## Three-particle scattering from numerical lattice QCD

Scattering from the lattice: applications to phenomenology and beyond

## Maxwell T. Hansen

May 14-I8th, 2018

## Review:

(I) Alternative two-particle derivation (Kim, Sachrajda, Sharpe)
$C_{L}(P)=(0) \cdot(O):(0) \geq C_{L}(P)=C_{\infty}(P)-A^{\prime} F \frac{1}{1+\mathcal{M}_{2 \rightarrow 2} F} A$ $+(0):(i B):(0)+$
IV Lellouch-Lüscher via pole matching
$\frac{L^{3}\langle 0| \mathcal{O}(0)|n, \vec{P}, L\rangle\langle n, \vec{P}, L| \mathcal{O}^{\dagger}(0)|0\rangle}{E-E_{n}} \frac{\langle 0| \mathcal{O}(0) \mid \pi \pi, \text { in }\rangle \mathcal{R}\left(E_{n}, \vec{P}, L\right)\langle\pi \pi, \text { out }| \mathcal{O}^{\dagger}(0)|0\rangle}{E-E_{n}}$

## Review:

I- Alternative two-particle derivation (Kim, Sachrajda, Sharpe)

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\begin{aligned}
C_{L}(P)=O^{+} \bullet(O) & +O^{\circ} \bullet(i B!O \\
& +O C_{L}(P)=C_{\infty}(P)-A^{\prime} F \frac{1}{1+\mathcal{M}_{2 \rightarrow 2} F} A
\end{aligned}
$$

(V) Lellouch-Lüscher via pole matching
$L^{3}\langle 0| \mathcal{O}(0)|n, \vec{P}, L\rangle\langle n, \vec{P}, L| \mathcal{O}^{\dagger}(0)|0\rangle$


■ A real, smooth, three-particle quantity ... $\mathcal{K}_{\mathrm{df}, 3} \not \supset \cdots \cdots \cdots \cdots \cdots \cdots$
I] Three-particle quantization condition
$c_{L}(E, \vec{P})=0=0+0=0+0=0=0+\cdots$


$$
C_{L}(E, \vec{P})=C_{\infty}(E, \vec{P})-A^{\prime} F_{3} \frac{1}{1+\mathcal{K}_{\mathrm{df}, 3} F_{3}} A
$$

IV Road to physics:
I. Use q.c. + energy levels to determine $\mathcal{K}_{\mathrm{df}, 3}$
II. Use known integral equation to relate $\mathcal{K}_{\mathrm{df}, 3}$ to $\mathcal{M}_{3}$

## Outline

$\square$ Warm up and definitions
$\square$ Basic set-up
$\square$ Finite-volume correlator
$\bar{\square}$ Three non-interacting particles
$\square$ Two particles in a box
IV Alternative derivation
Truncation and application
Relating matrix elements

- Three particles in a box


3-to-3 scattering (Sketch of) derivation
An unexpected infinite-volume quantity Relating energies to scattering
$\square$ Testing the result
D Know issues
D Large-volume expansion
D Effimov state in a box

## 口 Other methods

$\square$ Numerical explorations
$\square$ Truncation at low energies
D Toy solutions for various systems Unphysical solutions
$\square$ Looking forward

## Current status

Model- \& EFT-independent relation between finite-volume energies and relativistic two-and-three particle scattering


(a),(b) MTH and Sharpe (2015),(2016) (c) Briceño, MTH, Sharpe (2017)

## Smooth cutoff function

$\mathcal{K}_{\mathrm{df}, 3}$ and $F_{3}$ depend on a smooth cutoff function
To see why, consider one of the contributions to $C_{L}$...


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$\mathcal{K}_{\mathrm{df}, 3}$ and $F_{3}$ depend on a smooth cutoff function
To see why, consider one of the contributions to $C_{L \ldots}$


We choose to sum subdiagrams into $\mathcal{K}_{2}$
On-shell $\mathcal{K}_{2}$ gives important volume effects
No important effects far below threshold
Must connect the two regions

## Important limitation

Current formalism requires no poles in $\mathcal{K}_{2} \ldots$ Derivation assumes


Given that we are seeking an EFT-independent mapping... Is it intuitive that $\mathcal{K}_{2}$ poles need special treatment?

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Need to bridge the gap


## The most technical detail of all...

Far below threshold there is no ambiguity about which two-to-two scattering quantity appears in $C_{L}$


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Far below threshold there is no ambiguity about which two-to-two scattering quantity appears in $C_{L}$


Reason: $\frac{1}{L^{3}} \sum_{\vec{k}} \frac{1}{\left(2 \omega_{k}\right)^{2}\left(E_{\text {sub }}-2 \omega_{k}\right)}=\int_{\vec{k}} \frac{1}{\left(2 \omega_{k}\right)^{2}\left(E_{\text {sub }}-2 \omega_{k}\right)}=$ Analytic Continuation $\left[\int_{\vec{k}} \frac{1}{\left(2 \omega_{k}\right)^{2}\left(E-2 \omega_{k}+i \epsilon\right.}\right]$
This means that our subthreshold $\mathcal{K}_{2}$ is non-standard

$$
\mathcal{K}_{2}^{-1} \propto p^{*} \cot \delta\left(p^{*}\right)+[1-H(\vec{k})] \kappa\left(p^{*}\right)
$$

K matrix above threshold, smooth at threshold, interpolates to the amplitude below threshold
Why are you telling me this?
It is important because our formalism breaks down when there are poles in this definition of $\mathcal{K}_{2}$.

## Testing the formalism (Weak interactions)

[. Expansion is well known for small $a / L$

$$
E=3 m+\frac{12 \pi a}{m L^{3}}\left(1+c_{4} \frac{a}{L}+c_{5} \frac{a^{2}}{L^{2}}\right)+\mathcal{O}\left(1 / L^{6}\right)
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Huang and Yang (1957); Beane, Detmold, Savage, (2007); Tan(2007)

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\& First we recast the expression

$$
\begin{gathered}
\operatorname{det}\left[F_{3}(E, L)^{-1}+\mathcal{K}_{\mathrm{df}, 3}(E)\right]=0 \\
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To enhance an eigenvalue of $\mathcal{H}=\tilde{\mathcal{K}}_{2}^{-1}+\tilde{F}+\tilde{G}$

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8 Then we show that the solution comes from tuning E...
To enhance an eigenvalue of $\mathcal{H}=\tilde{\mathcal{K}}_{2}^{-1}+\tilde{F}+\tilde{G}$
\& The leading order follows from

$$
\mathcal{H}_{00}=-\frac{1}{64 \pi m^{2} a}+\frac{1}{16 L^{3} m^{3} \Delta E}+\frac{1}{8 m^{3} L^{3} \Delta E}+\cdots
$$

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We reproduce known results through $I / L^{5}$ and derive a relation at $I / L^{6}$ Note: Relativistic effects enter at $I / L^{6}$, same order as three-to-three

$$
\begin{gathered}
E=3 m+\frac{12 \pi a}{m L^{3}}\left(1+c_{4} \frac{a}{L}+\cdots\right)-\frac{\mathcal{M}_{\mathrm{thr}}}{48 m^{3} L^{6}}+\cdots \\
\text { MTH and Sharpe (2017) }
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We whecked this in $\lambda \phi^{4}$ through $\mathcal{O}\left(\lambda^{4}\right)$

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Meißner, Rìos and Rusetsky, Phys. Rev. Lett. 114, 091602 (2015) + erratum
The infinite-volume boundstate energy, $E_{B} \equiv 3 m-\frac{\kappa^{2}}{m}$ is shifted in finite volume by an amount $\quad m$

$$
\Delta E(L)=c|A|^{2} \frac{\kappa^{2}}{m} \frac{1}{(\kappa L)^{3 / 2}} e^{-2 \kappa L / \sqrt{3}}+\cdots\left\{\begin{array}{c}
c=-96.351 \cdots \\
\begin{array}{c}
\text { normalization correction factor } \\
\text { (close to one) }
\end{array} \\
\begin{array}{c}
c=-9 \text { Effimor wavefunction }
\end{array}
\end{array}\right.
$$

Assumes two-body potential, unitary limit, $\mathrm{P}=0$, s-wave only

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Our formalism gives a general relation between scattering amplitudes and energy levels. So we substitute...

$$
\mathcal{M}_{3} \sim-\frac{\Gamma \bar{\Gamma}}{E^{2}-E_{B}^{2}} \quad \mathcal{M}_{2}=-\frac{16 \pi E_{2}^{*}}{i p^{*}}
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and study the lowest three-particle finite-volume level

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and study the lowest three-particle finite-volume level
We aim to reproduce the exponent, leading power and overall constant using our relativistic formalism

## Reproducing the result...

1. Show that the relativistic quantization predicts (at leading order in I/L)

$$
\Delta E(L)=-\frac{1}{2 E_{B}}\left[\frac{1}{L^{3}} \sum_{\vec{k}}-\int_{\vec{k}}\right] \frac{\bar{\Gamma}^{(u)}(k) \Gamma^{(u)}(k)}{2 \omega_{k} \mathcal{M}_{2}(k)} \text { s-wave scattering amplitude }
$$

2. Derive the functional forms of the infinite-volume quantities

$$
\Gamma^{(u)}(k)=\frac{3^{3 / 8} \pi^{1 / 4}}{4} A \sqrt{-c} \mathcal{M}_{2}(k) \quad \mathcal{M}_{2}(k)=\frac{32 \pi m}{\kappa}\left[1+\frac{3 k^{2}}{4 \kappa^{2}}\right]^{-1 / 2}
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follows from matching to Effimov wavefunction
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3. Evaluate the sum-integral difference with Poisson summation

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& =c|A|^{2} \frac{\kappa^{2}}{m} \frac{1}{(\kappa L)^{3 / 2}} e^{-2 \kappa L / \sqrt{3}}+\cdots
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$$

We use the second form of the finite-volume correlator

$$
\begin{gathered}
\left.\mathcal{M}_{3, L}=\mathcal{S} \mathcal{D}_{L}^{(u, u)}+\mathcal{L}_{L}^{(u)} \mathcal{K}_{\mathrm{df}, 3} \frac{1}{1+F_{3} \mathcal{K}_{\mathrm{df}, 3}} \mathcal{R}_{L}^{(u)}\right] \\
=\mathcal{D}_{L}^{(u, u)}=\left[\begin{array}{c}
\left.\frac{1}{L^{3}} \sum_{\vec{k}}-\int_{\vec{k}}\right]\left[\begin{array}{c}
\text { here we use that } \\
\mathcal{M}_{G}
\end{array}\right. \\
\mathcal{D}_{L}^{(u, u)}=\mathcal{D}_{\infty}^{(u, u)}+\left[\frac{1}{L^{3}} \sum_{\vec{k}}-\int_{\vec{k}} \mathcal{D}_{\infty}^{(u, u)} \frac{1}{2 \omega_{k} \mathcal{M}_{2}(\vec{k})} \mathcal{D}_{L}^{(u, u)}\right.
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$$

Expansion and analysis of all terms shows that the same relation holds for the full (unsymmetrized) three-to-three scattering amplitude

$$
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$$

Substituting pole ansatz and solving gives the claimed result
$-\frac{1}{E^{2}-\left[E_{B}+\Delta E(L)\right]^{2}}=-\frac{1}{E^{2}-E_{B}^{2}}+\left[\frac{1}{L^{3}} \sum_{\vec{k}}-\int_{\vec{k}}\right] \frac{1}{E^{2}-E_{B}^{2}} \frac{\bar{\Gamma}^{(u)}(k) \Gamma^{(u)}(k)}{2 \omega_{k} \mathcal{M}_{2}(\vec{k})} \frac{1}{E^{2}-\left[E_{B}+\Delta E(L)\right]^{2}}$
finite-volume pole infinite-volume pole

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\Gamma^{(u)}(k)=\frac{3^{3 / 8} \pi^{1 / 4}}{4} A \sqrt{-c} \mathcal{M}_{2}(k) \quad \mathcal{M}_{2}(k)=\frac{32 \pi m}{\kappa}\left[1+\frac{3 k^{2}}{4 \kappa^{2}}\right]^{-1 / 2}
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follows from matching to Effimov wavefunction
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3. Evaluate the sum-integral difference with Poisson summation

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\begin{aligned}
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MTH and Sharpe (2017)

## Reproducing the result (more details)...

2. Derive the functional forms of the infinite-volume quantities

To derive the residue factor we match to the non-relativistic wavefunction

$$
\left[-\frac{1}{2 m} \sum_{i} \frac{\partial^{2}}{\partial \mathbf{r}_{i}^{2}}+\sum_{i j} V\left(\mathbf{r}_{i}-\mathbf{r}_{j}\right)\right] \psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)=-\frac{\kappa^{2}}{m} \psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)
$$

this can be re-expressed using the Faddeev equation

$$
\psi=\phi_{1}+\phi_{2}+\phi_{3} \quad\left[-\frac{1}{2 m} \sum_{i} \frac{\partial^{2}}{\partial \mathbf{r}_{i}^{2}}+\frac{\kappa^{2}}{m}\right] \phi_{3}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)=V\left(\mathbf{r}_{1}-\mathbf{r}_{2}\right) \psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)
$$

We have found that the unsymmetrized residue factor is given by

$$
\Gamma^{(u)}(k)=\lim _{\text {on shell }} 4 \sqrt{3} m^{2}\left(-\frac{\kappa^{2}}{m}-H_{0}\right) \tilde{\phi}_{3}
$$

Substituting the known wave function and expanding about the leading singularity, we find

$$
\Gamma^{(u)}(k)=\frac{3^{3 / 8} \pi^{1 / 4}}{4} A \sqrt{-c} \mathcal{M}_{2}(k)
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3. Evaluate the sum-integral difference with Poisson summation singularity from two-to-two amplitude

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&=c|A|^{2} \frac{\kappa^{2}}{m} \frac{1}{(\kappa L)^{3 / 2}} e^{-2 \kappa L / \sqrt{3}}+\cdots \\
& \text { MTH and Sharpe (2017) }
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$\square$ Truncation at low energies
D Toy solutions for various systems Unphysical solutions
$\square$ Looking forward

## Other methods...

## I A. Rusetsky, H.W. Hammer, J.-Y. Pang:

[ Non-relativistic
[ Based in a specific EFT, focuses on extracting LECs,
I Simpler derivation and formulae, can handle K-matrix poles
I Argued to be "diagramatically equivalent"
[] No t-channel cut, integrals go infinitely far below threshold

## — M. Mai and M. Döring

[ $]$ Relativistic
(]) Built on unitary constrains, replace imaginary cuts with volume cuts
I Cannot see the dropping of $\mathcal{O}\left(e^{-m L}\right)$
I Connection to our approach is not yet well understood

See also Polejaeva, Rusetksy (2012) and Briceño, Davoudi (2013)

## Usability?

"Despite this success, the quantization condition in these papers is not yet given in a form suitable for the analysis of the real lattice data"

Hammer, Pang and Rusetsky (2017)
We were motivated to challenge this claim...
We find that the "degree of usability" is comparable between the two approaches, provided one applies similar approximations.

How do we make the two-particle formalism usable?
Truncate partial waves
Single partial wave
$\mathcal{M}_{2}\left(E_{2}^{*}, \theta^{*}\right) \approx \sum_{\ell=0}^{N} P_{\ell}\left(\cos \theta^{*}\right) \mathcal{M}_{2, \ell}\left(E_{2}^{*}\right) \longrightarrow \mathcal{M}_{2}\left(E_{2}^{*}, \theta^{*}\right) \approx \mathcal{M}_{2, s}\left(E_{2}^{*}\right) \propto \frac{1}{p^{*} \cot \delta_{0}\left(p^{*}\right)-i p^{*}}$
Is there a three-particle analog?
$\mathcal{K}_{\mathrm{df}, 3}\left(E^{*}, \Omega_{3}^{\prime}, \Omega_{3}\right) \approx \sum_{n=0}^{N} \mathcal{P}_{n}\left(\Omega_{3}^{\prime}, \Omega_{3}\right) \mathcal{K}_{\mathrm{df}, 3, n}\left(E^{*}\right) \longrightarrow \mathcal{K}_{\mathrm{df}, 3}\left(E^{*}, \Omega_{3}^{\prime}, \Omega_{3}\right) \approx \mathcal{K}_{\mathrm{df}, 3}^{\mathrm{iso}}\left(E^{*}\right) \in \mathbb{R}$

At fixed energy $\underset{\mathcal{K}_{\mathrm{df}, 3}\left(E^{*}, \Omega_{3}^{\prime}, \Omega_{3}\right)}{ } \mathcal{M}_{2}\left(E_{2}^{*}, \theta^{*}\right)$ is a smooth function on a compact space.
Further investigation is needed to understand suppression of higher $\mathcal{K}_{\mathrm{df}, 3, n}\left(E^{*}\right)$.

## Numerics (keeping only s-wave and $\left.\mathcal{K}_{\mathrm{df}, 3}\left(E^{*}, \Omega_{3}^{\prime}, \Omega_{3}\right) \approx \mathcal{K}_{\mathrm{df}, 3}^{\text {iso }}\left(E^{*}\right)\right)$

$$
1 / \mathcal{K}_{\mathrm{dt}, 3}^{\mathrm{iso}}\left(E^{*}\right)=-F_{3}^{\mathrm{iso}}\left[E, \vec{P}, L, \mathcal{M}_{2}^{s}\right] \quad \mathcal{M}_{3}\left(E^{*}, \Omega_{3}^{\prime}, \Omega_{3}\right)=\mathcal{S}\left[\mathcal{D}+\mathcal{L} \frac{1}{1 / \mathcal{K}_{\mathrm{df}, 3}^{\mathrm{iso}}+F_{3, \infty}^{\mathrm{isos}}} \mathcal{R}\right]
$$

For the numerical approach we restrict attention to... $p^{*} \cot \delta_{0}\left(p^{*}\right)=-\frac{1}{a}, \quad \vec{P}=0$
Then the quantization condition is based on $F_{3}^{\text {iso }}(E, L, a)$


Finite-volume energies wherever these curves intersect $-1 / \mathcal{K}_{\mathrm{df}, 3}^{\text {iso }}(E)$

## $\mathcal{K}_{\mathrm{df}, 3}^{\mathrm{iso}}(E)=0$ solutions

Q Provides a useful benchmark: Deviations measure three-particle physics
Q Meaning for three-to-three scattering is clear

$$
i \mathcal{M}_{3}=\mathcal{S}[\underbrace{\mathrm{iM}_{2}}_{\left(i \mathcal{M}_{2}\right.}+\underbrace{\text { (iM2 }}
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## $\mathcal{K}_{\mathrm{d} \mathrm{d}, 3}^{\mathrm{iso}}(E)=0$ solutions

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Again: Non-interacting states $\left(\mathcal{M}_{2}=\mathcal{M}_{3}=0\right)$


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$$



## $\mathcal{K}_{\mathrm{df}, 3}^{\mathrm{iso}}(E)=0$ solutions

Straightforward to vary $a$ and to study large volumes




But, to avoid poles in $\mathcal{K}_{2}$, we must require $a<1 / m$

## Non-zero $\mathcal{K}_{\mathrm{df}, 3}^{\mathrm{iso}}(E)$ : Toy resonance

Here we consider a fun example for non-zero $\mathcal{K}_{\text {df }, 3}^{\text {iso }}$

$$
a=-10 \quad \mathcal{K}_{\mathrm{df}, 3}^{\mathrm{iso}}(E)=-\frac{c \times 10^{3}}{E^{2}-M_{R}^{2}}
$$

For small c we expect a narrow avoided level crossing, as cincreases the gap grows


Further investigation is needed to see if this gives a physical resonance description

## Unphysical solutions

Very large values of $\mathcal{K}_{\mathrm{df}, 3}^{\text {iso }}$ can lead to unphysical solutions


Unphysical input? Enhanced $\mathcal{O}\left(e^{-m L}\right)$ effects? Under investigation...

## Non-zero $\mathcal{K}_{\mathrm{df}, 3}(E)$ : Unitary bound state

The parameters $a=-10^{4}, \mathcal{K}_{\mathrm{df}, 3}^{\text {iso }}(E)=2500$ lead to a shallow bound state

$$
\kappa \approx 0.1 m \text { where } E_{B}=3 m-\kappa^{2} / m
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Finite-volume behavior of this state has a known asymptotic form
Meißner, Rios, Rusetsky (2015)

$$
E_{B}(L)=3 m-\frac{\kappa^{2}}{m}-(98.35 \cdots)|A|^{2} \frac{\kappa^{2}}{m} \frac{e^{-2 \kappa L / \sqrt{3}}}{(\kappa L)^{3 / 2}}\left[1+\mathcal{O}\left(\frac{1}{\kappa L}, \frac{\kappa^{2}}{m^{2}}, e^{-\alpha \kappa L}\right)\right]
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We fit our q.c. data over $60<m L<70$
$\longrightarrow \kappa=0.1068,|A|^{2}=0.948$
Close to one

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$$



## Converting to scattering amplitudes



## Converting to scattering amplitudes



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## Converting to scattering amplitudes



This only works below threshold... Relation above threshold crucially needed

## Converting to scattering amplitudes




## Back to the bound state



## Back to the bound state



## Back to the bound state




## Back to the bound state



## Outline

$\square$ Warm up and definitions
ㅁ Basic set-up
व/ Finite-volume correlator
ㅁ Three non-interacting particles
$\square$ Two particles in a box
Illernative derivation
Truncation and application
Relating matrix elements

- Three particles in a box


3-to-3 scattering (Sketch of) derivation
An unexpected infinite-volume quantity Relating energies to scattering

## I Testing the result

I- Know issues
Large-volume expansion
Effimov state in a box

## I] Other methods

## - Numerical explorations

I Truncation at low energies
I Toy solutions for various systems
Unphysical solutions
$\square$ Looking forward

## Still lots to do

$\square$ Finish result with intermediate twoparticle resonances
$\square$ Understand unphysical solutions
$\square$ Extend to non-identical, non-degenerate, multiple channels, spin
$\square$ Study subduction to finite-volume irreps
$\square$ Understand rigorous parametrizations for the infinite-volume observables
$\square$ Convince practitioners that the formalism is mature
$\square$ Reliably measure finite-volume spectra
$\square$ Extract three-particle scattering from LQCD

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## Big picture: making progress, but not quite there yet



## That's all folks!



Thanks to all the participants!

