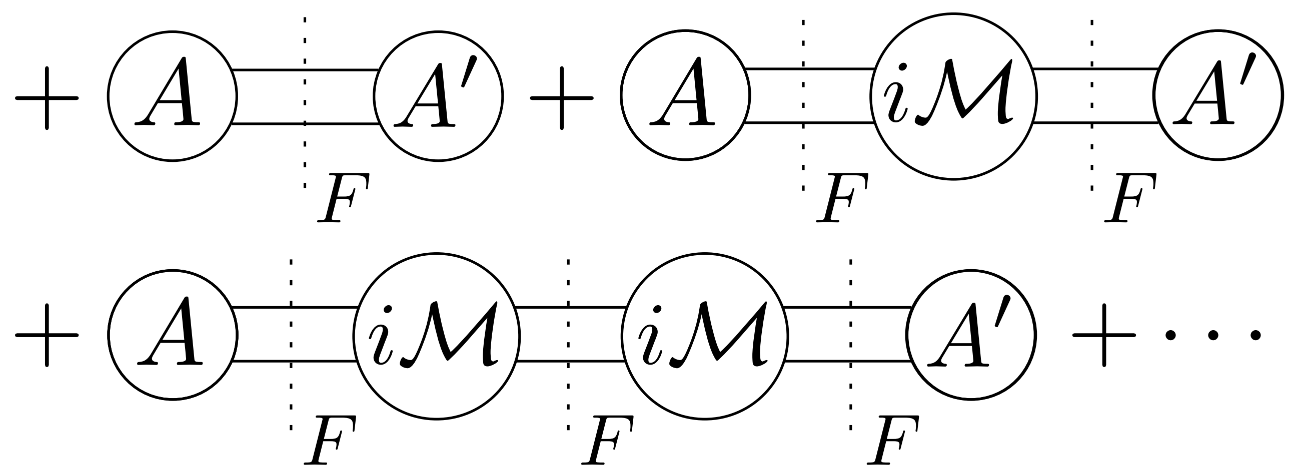
As Promised!
the infinite-volume, on-shell two-to-two scattering amplitude

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



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

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



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

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

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 result

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

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

where

$$4\pi Y_{\ell',m'}(\hat{k}'^*)\; i\mathcal{M}_{2\to 2;\ell',m';\ell,m}\; Y_{\ell,m}(\hat{k}^*) \equiv i\mathcal{M}_{2\to 2}(\hat{k}'^*, \hat{k}^*)$$

$$iF_{\ell',m';\ell,m} \equiv \frac{1}{2}\left[\frac{1}{L^3}\sum_{\vec{k}} - \int_{\vec{k}}\right] \frac{i4\pi Y_{\ell',m'}(\hat{k}^*) Y^*_{\ell,m}(\hat{k}^*)}{2\omega_k 2\omega_{P-k}(E - \omega_k - \omega_{P-k} + i\epsilon)}$$

with $\omega_k^2 = \vec{k}^2 + m^2$

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

First note $i\mathcal{M}_{2\to 2;\ell',m';\ell,m} \propto \delta_{\ell,\ell'}\delta_{m,m'}$

rotational invariance of infinite-volume theory

By contrast, $iF_{\ell',m';\ell,m}$ is not diagonal $\longrightarrow$ partial wave mixing

rotation symmetry broken by finite-volume

Nonetheless, if $i\mathcal{M}_{2\to 2;00;00}$ is the dominant contribution then only need to keep $iF_{00;00}$

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

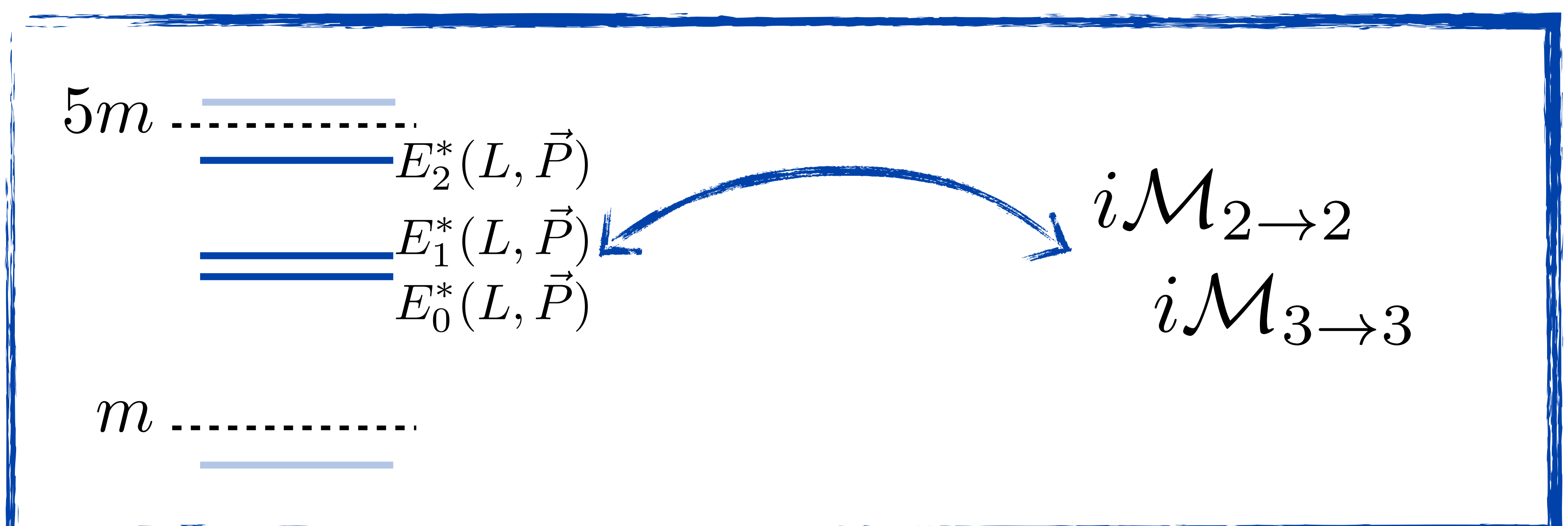
Now, three particles in a box

Require $m < E^* < 5m$

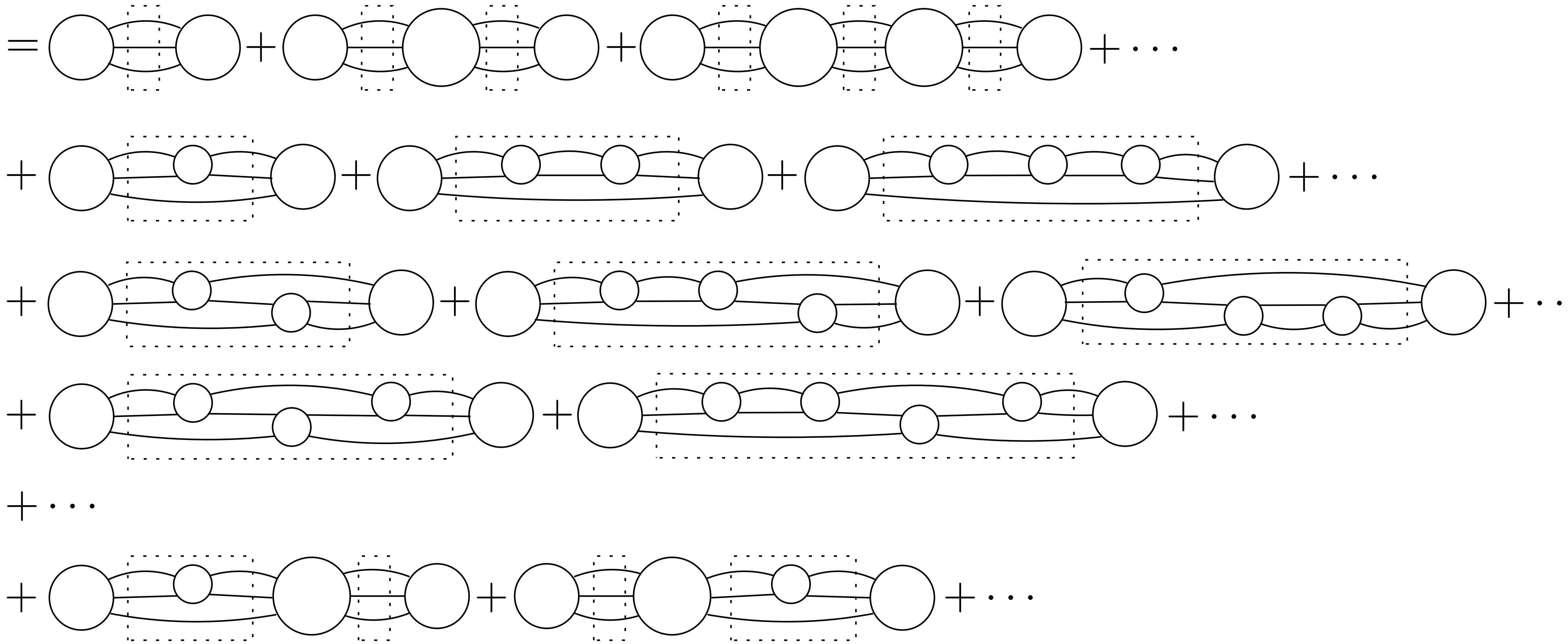
$$C_L(E, \vec{P}) \equiv \int_L d^4x\, e^{i(Ex^0 - \vec{P}\cdot\vec{x})} \langle 0|\mathrm{T}\sigma(x)\sigma^\dagger(0)|0\rangle$$

give interpolator odd-particle quantum numbers

Then two-to-two and three-to-three scattering enters result

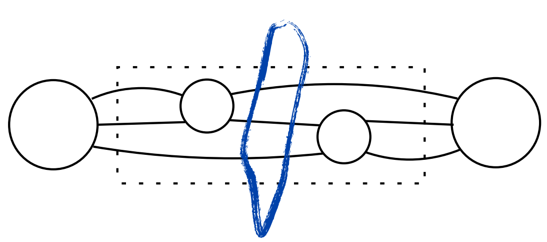


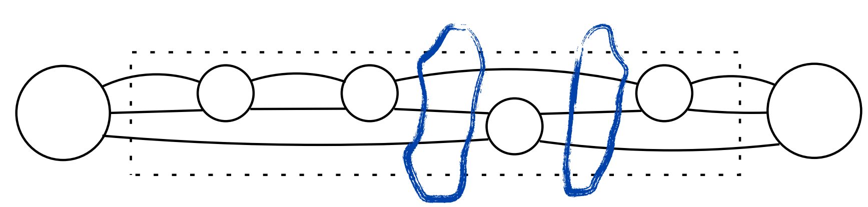
$C_L(E, \vec{P}) =$



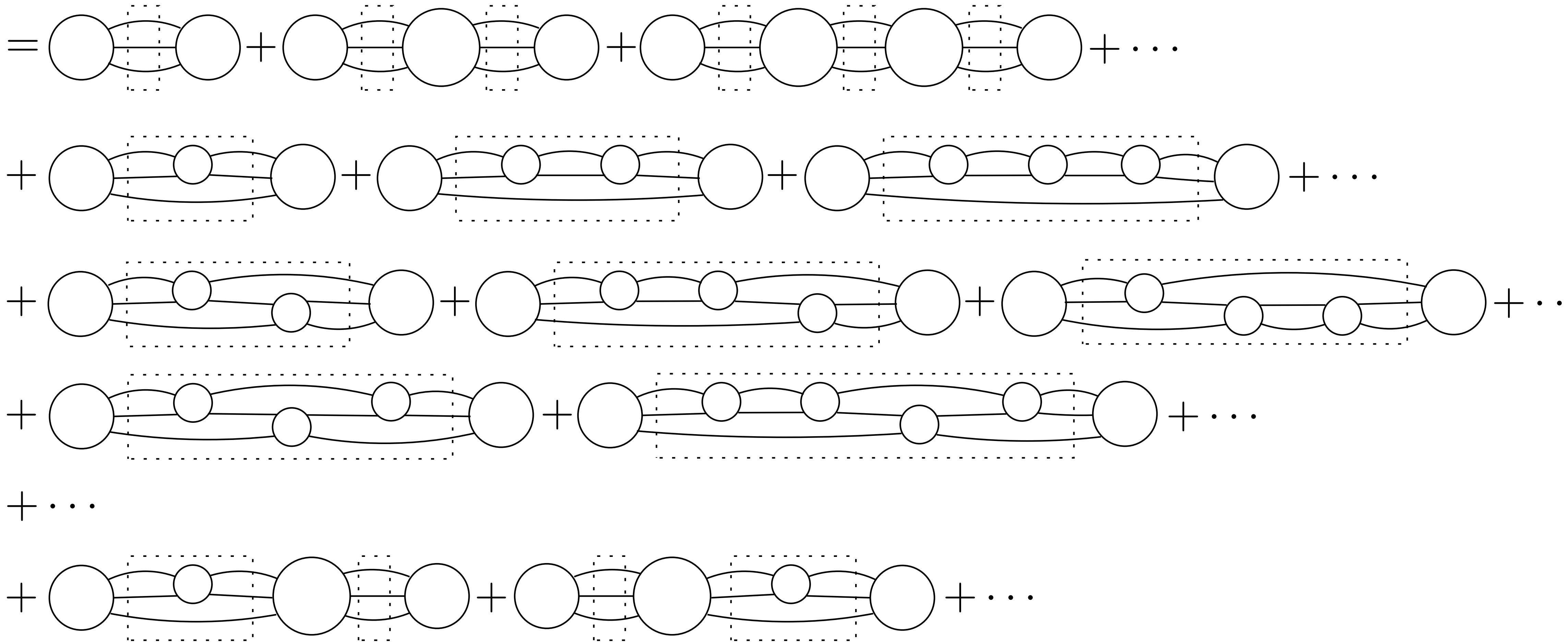
Top line can be summed following two-particle case.
But this approach does not easily generalize to include other diagrams.

Central difficulty comes from diagrams with
two-to-two insertions switching to different pair





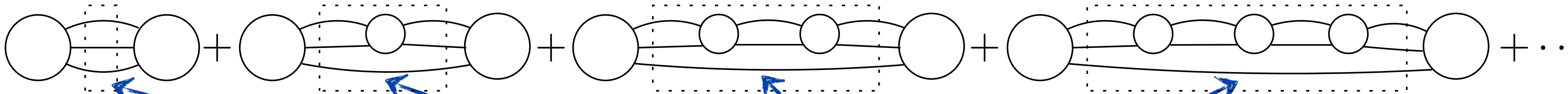
$C_L(E, \vec{P}) =$



Still, it is possible to sum all diagrams.
It is not, however, possible to explain the full story here.

Instead, focus here on two parts of derivation.
Each part contains an important lesson, needed to understand the final result.

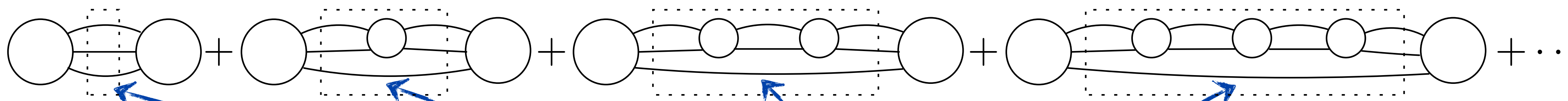
First Part: Sum "no-switch" diagrams

$C_L^{(1)} \equiv$ 

call the bottom momentum k

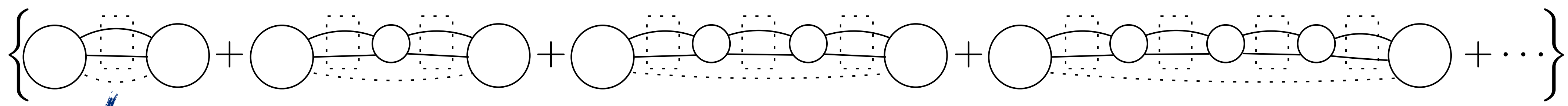
important finite-volume corrections only arise from $k^0 = \omega_k$

First Part: Sum “no-switch” diagrams

$C_L^{(1)} \equiv$ 

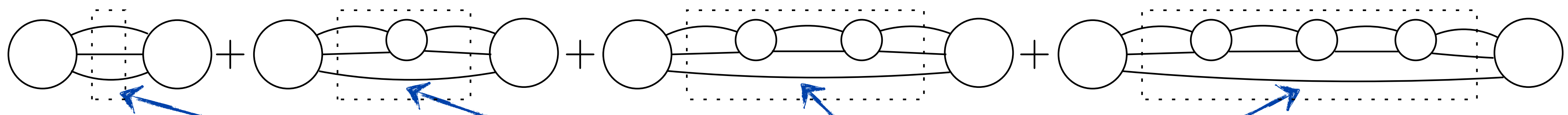
call the bottom momentum k

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

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

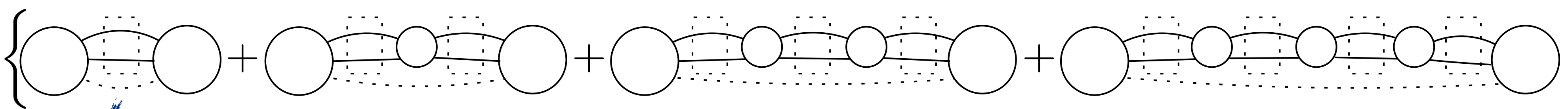
bottom propagator replaced with $1/(2\omega_k)$
and pulled out front

First Part: Sum "no-switch" diagrams

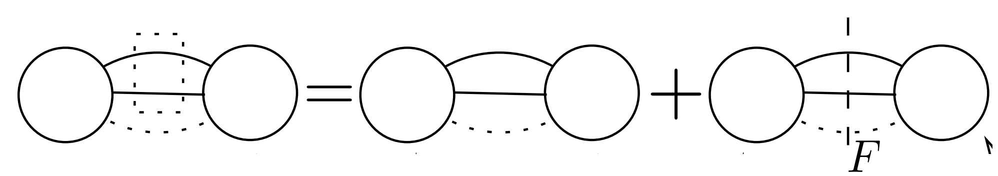
$C_L^{(1)} \equiv$  $+ \cdots$

call the bottom momentum k

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

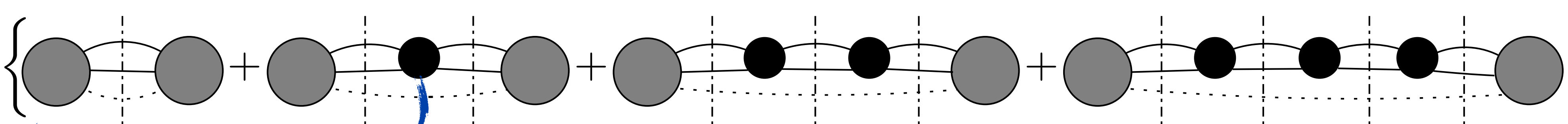
$C_L^{(1)} = \frac{1}{L^3}\sum_{\vec{k}} \frac{1}{2\omega_k}\Big\{$  $+ \cdots \Big\}$

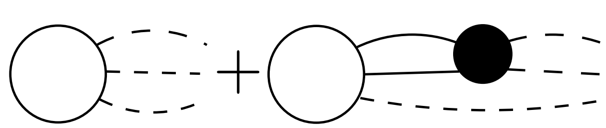
bottom propagator replaced with $1/(2\omega_k)$
and pulled out front

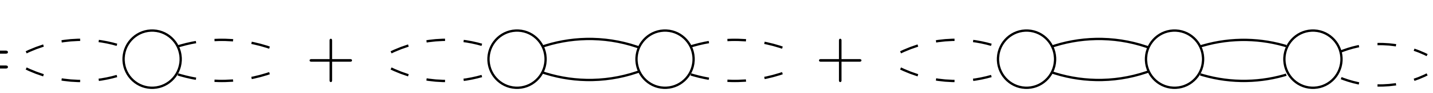
now substitute 

and rearrange by number of F insertions

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

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

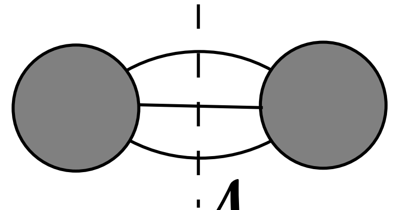
$=$ 

$=$  $+ \cdots$

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

Deduce

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

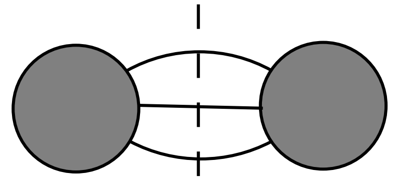


$\mathcal{A}$

$$[\mathcal{A}] = \frac{iF}{2\omega L^3} \frac{1}{1 - i\mathcal{M}_{2\to 2} iF}$$

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

Deduce

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

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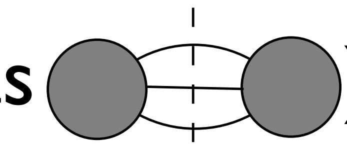
Main Lesson From Part One

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

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

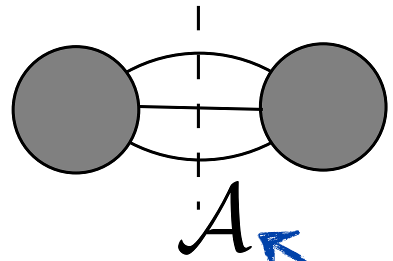
[finite-volume momentum]x[angular momentum]

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

$$iF_{k',\ell',m';k,\ell,m} = \delta_{k,k'}\ iF_{\ell',m';\ell,m}(E-\omega_k, \vec{P}-\vec{k})$$
$$i\mathcal{M}_{k',\ell',m';k,\ell,m} = \delta_{k,k'}\ i\mathcal{M}_{\ell',m';\ell,m}(E-\omega_k, \vec{P}-\vec{k})$$

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

Deduce

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

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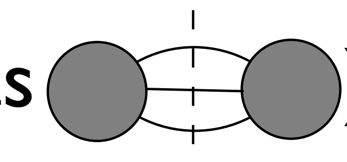
Finite volume residue terms (such as ) are of the form:

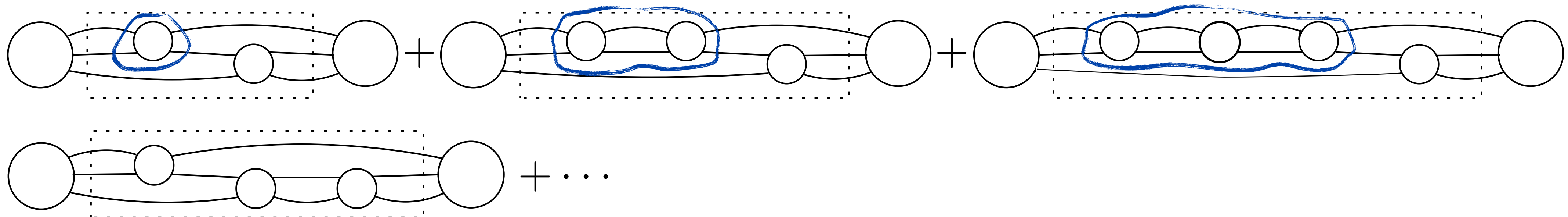
(row vector)x(matrix)x(column vector), acting on product space

[finite-volume momentum]x[angular momentum]

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

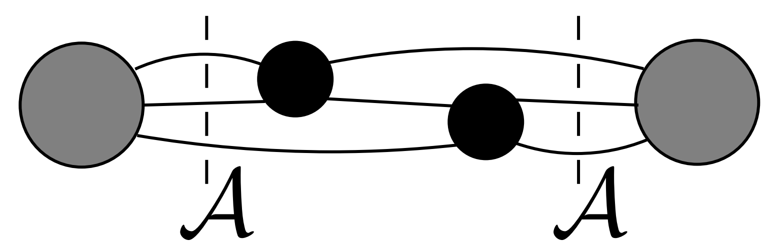
Second part: Sum "one-switch" diagrams

$$C_L^{(2)} =$$



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

$$C_L^{(2)} = C_\infty^{(2)} +$$

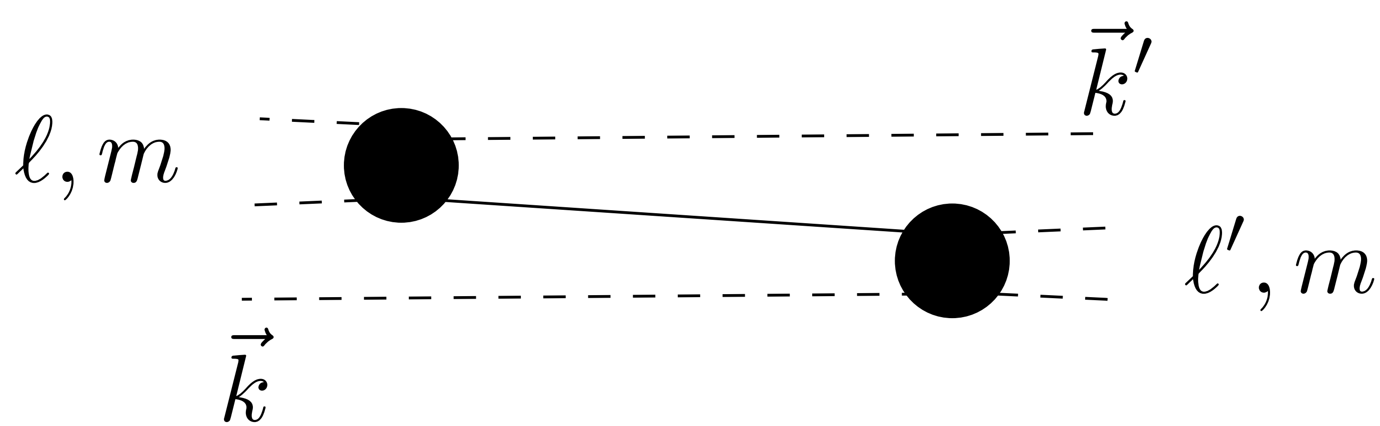


$$+ \cdots$$

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

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

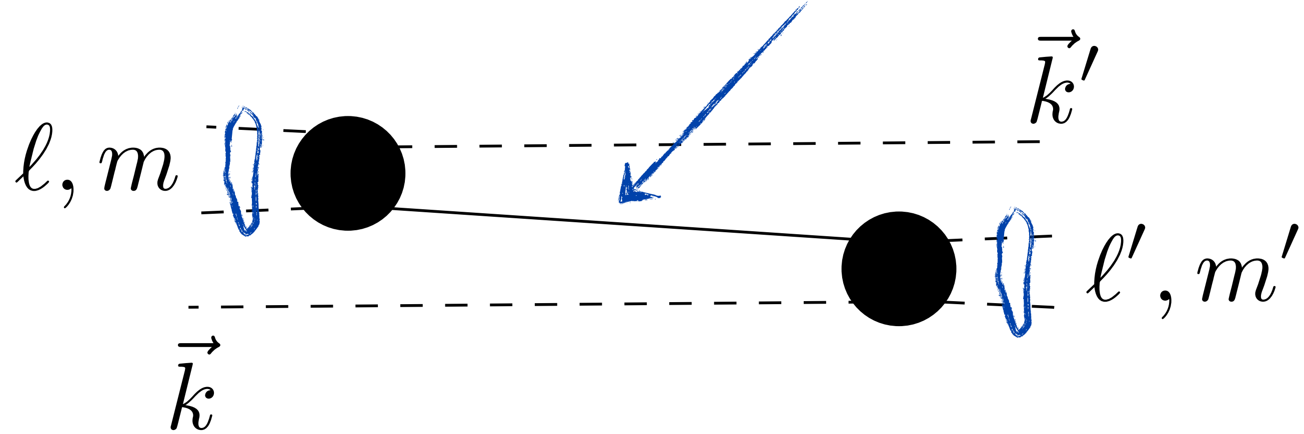
$$i\mathcal{M}^{(2,\mathrm{unsym})}_{3\to3;k',\ell',m';k,\ell,m} \equiv$$



Main Lesson From Part Two

Certain external moment put the intermediate propagator on-shell

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

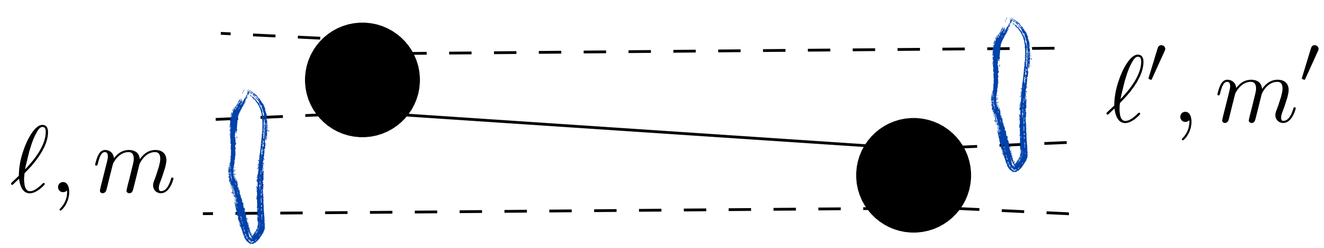


This implies that this diagram, and indeed also the full $i\mathcal{M}_{3\to 3}$ **has physical poles above threshold**

nothing to do with bound states

This is a problem because the amplitude is symmetric in external momenta

$$i\mathcal{M}_{3\to 3;k',\ell',m';k,\ell,m} \overset{!}{\supset}$$

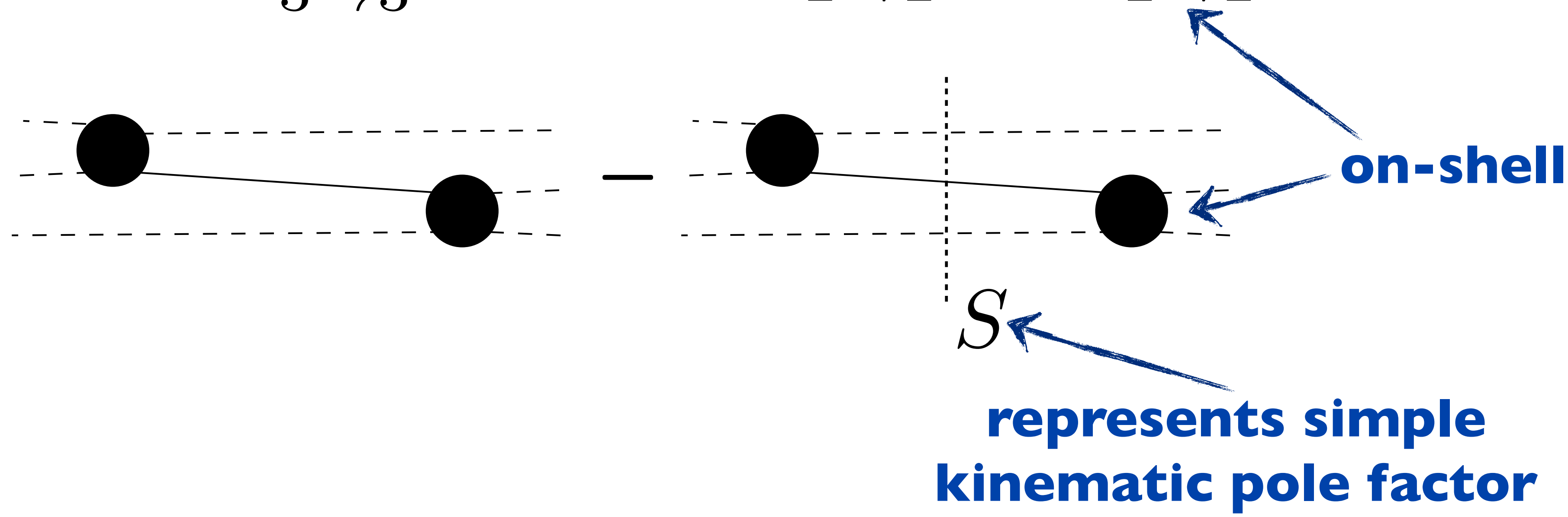


But this would demand decomposing a singular function in $Y_{\ell,m}$

The decomposition is not valid!

Resolution: Introduce

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



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

Can decompose in harmonics and truncate expansion at low energies

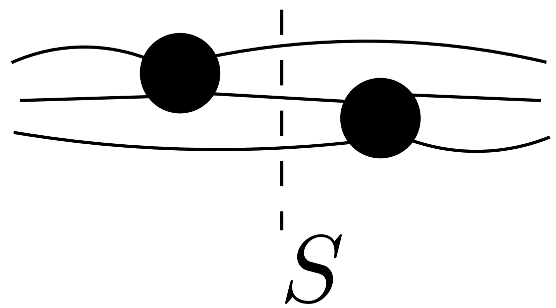
The approach of separating out singularities like this was first suggested over 40 years ago (Rubin et al. *PR 146-6* (1966))

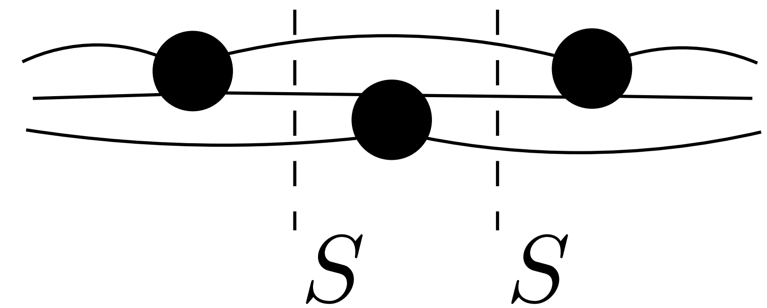
It makes sense to recover a singularity-free quantity from finite-volume spectrum. Then add singular terms back in.

This pattern of separating out singularities persists to all orders

Define

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





only on-shell amplitudes here

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

This definition arises from analyzing all two-to-two diagrams

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

is the observable to extract from the spectrum.

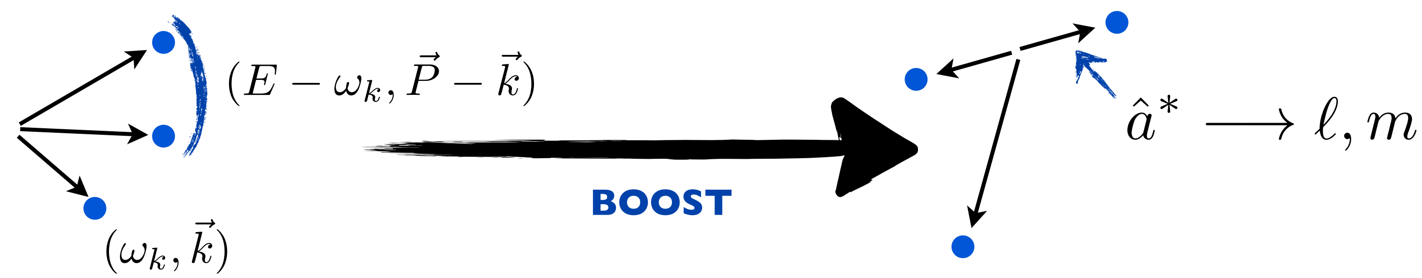
Review Lessons

1. In the three particle case, all matrices act on product space

[finite-volume momentum]x[angular momentum]

In other words, they have indices $\vec{k}, \ell, m$

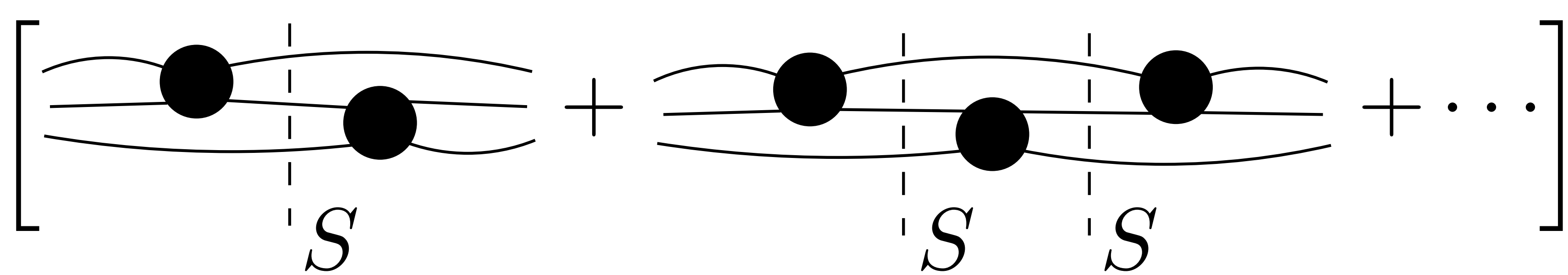
needed to describe three particles



2. Singularities in $i\mathcal{M}_{3\to3}$ invalidate decomposition in $Y_{\ell,m}$

Resolution is to introduce $i\mathcal{M}_{df,3\to3;k',\ell',m';k,\ell,m}$

$$i\mathcal{M}_{df,3\to3} \equiv i\mathcal{M}_{3\to3} -$$



This object arises naturally in finite-volume analysis.

Three-particle result

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

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

where

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

and

$$iF_{k,k'} \equiv \delta_{k,k'}\frac{1}{2}\left[\frac{1}{L^3}\sum_{\vec{a}} - \int_{\vec{a}}\right]\frac{i4\pi Y(\hat{a}^*)Y^*(\hat{a}^*)}{2\omega_a 2\omega_{P-k-a}(E - \omega_k - \omega_a - \omega_{P-k-a} + i\epsilon)}$$

$$iG_{k,p} \equiv \frac{1}{2\omega_p L^3}\frac{i4\pi Y(\hat{p}^*)Y^*(\hat{k}^*)}{2\omega_{P-p-k}(E - \omega_p - \omega_k - \omega_{P-p-k})}$$

Here harmonic indices are left implicit.

$\Delta_{L,P}(E) = \det[1 - i\mathcal{M}_{df,3\to3} iF_3] = 0$...is it useful?

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

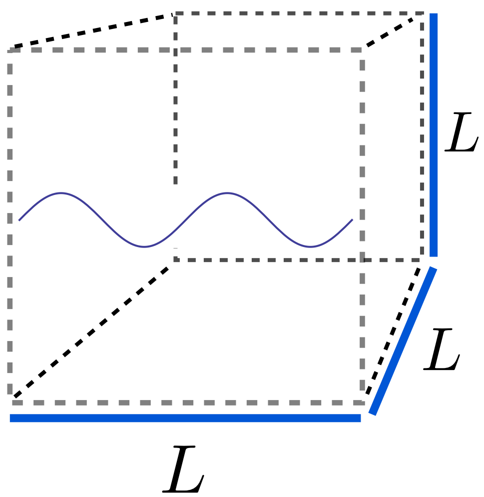
$$\boxed{i\mathcal{M}_{df,3\to3}(E_n^*) = [iF_{3,\text{iso}}(E_n, \vec{P}, L)]^{-1}}$$

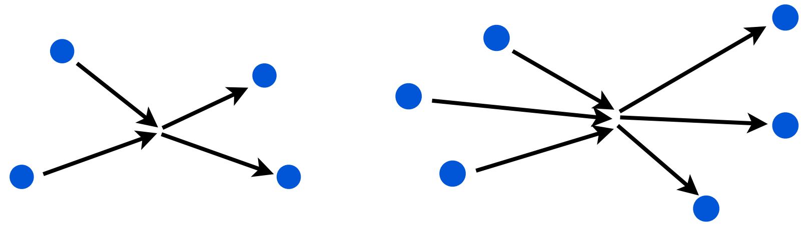
$$iF_{3,\text{iso}} \equiv \sum_{\vec{k},\vec{p}} iF_{3;k,p}$$

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

Conclusions

We have presented our result for extracting three-to-three scattering from finite-volume spectrum.





This is a necessary first step towards

$$D^0 \to \pi^+\pi^- \qquad D^0 \to K^+K^-$$

long distance part of $D^0 \longleftrightarrow \overline{D^0}$

More generally it is needed to extract any decay or scattering amplitude with more than two hadrons from Lattice QCD.

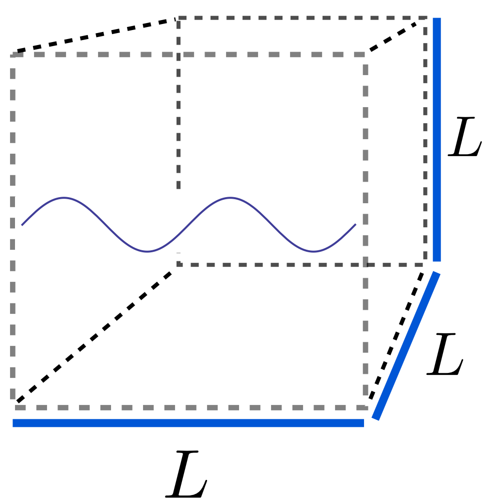
Future work and Applications

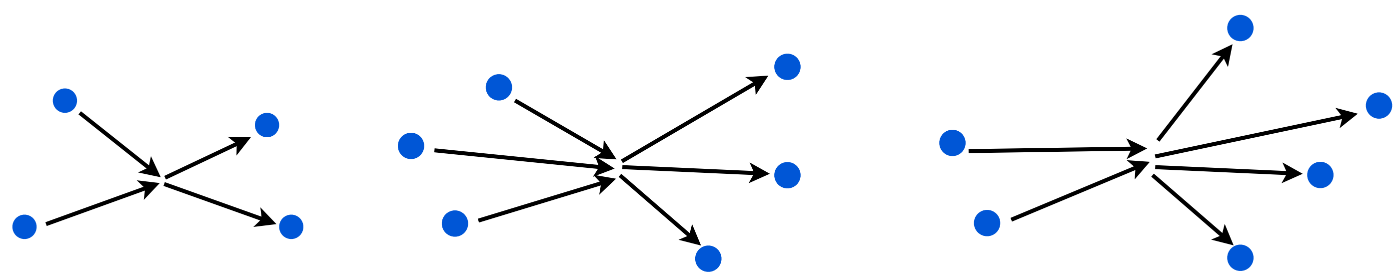
Generalize the Lellouch-Lüscher method, to find Lattice method for extracting weak decay into three particles

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

Generalize to accommodate non-identical and non-degenerate particles as well as spin.

Generalize mapping to accommodate four-particle states.





Identify as many channels as possible and begin program of extracting observables.