DWQ@25

BNL-HET & RBRC Joint Workshop

$K\pi$ scattering at physical pion mass using distillation

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THE UNIVERSITY *of* EDINBURGH

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Outline

Background

Smearing Radius
and N_{vec} Dependence

Exact and Stochastic Distillation

Conclusions and Outlook

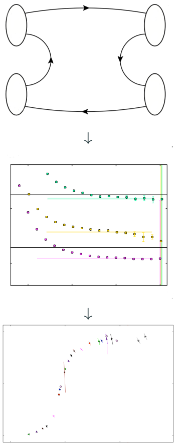
Background

Scattering on the lattice: $K\pi$

- Phenomenological motivations
  - rare decays, e.g. $B \to K^* l^+ l^- (\to K\pi l^+ l^-)$
  - multibody decays, e.g. $B \to K\pi\pi$
- Possible methodology
  - **correlator data**
  - energy spectrum
  - Lüscher analysis
- What can we get?
  - phase shifts
  - resonance parameters

$\to$ *this project: towards first physical pion mass $K\pi$ scattering*

Workflow illustration



[F. Erben 10.25358/openscience-3858]

Ensemble

- RBC-UKQCD $N_f = 2 + 1$ domain-wall fermion lattice [Blum et al. 10.1103/PhysRevD.93.074505]

volume	$48^3 \times 96$
L	≈ 5.5 fm
a	≈ 0.11 fm
$m_\pi L$	≈ 3.8
m_π	≈ 139 MeV
m_K	≈ 499 MeV

- Ensemble exploration
  - several datasets with measurements over 9 configurations (40 MC steps)
  - Dirac operator (D) inversions on 12 time sources per configuration (every $8th$)
  - low statistics: treat correlators obtained from different time sources as uncorrelated samples (but bin later)

* done using DiRAC Extreme Scaling HPC Service (aka Tesseract) [https://www.dirac.ac.uk]

Distillation [M. Peardon et al. 10.1103/PhysRevD.80.054506]

- Gauge-covariant $3D$-Laplacian

$$-\nabla^2_{\mathbf{x},\mathbf{y}}(t) = 6\delta_{\mathbf{xy}} - \sum_{j=1}^{N_{\text{vec}}} \left[U_j(\mathbf{x},t)\delta_{\mathbf{x}+\hat{j},\mathbf{y}} + U_j^\dagger(\mathbf{x}-\hat{j},t)\delta_{\mathbf{x}-\hat{j},\mathbf{y}} \right] \tag{1}$$

- Projects quark fields onto low-lying $-\nabla^2$ space

$$\mathcal{S}_{\mathbf{xy}}(t) = \sum_{i=1}^{N_{\text{vec}}} v_k(\mathbf{x};t)v_k(\mathbf{y};t)^\dagger, \quad \text{eigenvectors } v_k \text{ and eigenvalues } \lambda_1 < \lambda_2 < \ldots < \lambda_{N_{\text{vec}}} \text{ of } -\nabla^2 \tag{2}$$

- Distilled propagator

$$S(\mathbf{x},t_f;\mathbf{y},t) \equiv \left[\mathcal{S}D^{-1}\mathcal{S}^\dagger\right](\mathbf{x},t_f;\mathbf{y},t) = \sum_{k,l=1}^{N_{\text{vec}}} v_k(\mathbf{x};t_f) \underbrace{\tau_{kl}(t_f,t)}_{perambulator} v_l(\mathbf{y};t)^\dagger, \tag{3}$$

$\rightarrow$ number of Dirac operator inversions $N_{\text{inv}} \propto N_{\text{vec}}$ (*exact distillation*)

- Further: *stochastic distillation* [C. Morningstar et al. 10.1103/PhysRevD.83.114505]
    - introduce Lap-spin-time stochastic noises $\eta^r, r = 1, 2, \ldots, N_\eta$
    - efficient when the stochastic noise $\lesssim$ gauge noise

$\to N_{\text{inv}} \propto N_\eta$

- Variance reduction: dilution projectors [C. Morningstar et al. 10.1103/PhysRevD.83.114505]
    - introduce Lap-spin-time dilution projectors $P^L P^S P^T$ and define partitioned noises as

$$\eta^{r,LST} = P^L P^S P^T \eta^r \tag{4}$$

- example: Lap interlaced dilution ($N_{\text{vec}} = 6$, $LI = 3$ Lap-dilution sources)

$$\text{dilution partitions: } \Big\{ \underbrace{\{1,4\}}_{\text{source } L=1}, \underbrace{\{2,5\}}_{\text{source } L=2}, \underbrace{\{3,6\}}_{\text{source } L=3} \Big\} \tag{5}$$

$\to N_{\text{inv}} \propto N_\eta LI$

Code

- `Grid`: data parallel C++ lattice library
- `Hadrons`: Grid-based workflow management system for lattice simulations
- Open-source and free software

`github.com/paboyle/Grid`

`github.com/aportelli/Hadrons`

Distillation within `Grid` and `Hadrons`

- Started in 2019 by Marshall M. and Erben F. [P. Boyle et al. arxiv:1912.07563]
- Refactorisation: meson fields (disk space and efficiency)
- Proper documentation and file specification

Code: Distillation Meson Fields (`MDistil` at `github.com/aportelli/Hadrons`)

- Accounts for time-dilution sparsity of ϱ vectors
- Example of exact distillation workflow (`aportelli.github.io/Hadrons-doc/`)

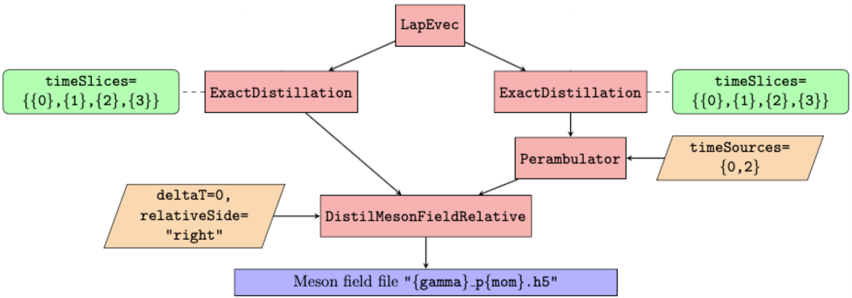
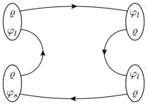


Figure 2: Exact distillation on a $N_t = 4$ lattice. N_{vec} encoded in Laplacian eigenpack (`LapEvec`).

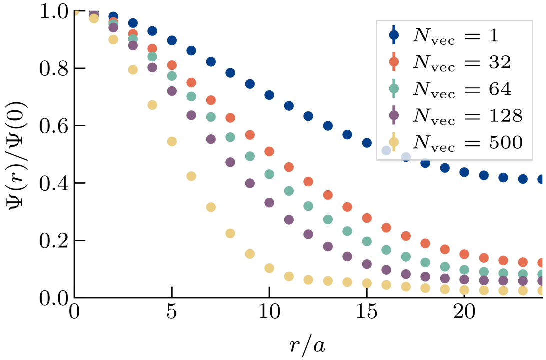
- Computation of backtracking quark lines, e.g. appearing on



Smearing Radius and N_{vec} Dependence

Spatial distribution [M. Peardon et al. 10.1103/PhysRevD.80.054506]

$$\Psi(r) = \sum_{\mathbf{x},t} \sqrt{\text{tr}\, \mathcal{S}_{\mathbf{x},\mathbf{x}+\mathbf{r}}(t)\mathcal{S}_{\mathbf{x}+\mathbf{r},\mathbf{x}}(t)} \quad (6)$$



- Smearing profile for several values of N_{vec}
- Larger N_{vec} approaches point source ✓

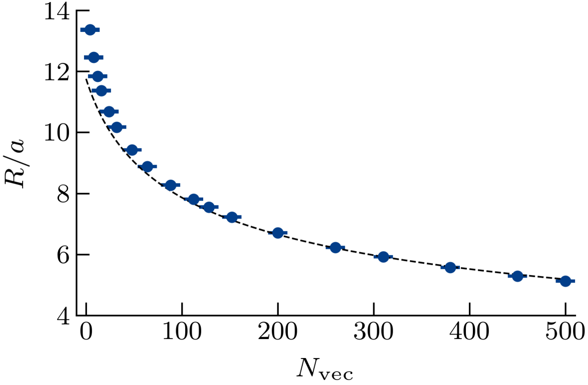
* stout-smearing parameters $\rho = 0.2, n = 3$

Smearing Radius

- Define R:

$$\frac{\int_0^R \Psi(r)\,dr}{2\int_0^{aL/2} \Psi(r)\,dr} = 0.341 \qquad (7)$$

Study dependence on $N_{\text{vec}} \longrightarrow$



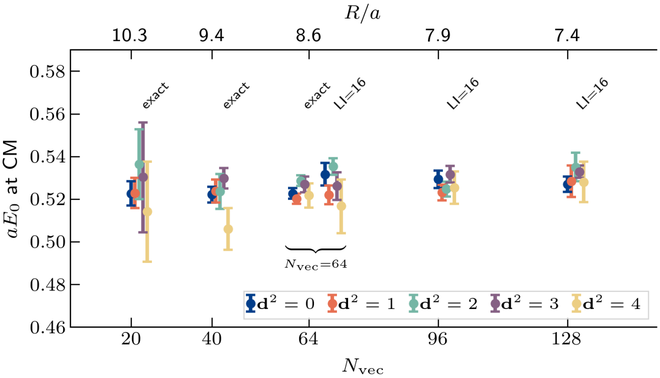
- Curve flattening: simple fit to $A(B + N_{\text{vec}})^C$, with $C \approx -0.3$
- Given such flattening and overall cost $\propto N_{\text{vec}}$, reasonable to explore $N_{\text{vec}} \sim 100$
- Schemes

	$LI = 4$	$LI = 8$	$LI = 16$	$LI = 32$	exact	exact	exact
N_{vec}	64	64	64, 96, 128	64	20	40	64
N_{inv}	32	64	128	256	80	160	256

* stochastic distillation with $N_\eta = 2$ noise vectors and full time-spin dilution

Vector-to-vector correlators $(\bar{s}\gamma_i l)$

- Fit to $Z_0\left(e^{-E_0 t} + e^{-(N_t - t)E_0}\right)$ for now
- Use exact distillation fit ranges as reference
- Boost E_0 from moving frames (A1 irrep) to center-of-momentum frame



→ E_0 roughly consistent for $N_{\text{vec}} \gtrsim 60$ across moving frames (from dispersion relation)

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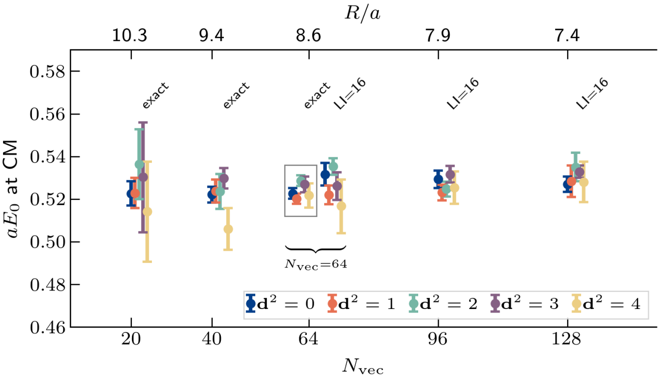
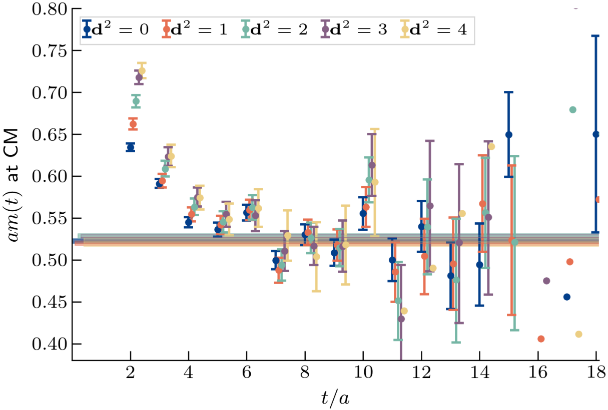


$\rightarrow$ E_0 roughly consistent for $N_{\text{vec}} \gtrsim 60$ across moving frames (from dispersion relation)

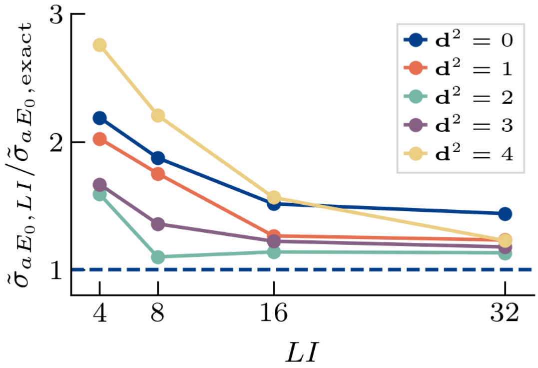
- **Effective mass** at $N_{\text{vec}} = 64$ (exact distillation)
  - Fit result: E_0 bands



- Caveats:
  - low-statistics and correlations
  - excited states

Exact and Stochastic Distillation

Exact and Stochastic Distillation at $N_{\text{vec}} = 64$



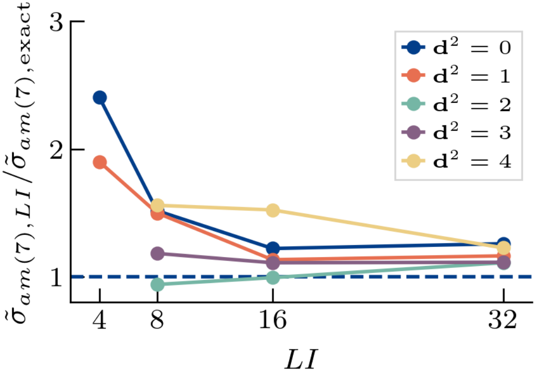
Cost comparison: normalised standard deviation

- Cost-normalised standard deviation $\tilde{\sigma} \equiv \sigma\sqrt{N_{\text{inv}}}$
- Ratio to exact distillation (only MC noise at dashed line)

- $N_{\text{noise}} = 2$ here ; would need at least 4 in the full analysis

$\rightarrow$ $LI = 16$ less efficient than exact distillation *at* $N_{\text{vec}} = 64$

Exact and Stochastic Distillation at $N_{\text{vec}} = 64$



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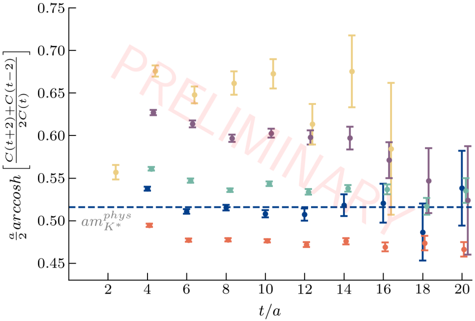
Preliminary GEVP

- Exact distillation data at $N_{\text{vec}} = 64$ (extended to every 2nd time slice), attempt GEVP

$$C(t)u(t,t_0) = \lambda(t,t_0)C(t_0)u(t,t_0) \tag{8}$$

- Rest-frame operators

$$\bar{s}\gamma^z l(\mathbf{p}=0) \text{ and } K\pi(\mathbf{p},-\mathbf{p}), \mathbf{p} = (1,0,0), (1,1,0), (1,1,1), (2,0,0) \tag{9}$$



- Preliminary fixed-t_0 GEVP ($t_0 = 2$) for a 5×5 correlator matrix (T_{1u} irrep).

$\rightarrow$ moving frames, especially irreps $B_2(1,1,0)$, $B_3(1,1,0)$, $E(1,1,1)$ and A_1

Conclusions and Outlook

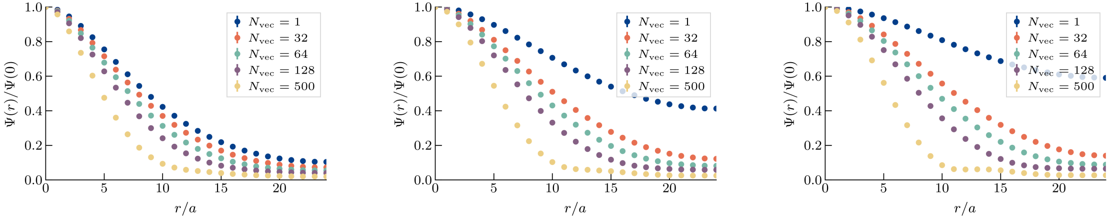
Conclusions and Outlook

- `Grid/Hadrons` distillation code for large-scale simulations (open source)
- N_{vec} **dependence of smearing radius and single-particle correlators**
  - tune N_{vec} directly on the physical pion mass $48^3 \times 96$ ensemble
  - smearing radius curve flattening
  - to resolve momenta $\mathbf{d}^2 \leq 4$ at correlator level, no clear benefit seen going above $N_{\text{vec}} = 64$
- **Comparison between several distillation schemes at** $N_{\text{vec}} = 64$
  - cost comparison between exact and stochastic distillation ($N_{\text{noise}} = 2$)
  - exact has better cost-benefit at correlator level, besides being simpler to handle
- **Next**
  - progressively higher statistics, inversions on every time slice
  - refine variational analysis and moving frames
  - Lüscher analysis and $K^*(892)$ resonance parameters

Thanks for the attention. Questions or comments?

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme under grant agreement No 813942.

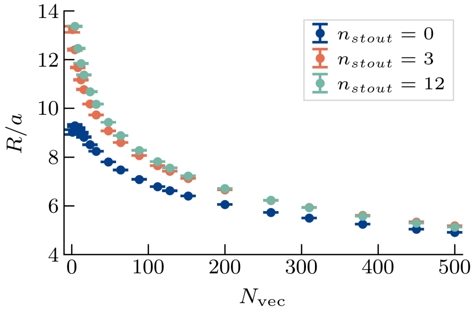
Smearing spatial distribution for $n_{\text{stout}} = 0, \mathbf{3}, 12$ $(\rho = \mathbf{0.2})$



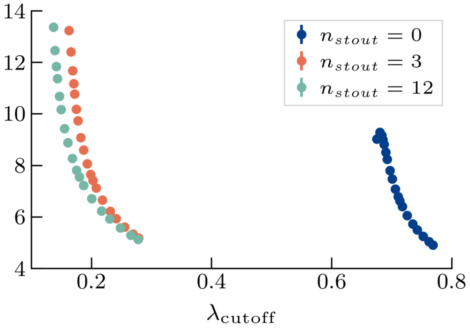
$n_{\text{stout}} = 0$ | $\mathbf{n_{\text{stout}} = 3}$ | $n_{\text{stout}} = 12$

Backup

Smearing radius for $n_{\text{stout}} = 0, \mathbf{3}, 12$ $(\rho = \mathbf{0.2})$

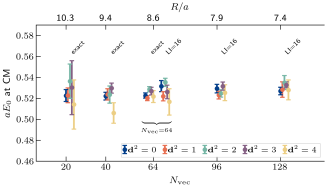


radius vs N_{vec}

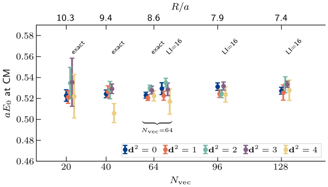


radius vs λ_{cutoff}

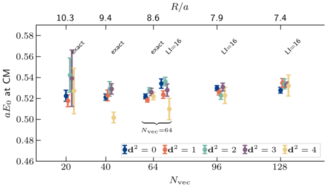
Varying bin size (E_0 vs N_{vec})



bin size=1



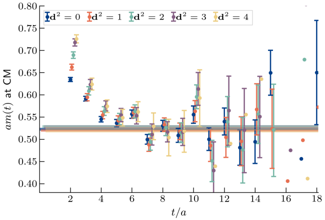
bin size=2



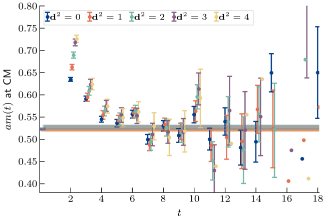
bin size=4

Backup

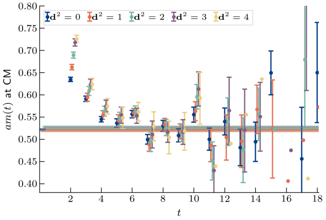
Varying bin size (m_{eff} vs t)



bin size=1

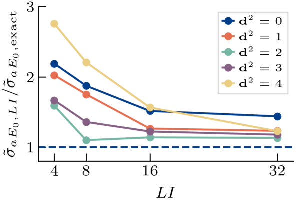


bin size=2



bin size=4

Varying bin size ($\frac{\sigma_{E_0, LI}\sqrt{N_{\mathrm{inv}, LI}}}{\sigma_{E_0, exact}\sqrt{N_{\mathrm{inv}, exact}}}$ vs LI)



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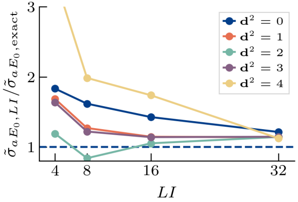

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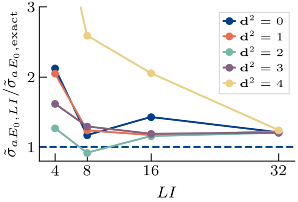
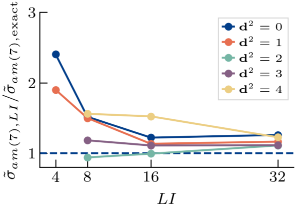


bin size=4

Fluctuates but it is not changing conclusions

Backup

Varying bin size $\left(\frac{\sigma_{m_{\text{eff}}(t=7),LI}\sqrt{N_{\text{inv},LI}}}{\sigma_{m_{\text{eff}}(t=7),exact}\sqrt{N_{\text{inv},exact}}}\right)$ vs LI)



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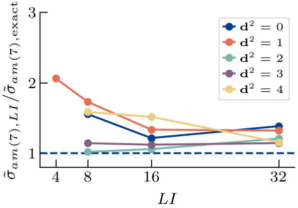

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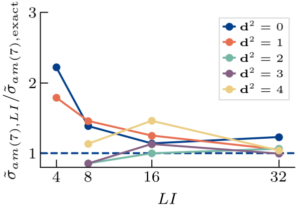
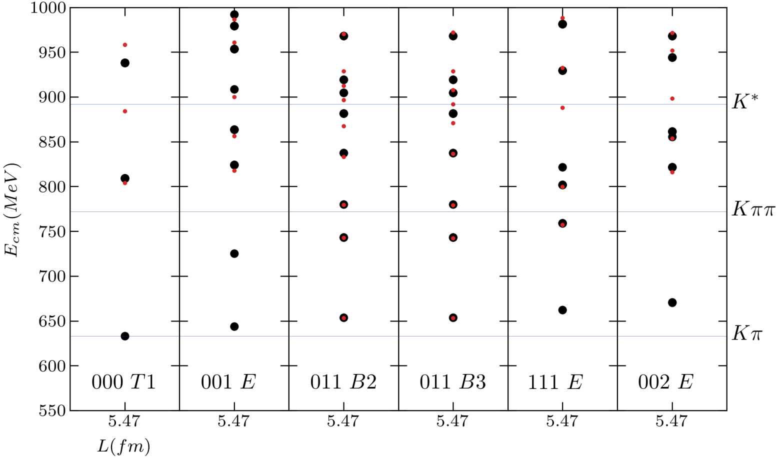


bin size=4

Fluctuates but it is not changing conclusions

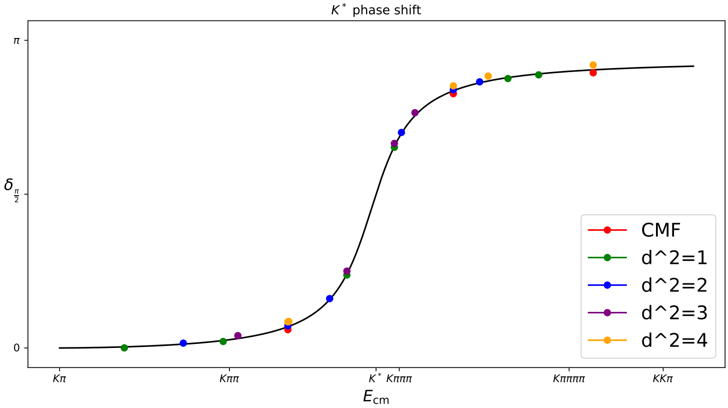
Backup

Irreps with $l = 1, \ldots$



Backup

Non-interacting energies



(courtesy of F. Erben)