

# Excited states from Lattice QCD

“something about excited states/exotica, which uses techniques which could potentially be useful for finite T as well”

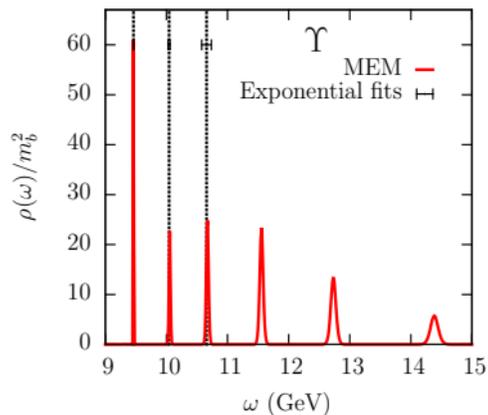
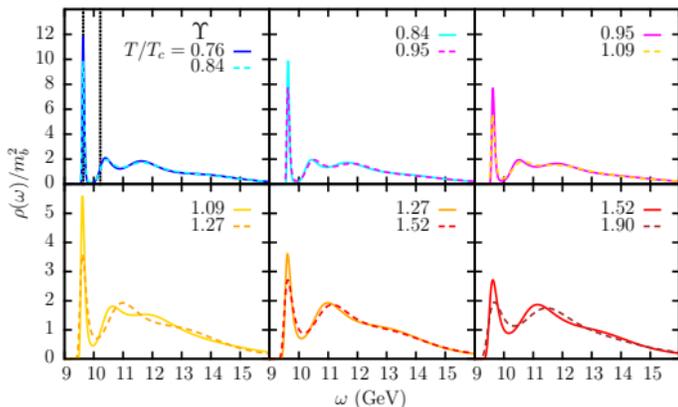
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THOR Cost Meeting, Swansea, September 2017

# SPECTROSCOPY AT ZERO AND FINITE TEMPERATURE

MEM is the method of choice at  $T > 0$  - where focus is on e.g. patterns of melting/suppression in ground states of S and P waves.



Focus is rather different at  $T = 0$  and there has been a lot of rapid progress in the last few years: experimental and in lattice techniques.

## LATTICE SPECTROSCOPY: TWO STRATEGIES FOR PROGRESS

Below thresholds: “gold-plated” quantities characterised by

- Using well-trying and tested and validated methods
- High statistics and improved actions for precise results
- Different actions in agreement
- Most/All systematic errors accounted for e.g. continuum extrapolation, finite volume, physical light quark masses,  $N_f$ , EM effects

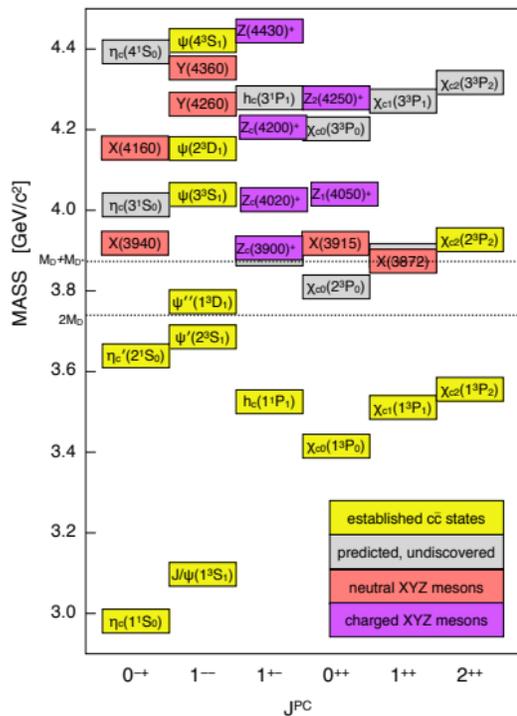
Above thresholds: calculation of high spin & exotic states relatively new

- Physics of molecular/multi hadron states needs relevant operators.
- No continuum extrapolation
- Relatively heavy pions ← already changing
- Improvements underway now that methods are proven

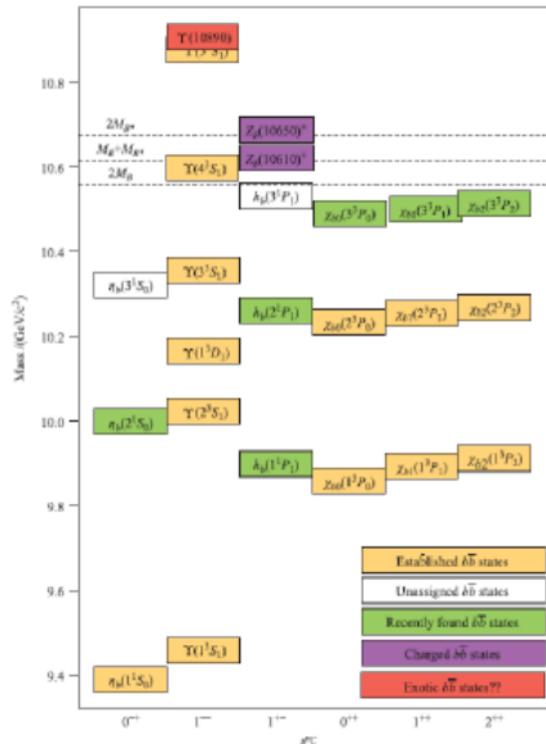
new ideas crucial

- Distillation - quark propagation enabling isoscalars, precision spectroscopy ...
- Framework for scattering & coupled channels

# A CHARMING AND BEAUTIFUL RENAISSANCE

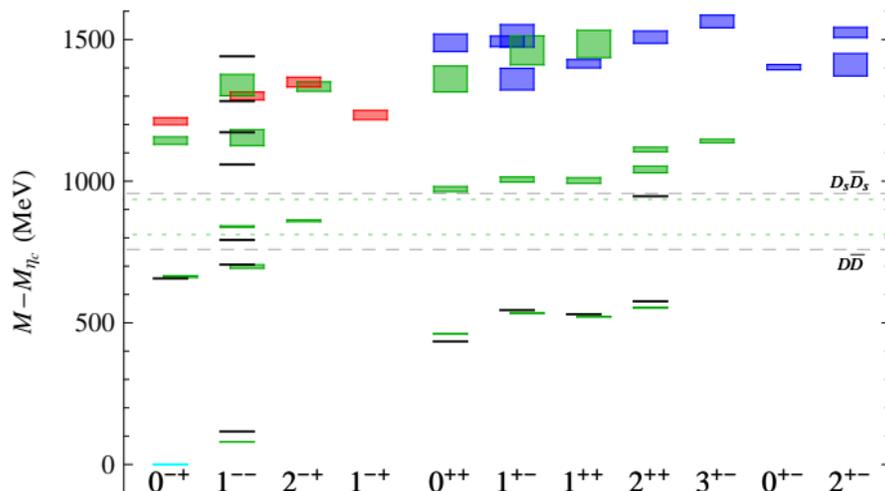


from Ryan Mitchell via Steve Olsen



from X-H Liu, ECT\* 2017

# PRECISION SPECTROSCOPY OF HYBRIDS: CHARMONIUM



- Not all fit quark model: **spin-exotic (and non-exotic) hybrids determined.**
- Same pattern and energy scale in mesons and baryons - heavy and light.
- Very little bottomonium spectroscopy yet ...



# LATTICE HADRON SPECTROSCOPY, $T=0$

In principle, provides a model-independent ab initio description of the QCD spectrum.

Lots of progress and new ideas to tackle spectroscopy

- Algorithms for quark propagation: all-to-all propagators and distillation
- Extracting energies of excited and exotic states
  - Bayesian analysis,  $\chi^2$ -histogram analysis, variational analysis, ...
- Using symmetries and operator overlaps to identify states at  $J \geq 2$
- Extension of Lüscher's finite volume idea for scattering including coupled channels and resonant transitions.
- Despite huge progress the nature of the XYZ states still unclear.

## Questions

Does it make sense to study hybrids and/or exotica at finite temperature?

Can we use the techniques from zero temperature to improve spectroscopy?

- smearing plays a key role.

# **Making Measurements**

# A RECIPE FOR (MESON) SPECTROSCOPY

Let's look at the basic ideas for extracting energies:

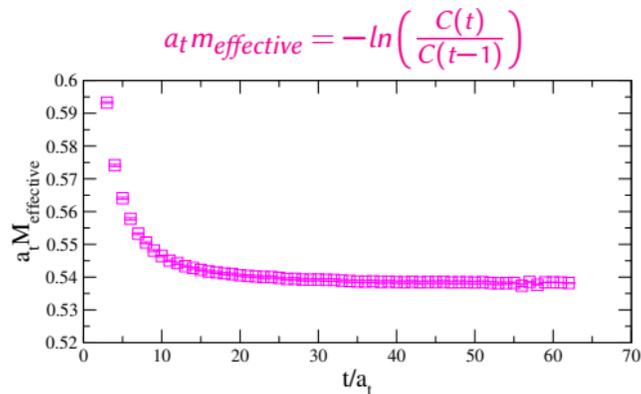
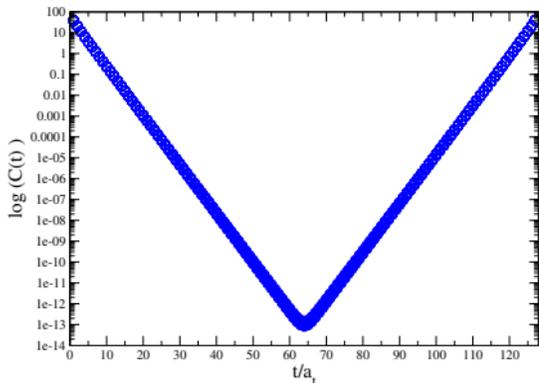
- Ground state energies found from  $t \rightarrow \infty$  limit of a Euclidean-time correlation function

$$\begin{aligned} C(t) &= \langle 0 | \phi(t) \phi^\dagger(0) | 0 \rangle \\ &= \sum_{k, k'} \langle 0 | \phi | k \rangle \langle k | e^{-\hat{H}t} | k' \rangle \langle k' | \phi^\dagger | 0 \rangle \\ &= \sum_k |\langle 0 | \phi | k \rangle|^2 e^{-E_k t} \end{aligned}$$

- So,  $\lim_{t \rightarrow \infty} C(t) = Z e^{-E_0 t}$  and ground states are reliably determined from exponential fits.

# FROM CORRELATORS TO ENERGIES

- In general works well for extracting ground states
- Higher excitation energies hard to extract by just fitting to exponentials.



- The correlator and effective mass of the  $J/\psi$  meson.
- For  $\mathcal{O}_i = \mathcal{O}_j$  the correlation function is positive definite and  $a_t m_{effective}$  converges monotonically from above.
- Bayesian fitting methods improve multi-exponential fits but not enough to determine/disentangle high-spin states.

## EXCITED STATES

To go beyond ground state spectroscopy the method of choice is the **variational idea**: find operator  $\phi$  to maximise  $C(t)/C(t_0)$  from sum of basis operators  $\phi = \sum_a v_a \phi_a$

[C. Michael & I. Teasdale. NPB215 (1983) 433]; [M. Lüscher & U. Wolff. NPB339 (1990) 222]

### Variational method

If we can measure  $C_{ab}(t) = \langle 0 | \phi_a(t) \phi_b^\dagger(0) | 0 \rangle$  for all  $a, b$  and solve the generalised eigenvalue problem

$$C_{ij}(t) v_j^{(n)} = \lambda^{(n)}(t) C_{ij}(t_0) v_j^{(n)},$$

then

- eigenvalues:  $\lambda^{(n)}(t) \sim e^{-E_n t} [1 + O(e^{-\Delta E t})]$ ,  $t \geq t_0/2$  - gives principal correlator.
- eigenvectors: related to overlaps  $Z_i^{(n)} = \sqrt{2E_n} e^{E_n t_0/2} v_i^{(n)\dagger} C_{ji}(t_0)$ .

For this to be practical, we need

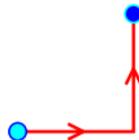
- a “good” basis set that resembles the states of interest
- all elements of this correlation matrix measured

[Blossier et al JHEP 0904 (2009) 094]

# VARIATIONAL METHOD: A METHOD NOT A MAGIC WAND!

Good information in gets good information out!

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.



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

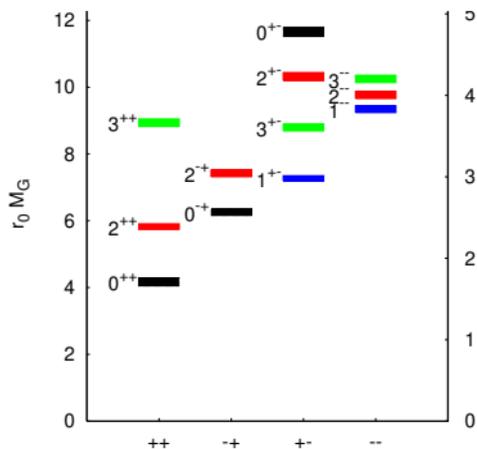
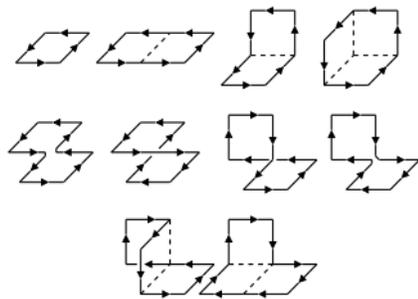
A good operator:

- An operator of definite momentum that transforms under a lattice irrep
- An operator that has strong overlap with the (continuum) state of interest.
- An operator is not noisy ie that produces an acceptable correlator

# GLUEBALLS - AN EARLY SUCCESS

- QCD nonAbelian  $\Rightarrow$  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

[Morningstar and Peardon]



## DESIGNING GOOD LATTICE OPERATORS - A TALE OF TWO SYMMETRIES



- Lorentz symmetry broken at  $a \neq 0$  so  $SO(4)$  rotation group broken to discrete rotation group of a hypercube.
- Classify states by irreps of  $O_h$  and relate by subduction to  $J$  values of  $O(3)$ .
- 5 irreps of  $O(3)$  and an infinite number for  $J^P$  so values are distributed across lattice irreps.

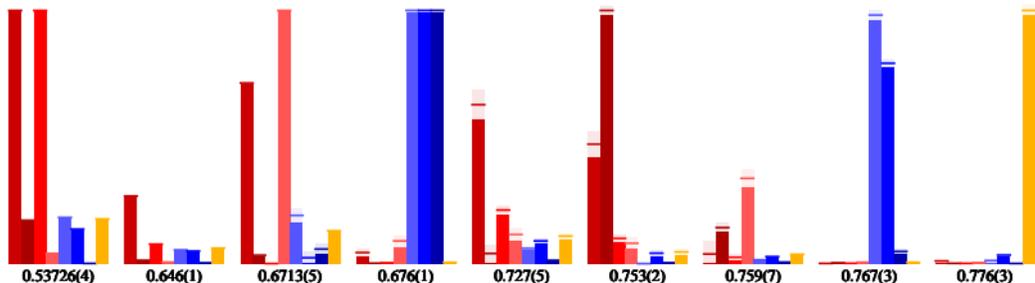
- start with continuum operators, built from  $n$  derivatives:  

$$\phi = \bar{\psi} \Gamma (D_{i_1} D_{i_2} D_{i_3} \dots D_{i_n}) \psi$$
- Construct irreps of  $SO(3)$ , then subduce these representations to  $O_h$
- Replace derivative with lattice differences:
- A subduced irrep carries a “memory” of continuum spin  $J$  from which it was subduced - it **overlaps** predominantly with states of this  $J$ .

J	0	1	2	3	4
$A_1$	1	0	0	0	1
$A_2$	0	0	0	1	0
$E$	0	0	1	0	1
$T_1$	0	1	0	1	1
$T_2$	0	0	1	1	1

# USING GEVP EIGENVALUES - OPERATOR OVERLAPS

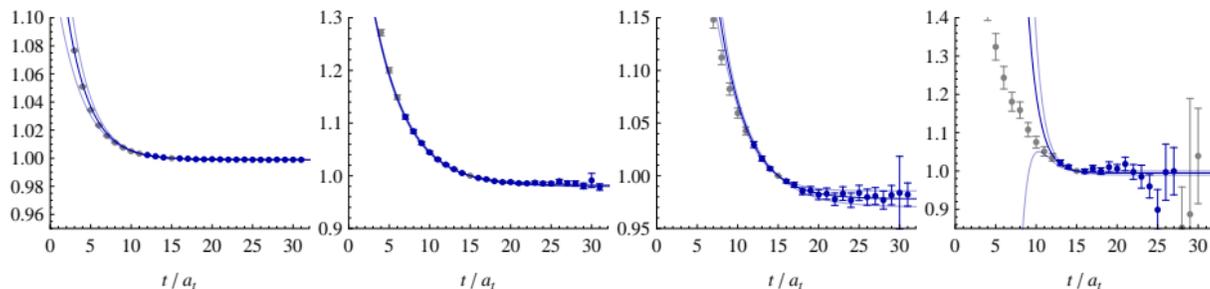
- Using  $Z = \langle 0|\Phi|k\rangle$ , helps to identify continuum spins
- For high spins, can look for agreement between irreps
- Data below for  $T_1^-$  irrep, colour-coding is **Spin 1**, **Spin 2**, **Spin 3** and **Spin 4**.





## 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.
- Anisotropy helps the variational method: improving resolution in the temporal direction.
- Smearing crucial.

# VARIATIONAL IDEAS AT FINITE T

- WHOT-QCD collaboration have explored variational ideas to extract excited states at finite T.
  - 0810.1567, Umeda et al: Ground and first excited states of  $J/\Psi, \chi_c$  from a basis of smeared source and sink operators.  
Studied the shape and vol-dependence of BS wavefunctions to distinguish bound and scattering states.
  - 1104.33842, Ejiri et al: Adapted variational method to calculate locations and heights of spectral functions - and compared to MEM.  
Very dependent on “good” operators to resolve a signal in the range of available  $t$  at high temperatures. Using point-smeared operators.
- At T=0, much of the progress has come from looking again at the hadronic building blocks - the propagators.

# **Making Propagators**

## LOOKING BACK AT PROPAGATION

Exploiting techniques for excited states requires **efficient** and **precise** determination of propagators.

What's on the market?

- Point propagators - used extensively at finite  $T$ , rarely (at least in isolation) at  $T=0$ .
- Smearred propagators - via Gaussian, Jacobi etc smearing.
- All to all propagators + smearing.
- Distillation - a “redefinition” of smearing.

How useful can smearing be at finite temperature? Can zero temperature methods be useful?

# POINT PROPAGATORS

For better simulations of hadronic quantities look again at the building blocks: **the quark propagators**

## Point (to-all) propagator pros

- doesn't require vast computing resources

## Point (to-all) propagator cons

- **restricts the accessible physics**
  - flavour singlets and condensates impossible: quark loops need props w sources everywhere in space
- **restricts the interpolating basis used**
  - a new inversion needed for every operator that is not restricted to a single lattice point
- **entangles propagator calculation and operator construction**
- **not using all information encoded in configurations**

# SOLUTIONS?

- Improve the determination point props to access the physics of interest: **smearing**. Lots of examples around.
- Compute all elements of the quark propagator: **all-to-all propagators**. **Problem** It's expensive - needs and unrealistic number of inversions.
- **Work around**: Use **stochastic estimators** (with variance reduction).
- Rethink the problem: combine smearing and propagation ie **distillation**

I'm just picking a couple of ideas to focus on.

## **All-to-all propagators**

## ABOUT ALL-TO-ALL PROPAGATORS

- Computing **all** elements of the quark propagator would require full knowledge of the inverse - this is prohibitively expensive
- The lattice representation of the Dirac operator is a large, but very sparse matrix.
- If we are satisfied with an *unbiased estimator* of all elements then sparse matrix methods can be used. Stochastic estimation should be acceptable - we are already using it to generate gauge fields!
- Variance reduction will be crucial

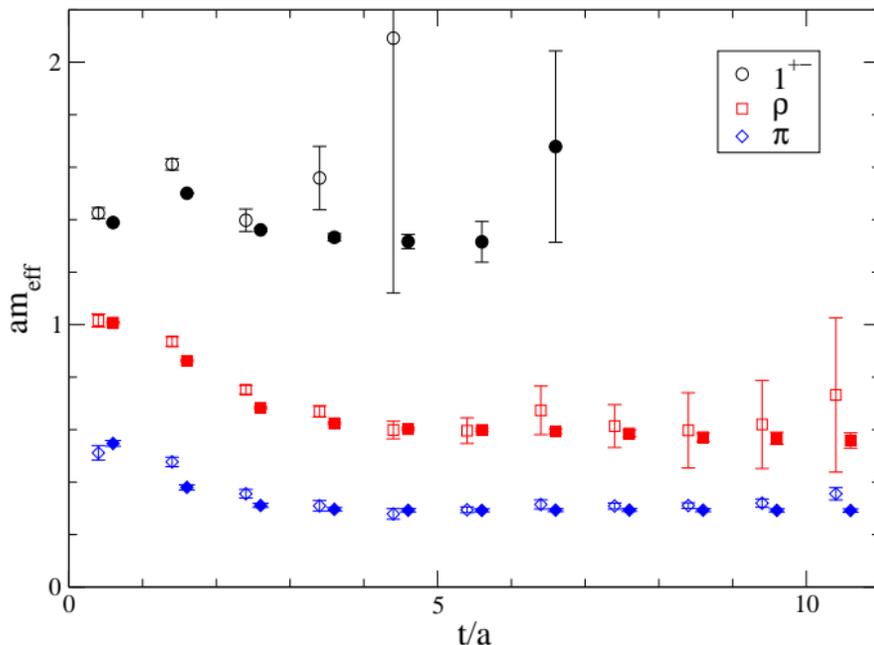
# ALL-TO-ALL QUARK PROPAGATORS

- Start with a spectral representation of  $Q = \gamma_5 M$  (hermitian so eigenvalues are easier to compute).
- If we can compute all the eigenvectors and eigenvalues,  $\{\lambda^{(i)}, v^{(i)}\}$  of

$$Q = \sum_{i=1}^N \lambda^{(i)} v^{(i)} \otimes v^{*(i)} \quad \text{then} \quad Q^{-1} = \sum_{i=1}^N \frac{1}{\lambda^{(i)}} v^{(i)} \otimes v^{*(i)}$$

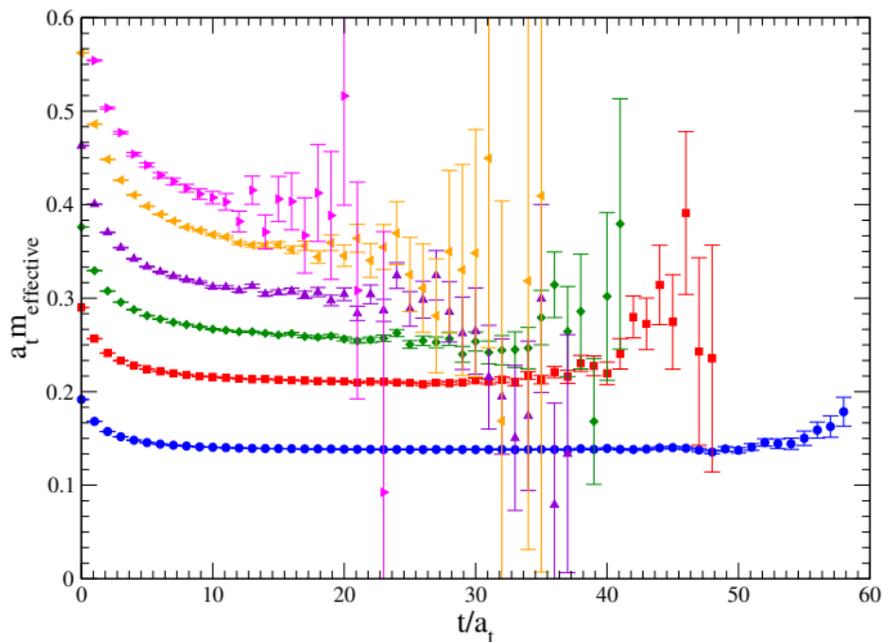
- Even a small sub-set of eigenvectors is computationally expensive, so truncate at  $N_{\text{ev}} \ll N$
- Truncated sum violates **reflection positivity**.
- Use stochastic methods (dilution) to estimate the truncated part.

## COMPARING METHODS: POINT AND ALL-TO-ALL



- $\beta = 5.7$ ,  $12^3 \times 24$ ,  $m_\pi/m_\rho = 0.50$ , 75 configs and 100 eigenvectors with time/even-odd/spin dilution.
- Dramatic improvement in precision - especially for higher-lying states.

# EXTRACTING EXCITED STATES ENERGIES



$N_f = 2, 12^3 \times 80$  Wilson fermions, static-light meson energies. Jacobi smearing is used to create a basis of operators for a variational analysis.

# Distillation

# DISTILLATION DISTILLED...

- A smeared quark field is  $\tilde{\psi} = \square\psi$ .
- **Define** smearing to be explicitly a very low-rank operator. Rank is  $N_D (\ll N_S \times N_C)$ .

Distillation operator

$$\square(t) = V(t)V^\dagger(t)$$

with  $V_{\underline{x},c}^a(t)$  a  $N_D \times (N_S \times N_C)$  matrix

- Example (used to date):  $\square_\nabla$  the **projection operator into  $\mathcal{D}_\nabla$ , the space spanned by the lowest eigenmodes of the 3-D laplacian**
- Eigenvectors of  $\nabla^2$  not the only choice...

- Consider an isovector meson two-point function:

$$C_M(t_1 - t_0) = \langle\langle \bar{u}(t_1) \square_{t_1} \Gamma_{t_1} \square_{t_1} d(t_1) \quad \bar{d}(t_0) \square_{t_0} \Gamma_{t_0} \square_{t_0} u(t_0) \rangle\rangle$$

- Substituting the low-rank distillation operator  $\square$  reduces this to a **much smaller** trace:

$$C_M(t_1 - t_0) = \langle \text{Tr}_{\{\sigma, \mathcal{D}\}} [\Phi(t_1) \tau(t_1, t_0) \Phi(t_0) \tau(t_0, t_1)] \rangle$$

- $\Phi_{\beta, b}^{\alpha, a}$  and  $\tau_{\beta, b}^{\alpha, a}$  are  $(N_\sigma \times N_{\mathcal{D}}) \times (N_\sigma \times N_{\mathcal{D}})$  matrices.

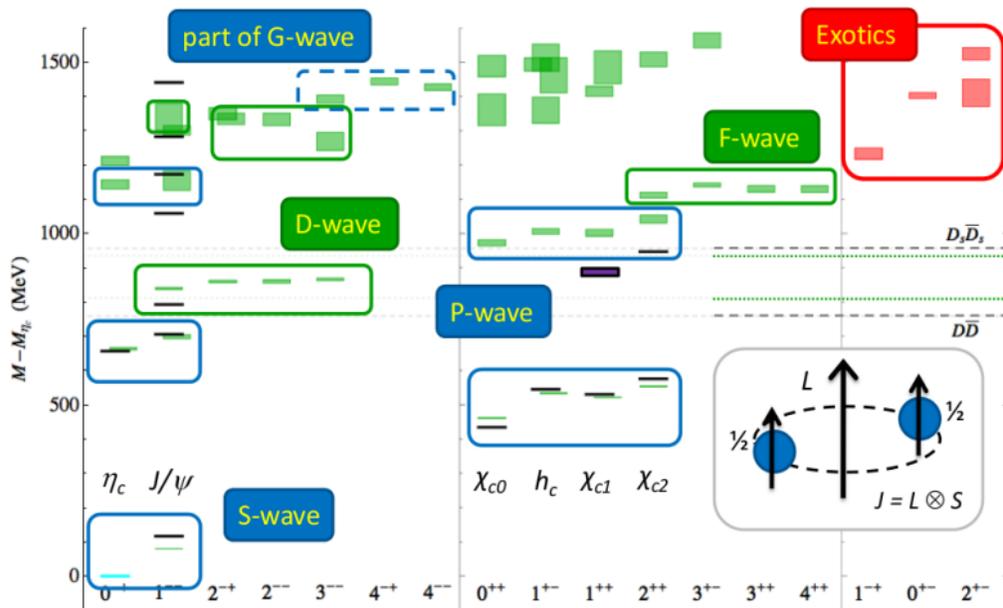
$$\Phi(t) = V^\dagger(t) \Gamma_t V(t)$$

$$\tau(t, t') = V^\dagger(t) M^{-1}(t, t') V(t')$$

The “perambulator”

- Note that propagation (via perambulators) and operator construction are separated. Perambulators can be stored and reused for any later operators of interest.

## CHARMONIUM WITH DISTILLATION

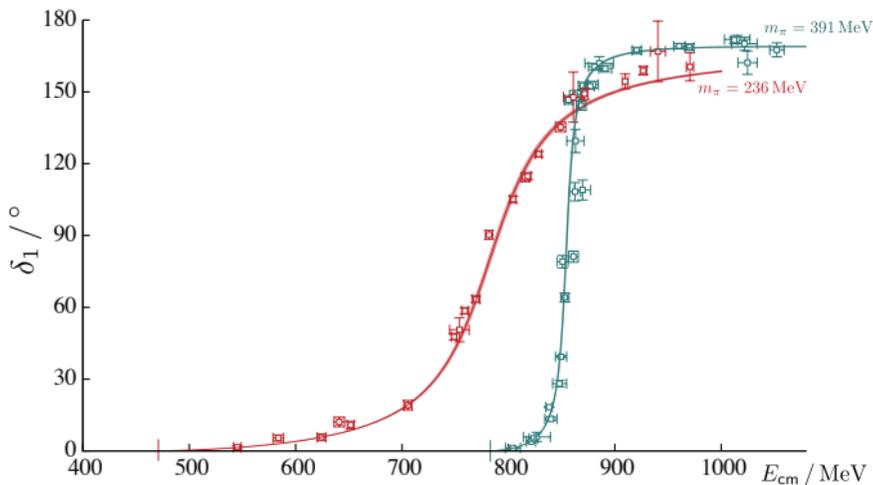


$N_f = 2 + 1$ ,  $m_\pi \sim 400\text{MeV}$ . Single hadron operators ie no scattering analysis. Lattice irreps have  $\sim 10\text{-}20$  operators in basis.

## EXTRACTING SCATTERING INFORMATION

- Use the finite volume as a tool
- Related **lattice energy levels in a finite volume** to a decomposition of the scattering amplitude in **partial waves in infinite volume**

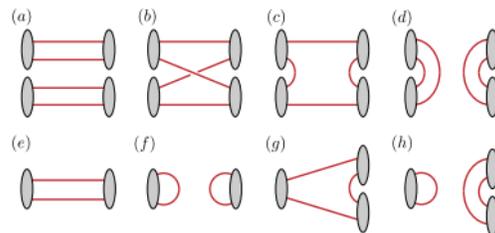
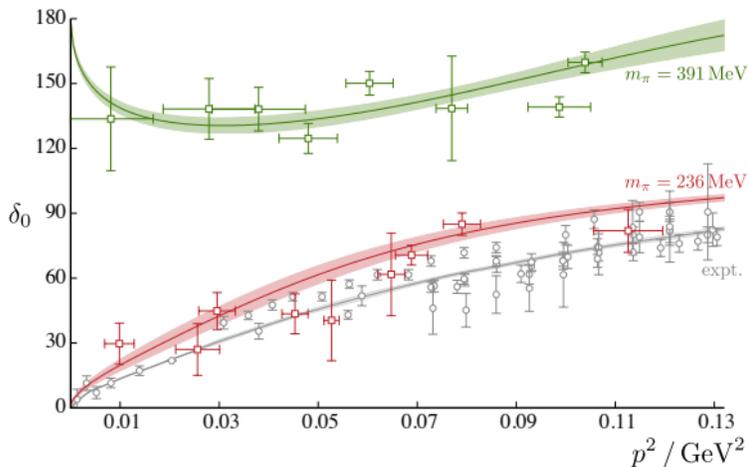
$$\det \left[ \cot \delta(E_n^*) + \cot \phi(E_n, \vec{P}, L) \right] = 0$$



- Includes coupled channels, all disconnected diagrams
- See “HadSpec” for more eg  $a_0$ ,  $\sigma$  meson etc

# SIGMA MESON

Isoscalar  $\pi\pi$  scattering including all diagrams.

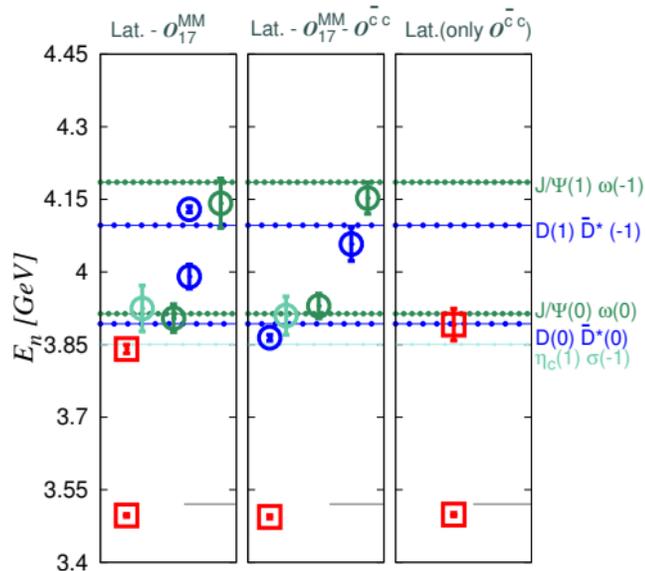
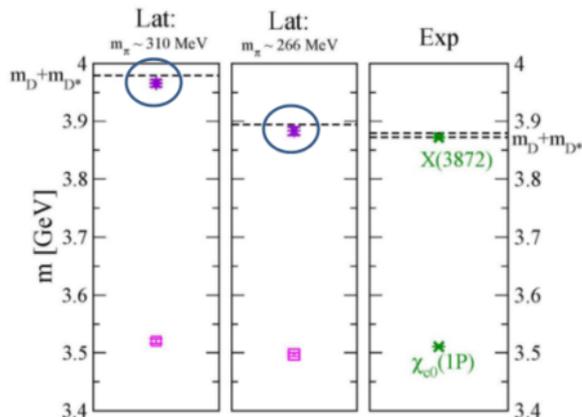


From  $m_\pi = 236, 391$  MeV resolve a  $\sigma$  that evolves from a bound-state below  $\pi\pi$  threshold at heavier mass to a broad resonance at lighter mass.  
Note that lattice can also be a tool to study mass-dependence!

# THE XYZs: X(3872) - A FIRST LOOK (NO COUPLED CHANNELS)

Prelovsek & Leskovec 1307.5172

Padmanath, Lang, Prelovsek 1503.03257



Ground state:  $\chi_{c1}(1P)$   
 $D\bar{D}^*$  scattering mx: pole just below thr.  
 Threshold location? Finite vol effects?

X(3872) not found if  $c\bar{c}$  not in basis.

Within 1MeV of  $D^0\bar{D}^{0*}$  and 8MeV of  $D^+D^*$  thresholds: isospin breaking effects important?

# SUMMARY

- Hadronic spectroscopy has changed dramatically in recent years at zero and finite temperature.
- Progress has come from improvements to quite different methods - Bayesian methods at  $T=0$  and variational analysis and quark propagation at  $T>0$ .
- At  $T=0$ , excited and exotic hadronic states are determined with high precision and the finite volume is used to extract scattering information in increasingly complex scenarios.
- New(ish) methods imply a cost: - all-to-all, eigenvectors for distillation, many operators for variational. But typical improvements in spectroscopic quantities could not otherwise be achieved.
- Multi-hadron and scattering calculations (not discussed) are now quite sophisticated, using these methods - is this useful at finite temperature?
- Can we import some ideas to finite temperature spectroscopy?

## EXAMPLE: $J^{PC} = 2^{++}$ MESON CREATION OPERATOR

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

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

- Lattice: Substitute gauge-covariant lattice finite-difference  $D_{latt}$  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:

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

# BAD NEWS: THE BILL!

- For constant resolution distillation space scales with  $N_s$
- The cost of a calculation scales with  $V^2$

## The problem:

- To maintain constant resolution, need  $N_D \propto N_s$

- **Budget:**

Fermion solutions	construct $\tau$	$\mathcal{O}(N_s^2)$
Operator constructions	construct $\Phi$	$\mathcal{O}(N_s^2)$
Meson contractions	$\text{Tr}[\Phi\tau\Phi\tau]$	$\mathcal{O}(N_s^3)$
Baryon contractions	$\bar{B}\tau\tau\tau B$	$\mathcal{O}(N_s^4)$

- Ok for reasonable lattices (eg with  $N_s = 16^3$ ,  $N_D = 64$ ) but scaling this to a  $32^3$  volume requires  $N_D = 512$ . Expensive.
- Distillation does not preclude stochastic estimation - use both for large  $V$ .