

B05 – A novel approach to the baryon spectrum based on stochastic methods

NuMeriQS Retreat

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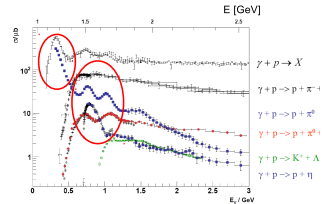
HPC support by Jülich Supercomputing Centre

Baryon spectroscopy

Extract the spectrum of excited states from experimental data

→ What are those bumps?

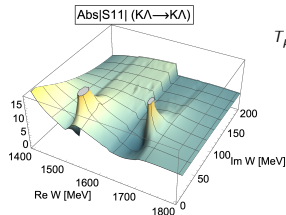
- energy & angular momentum excitations of baryons (resonances)?
- conventional 3 quark baryons or more complicated objects?
- ...



- **Theoretical challenge:** build a model that includes as many constraints from symmetries of nature as possible

$$T_{\mu\nu}(q, p', W) = V_{\mu\nu}(q, p', W) + \sum_{\kappa} \int_0^{\infty} dp p^2 V_{\mu\kappa}(q, p, W) G_{\kappa}(p, W) T_{\kappa\nu}(p, p', W)$$

- **Numerical challenge:** large number of free model parameters, heterogeneous data base, uncertainty quantification, ...



source: ELSA; data: ELSA, JLab, MAMI

→ use HMC and Bayesian inference to sample parameter space

→ determine resonance uncertainties from samples (means, standard deviation)

Bayesian parameter estimation with HMC

Bayes':

$$\log \pi(\theta | D) \propto \log L(D | \theta) + \log \pi(\theta) = -\frac{1}{2}\chi^2(D, \theta) + \log \pi(\theta)$$

$D \sim \text{data}$

$\theta \sim \text{vector of model parameters,}$
 $\text{dim} \sim 900$

(assumed gaussian likelihood)

Hamilton's equations:

$$\text{with } H = \frac{1}{2}p^T M^{-1}p + \frac{1}{2}\chi^2(\theta)$$

$$\frac{d\theta}{dt} = M^{-1}p, \quad \frac{dp}{dt} = \nabla_{\theta_i} \left(\frac{1}{2}\chi^2(\theta) - \log \pi(\theta) \right)$$

- leapfrog to propose updates for the Markov chain \rightarrow need **numerical gradient** of $\chi^2(\theta)$
(costly in high-dim parameter space)

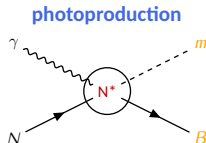
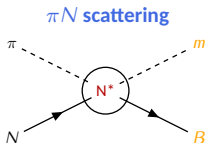
Idea: reevaluate gradient only every n -th step?

- Mass matrix M (parameters are highly correlated)
 $\rightarrow (M = 1,) M = \text{diag}(\text{Cov}(\theta))$ or $M = \text{Cov}(\theta)$ (from warm-up phase, Euclidean HMC)?
or beyond "vanilla" HMC: Riemannian kinetic energy?
- Integration time: \rightarrow hand-tuned to achieve a good acceptance rate
or beyond "vanilla" HMC: No-U-Turn sampler

Further challenges specific to our problem

(Besides the costly gradient)

- Diverse data base, different production mechanisms:



partially inconsistent data, very different quantity & quality

→ weights in χ^2 to account for limited # of data points

(so far: adjusted as needed to achieve a good description of all data)

- Identify pathological solutions: good χ^2 but “unnatural” amplitudes (sharp rises/drops, wiggles)
→ penalties?
- Systematic uncertainties: model uncertainties as, e.g., # of resonance states
→ Bayesian evidence for model w/ vs. w/o a certain state
→ full HMC run for model w/o state?
- Practical challenge: hand-coded HMC in Fortran 90