# Lattice Methods for Hadron Spectroscopy: building operators and extracting energies

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# Plan

- Operator construction
  - types of operator
  - what makes a good operator?
  - operators on the lattice and the continuum
- Fitting correlator data
  - single correlators and single exponentials
  - general remarks on fitting and errors
  - extracting excited states
- Anisotropic lattices
- Systematic errors

# Interpolating Operators

# The interpolating operators

- We have spent some time looking at methods for quark propagation
- What about the operators $\mathcal{O} = \bar{\Psi}_{i\alpha}(\vec{x},t)\Gamma_{\alpha\beta}\Psi_{i\beta}(\vec{x},t)$?
- The simplest objects are colour-singlet local fermion bilinears:

$$\mathcal{O}_\pi = \bar{d}\gamma_5 u,\ \mathcal{O}_\rho = \bar{d}\gamma_i u,\ \mathcal{O}_N = \epsilon^{abc}\left(u^a C\gamma_5 d^b\right)u^c,$$

$$\mathcal{O}_\Delta = \epsilon^{abc}\left(u^a C\gamma_n u d^b\right)u^c$$

or more correctly!

$$\mathcal{O}_{A_1} = \bar{d}\gamma_5 u,\ \mathcal{O}_{T_1} = \bar{d}\gamma_i u,\ \mathcal{O}_{G_1} = \epsilon^{abc}\left(u^a C\gamma_5 d^b\right)u^c,$$

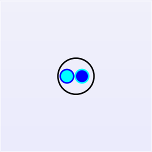
$$\mathcal{O}_H = \epsilon^{abc}\left(u^a C\gamma_n u d^b\right)u^c$$

Access to $J^{PC} = 0^{-+}, 0^{++}, 1^{--}, 1^{++}, 1^{+-}, 1/2, 3/2$

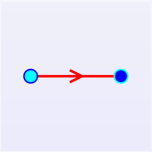
# Extended operators

- We would like to access states with $J > 1$
- Would like many more operators that all transform irreducibly under some irrep enabling variational analysis.
- Lattice operators are bilinears with path-ordered products between the quark and anti-quark field; different offsets, connecting paths and spin contractions give different projections into lattice irreps.

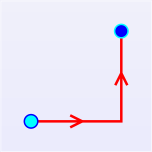
Meson operators examples



$\mathcal{O}_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)\psi_\beta(x)$



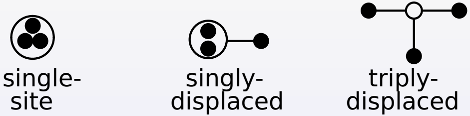
$\mathcal{O}^i_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)U_i(x)\psi_\beta(x+\hat{\imath})$



$\mathcal{O}^{ij}_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)U_i(x)U_j(x+\hat{\imath})\psi_\beta(x+\hat{\imath}$

# Extended baryon operators

- The same idea for baryons gives prototype extended operators

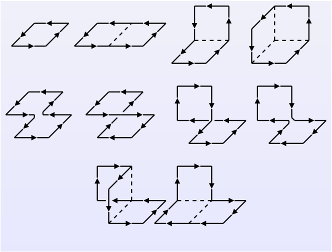


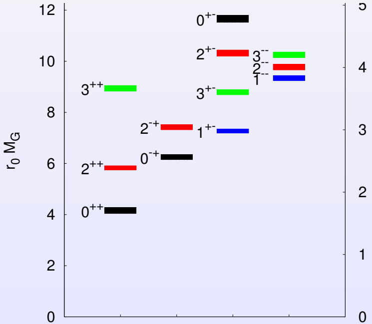

With thanks: 0810.1469

- We can make arbitrarily complicated operators in this way
- An early success was glueball calculations

# Glueballs

- QCD nonAbelian ⇒ allows bound states of glue
- Candidates observed experimentally: $f_0(1370), f_0(1500), f_0(2220)$
- Glueballs can be calculated in lattice QCD
- The interpolating fields are purely gluonic, built from Wilson loops





# Good operators

- What makes a good operator?
- An operator of definite momentum that transforms under a lattice irrep
- An operator that has strong overlap with the (continuum) state you are interested in.
- An operator is not noisy ie that produces an acceptable correlator
- Note that smearing and distillation are rotationally symmetric operations and do not change the quantum numbers.

- But recall from earlier that subduction leads to

| Lattice irrep, $\Lambda$ | Dimension | Continuum irreps, $J$ |
|---|---|---|
| $A_1$ | 1 | 0, 4, ... |
| $A_2$ | 1 | 3, 5, ... |
| $E$ | 2 | 2, 4, ... |
| $T_1$ | 3 | 1, 3, ... |
| $T_2$ | 4 | 2, 3, ... |
| $G_1$ | 3 | 1/2, 7/2, ... |
| $G_2$ | 3 | 5/2, 7/2, ... |
| $H$ | 4 | 3/2, 5/2, ... |

- So a correlator $C(t) = \langle 0|\phi(t)\phi^\dagger(0)|0\rangle$ contains in principle information about all (continuum) spin states in $\Lambda^{PC}$.

# Operator basis — derivative construction

- A closer link to (or “memory” of) the continuum would be good
- There are different approaches to optimise lattice operators. This is one.

# Operator basis — derivative construction

- A closer link to (or “memory” of) the continuum would be good
- There are different approaches to optimise lattice operators. This is one.
- Start with continuum operators, built from $n$ derivatives:

$$\Phi = \bar{\psi}\,\Gamma\left(D_{i_1} D_{i_2} D_{i_3} \dots D_{i_n}\right)\psi$$

- Construct irreps of $SO(3)$, then subduce these representations to $O_h$
- Now replace the derivatives with lattice finite differences:

$$D_j\psi(x) \rightarrow \frac{1}{a}\left(U_j(x)\psi(x+\hat{j}) - U_j^{\dagger}(x-\hat{j})\psi(x-\hat{j})\right)$$

- On a discrete lattice covariant derivative become finite displacements of quark fields connected by links

arXiV:0707.4162

# Example: $J^{PC} = 2^{++}$ meson creation operator

- Trying to gain more information to discriminate spins. Consider continuum operator that creates a $2^{++}$ meson:

$$\Phi_{ij} = \bar{\psi}\left(\gamma_i D_j + \gamma_j D_i - \frac{2}{3}\delta_{ij}\gamma \cdot D\right)\psi$$

- Lattice: Substitute gauge-covariant lattice finite-difference $D_{\rm latt}$ for $D$
- A reducible representation:

$$\Phi^{T_2} = \{\Phi_{12}, \Phi_{23}, \Phi_{31}\}$$

$$\Phi^{E} = \left\{\frac{1}{\sqrt{2}}(\Phi_{11} - \Phi_{22}), \frac{1}{\sqrt{6}}(\Phi_{11} + \Phi_{22} - 2\Phi_{33})\right\}$$

- Look for signature of continuum symmetry:

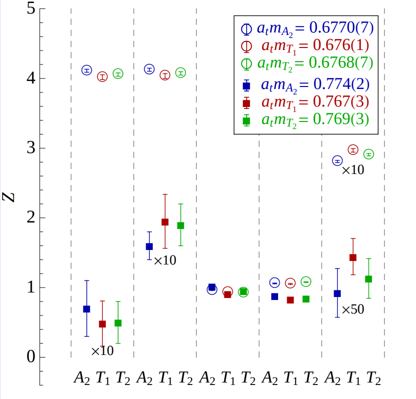
$$\mathcal{Z} = \langle 0|\Phi^{(T_2)}|2^{++(T_2)}\rangle = \langle 0|\Phi^{(E)}|2^{++(E)}\rangle$$

up to rotation-breaking effects

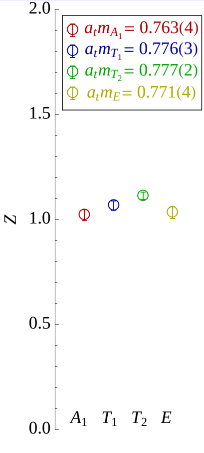
# This idea appears to work well

arXiv:1204.5425

## Spin-3 identification




## Spin-4 identification




$J = 3$ in $A_2, T_1, T_2$
$J = 4$ in $A_1, T_1, T_2, E$

# Extracting Energies
# aka
# The Dark Art of Fitting Data

# Hadron masses

Hadron energies determined from 2-pt correlation functions.
Begin with a simple correlator

$$C(t, \mathbf{p}) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \langle \mathcal{O}(\mathbf{x}, t) \mathcal{O}^\dagger(\mathbf{0}, t) \rangle.$$

where $\mathcal{O}$ is a single interpolating operator for the hadron of interest. Recall that by inserting a complete set of energy eigenstates $|n\rangle$ and assuming a discrete energy spectrum as $t \to \infty$ and for hadrons at rest

$$C(t) \to \frac{1}{2E_n} |\langle 0|\mathcal{O}|n_o\rangle|^2 e^{-E_0 t},$$

where $n_0$ is the lightest state that couples to $\mathcal{O}$ and $E_0$ is its energy.

# The effective mass

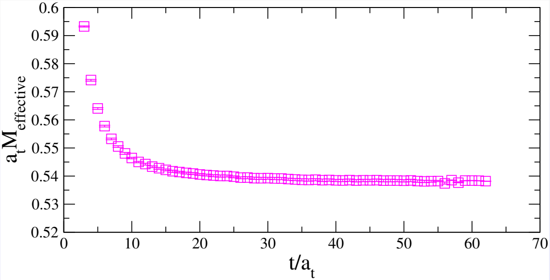
A useful quantity is the effective mass

$$a_t M_{\text{eff}}(t) = \ln\left(\frac{C(t)}{C(t+1)}\right)$$

- A useful quantity to see ground state dominance: $m_{eff} \rightarrow$ constant - the plateau
- The onset and length of the plateau depends on $\mathcal{O}$
- The hadron mass is extracted from a fit to correlator data in the plateau region
- statistical errors grow exponentially with $t$, except for the pion

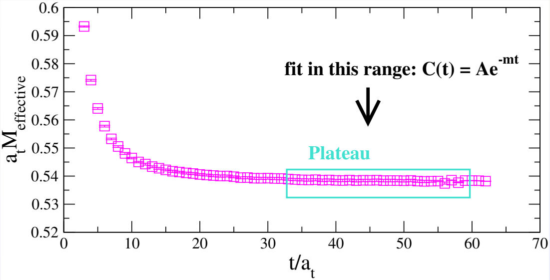
# An effective mass plot

At large times, effective mass converges to the ground state energy - see a plateau in the effective mass plot as a function of time.



# An effective mass plot (2)

At large times, effective mass converges to the ground state energy - see a plateau in the effective mass plot as a function of time.




- The correlator data is fitted to the expected $C(t) = Ae^{-E_0 t}$ form. Eg using a $\chi^2$ minimisation algorithm with $A$ and $E_0$ free parameters and for some “reasonable” choice of time range.
- Errors are estimated by bootstrap or jackknife.

# Resampling techniques

- Two methods: Bootstrap and Jackknife
  - Jackknife from Quenouille (1956) and Tukey (1957)
  - Consider $N$ measurements, remove the first leaving a jackknifed set of $N-1$ "resampled" measurements.
  - Repeat analysis (fits) on this reduced set, giving parameters $\alpha_{J(1)}$.
  - Repeat resampling, throwing out 2nd measurement etc to get $\alpha_{J^i}, i = 1, \ldots, N$.
  - Then

$$\sigma_J^2 = \frac{(N-1)}{N} \sum_{i=1}^{N} (\alpha_{J(i)} - \alpha)^2$$

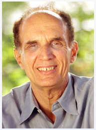
where $\alpha$ is the result from fitting the full dataset.

John Tukey: also gave us FFT and box plots!

# Resampling techniques (2): bootstrap

Bootstrap from Efron (late '70s). See Numerical Recipes and Efron's book An Introduction to the Bootstrap

- A resampling technique.
- Create a new dataset by drawing $N$ datapoints with replacement from the original dataset, size $N$.
- Replacement means you do not get the original set each time - but a set with a random fraction of the original points.
- As for jackknife repeat analysis on each new set.



Bradley Efron

Numerical Recipes in C says
*Offered the choice between mastery of a five-foot shelf of analytical statistics books and middling ability at performing statistical Monte Carlo simulations, we would surely choose to have the latter skill.*

# How to choose a fit range

When fitting the correlator data we are looking for:

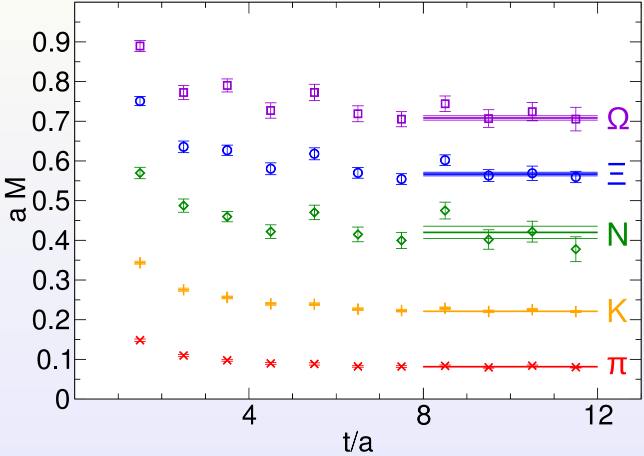
- a good $\chi^2/N_{d.o.f.}$
- a “reasonable” range in $t$
- a “reasonable” fit error
- a fit that is stable with respect to the choice of $t$. In particular with respect to small changes in $t_{min}$ the minimum timeslice included in the fit.

Common quantities to look at

- a sliding window: plot the fitted mass as a function of $t_{min}$
- a fit-histogram: plot $QN_{dof}/(\Delta m)$ for each $(t_{min}, t_{max})$ and $Q = \Gamma[(interval - N_{param})/2, \chi^2/2]$. Choose the $(t_{min}, t_{max})$ that maximises this quantity.
- A good idea to check your fit range looks reasonable on the effective mass plot

# Effective mass plots

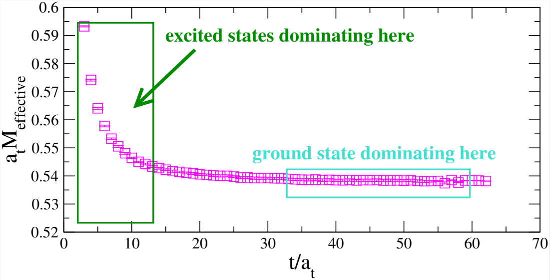
BMW Collaboration (Dürr et al) 0906.3599v1




- $L/a = 48, a = 0.085fm, m_\pi = 190$MeV

# The effective mass (again)

At large times, effective mass converges to the ground state energy - see a plateau in the effective mass plot as a function of time.




- How can we determine excited state energies?
- First guess: fit to 2 exponentials - $C(t) = Ae^{-E_0 t} + Be^{-E_1 t}$, where $A, B, E_0, E_1$ are fit parameters.
- Since the regions where $E_0$ and $E_1$ are relevant are different: fit for $E_0$ and freeze its value in a fit for $E_1$.
- Notoriously unstable fits.
- Different approach needed

# Extracting excited state energies

There are a number of ideas on the market

- Bayesian analysis
- $\chi^2$-histogram analysis
- Variational analysis
- $\vdots$

# Variational analysis

- Consider a basis of operators $\mathcal{O}_i, i = 1, \ldots, N$ in a given lattice irrep.
- Form a matrix of correlators

$$C_{ij}(t) = \langle \mathcal{O}_i(t) \mathcal{O}_j^\dagger(0) \rangle$$

- Treat as a generalised eigenvalue problem (GEVP):

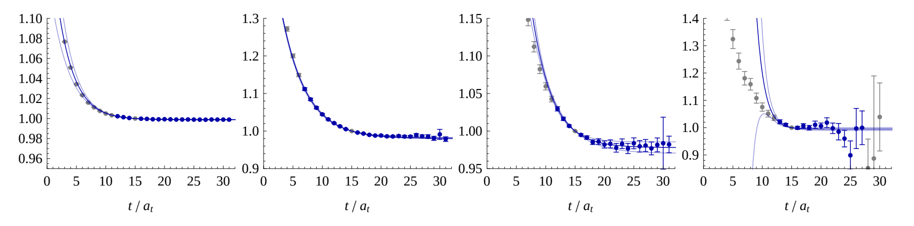
$$C(t) v_n(t, t_0) = \lambda_n(t, t_0) C(t_0) v_n(t, t_0)$$

  where $t_0$ is a refence timeslice (you choose)
- The vectors $v_n$ diagonalise $C(t)$
- For finite $N$ one can prove [Lüscher & Wolff 1990]

$$E_n^{eff}(t, t_0) = -\partial_t \log \lambda_n(t, t_0) = E_n + O(e^{-\Delta E_n t})$$

# Fitting principal correlators

- Typical fits for a set of excited states in the $T_1^{--}$ irrep in charmonium (26 operators!) are




- plotting $\lambda_n(t) \cdot e^{m_n(t_1 - t_0)}$ with $t_0 = 15$.
- Expect a plateau at 1.0 if single-exp dominates.

# Improving resolution: anisotropic lattices

# Improving resolution - the anisotropic lattice

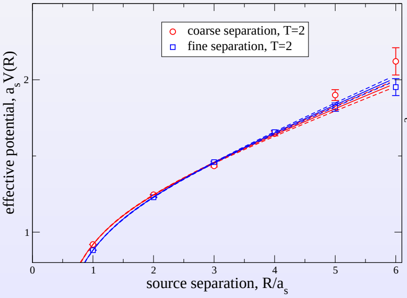
- If we can build a good basis of operators, we can extract energies of low-lying states from the correlator at short distances.
- The lattice correlator can only be sampled at discrete values of $t$ and signal falls quickly for a massive state, while the statistical noise does not. Reducing the lattice spacing is extremely computationally expensive
- Mitigate this cost by reducing just the temporal lattice spacing, keeping the spatial mesh coarser; the anisotropic lattice.
- Unfortunately this reduces the symmetries of the theory from the hypercubic to the cubic point group. The dimension four operators on the lattice now split;

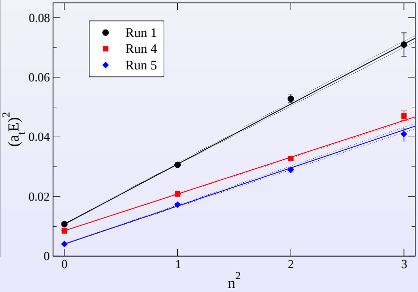
$$\begin{aligned}\mathrm{Tr}\, F_{\mu\nu}F_{\mu\nu} &\rightarrow \left\{\mathrm{Tr}\, F_{ij}F_{ij}, \mathrm{Tr}\, F_{i0}F_{i0}\right\} \\ \bar{\psi}\gamma_\mu D_\mu \psi &\rightarrow \left\{\bar{\psi}\gamma_i D_i \psi, \bar{\psi}\gamma_0 D_0 \psi\right\}\end{aligned}$$

- On $3 \oplus 1$ anisotropic lattices, spatial symmetries unchanged.

# QCD and the anisotropic lattice

- The space-time symmetry breaking in QCD introduces extra bare parameters in the lagrangian, that must be tuned to restore Euclidean rotational invariance in the continuum limit.
- For QCD, both the quarks and gluons must "feel" the same anisotropy; this requires tuning *a priori*.
- Two physical conditions are satisfied simultaneously, derived from the "sideways" potential and the pion dispersion relation.



# Systematic Uncertainties

## lattice artefacts

$$\left.\frac{m_N}{m_\Omega}\right|_{lat} = \left.\frac{m_N}{m_\Omega}\right|_{cont} + \mathcal{O}(a^p),\ p \geq 1$$

requires extrapolation to the continuum limit, $a \to 0$

## finite volume effects

- Energy measurements can be distorted by the finite box
- Rule of thumb: $m_\pi L > 3$ ok for many things ...

## Unphysically heavy pions

- Simulations at the physical point have started but most calculations rely on chiral extrapolation to reach physical $m_u, m_d$
- Use Chiral Perturbation Theory (ChPT) to guide the extrapolations. Are chiral corrections reliably described by ChPT?

## Fitting

- Uncertainties from the choice of fit range, $t_0$ etc.

# Summary

- Constructing operators to have good overlap with states is important
  - Extended operators give access to $J > 1$ states and allow variational analysis
  - Operators subduced from the continuum retain a memory of continuum spin - see this in the operator overlaps
  - Other methods on the market also and it is early days in this sort of spectroscopy
- Fitting data requires an understanding of the underlying physics. No rules for picking a fit range but there are guidelines ...
- Anisotropic lattices give extra resolution and have been successfully used in spectroscopy
- Systematic errors should be dealt with (or at least acknowledged)
  - Precision spectroscopy of ground states usually includes continuum and chiral extrapolations in large volumes
  - Spectroscopy for higher-lying states not as mature. There are precision calculations at finite lattice spacing and unphysical quark mass.