

# Spectroscopy

in Euclidean space, a) choose a time direction: e.g.  $\hat{t} = (0, 0, 0, 1)$

b) identify fermion fields  $\psi^+ = \bar{\psi} \gamma^+ = \bar{\psi} \gamma_4$

c) use a time extent  $L_t$  with (anti)periodic boundary conditions

if we let  $\mathcal{O}(t)$  and  $\mathcal{O}'(t)$  be functions of the fields at time  $t$

$$\text{then } C(t) \equiv \langle \mathcal{O}'(t) \mathcal{O}^+(0) \rangle = \frac{\text{tr} [e^{-(L_t-t)\hat{H}} \mathcal{O}' e^{-t\hat{H}} \mathcal{O}^+]}{\text{tr} [e^{-L_t\hat{H}}]} \quad \text{for } t > 0$$

$$\xrightarrow{L_t \rightarrow \infty} \sum_{n=0}^{\infty} \underbrace{\langle \mathcal{O}' |}_{\text{vacuum}} \langle n | \underbrace{\mathcal{O}^+}_{\text{energy eigenstates (discrete in finite volume)}} | n \rangle e^{-E_n t}$$

restrict sum to states with  $\langle \mathcal{O}' | \mathcal{O}^+ | n \rangle \neq 0 \neq \langle \mathcal{O} | \mathcal{O}^+ | n \rangle$

and order energies  $E_0 < E_1 < E_2 < \dots$

$$\Rightarrow -\frac{d}{dt} \log C(t) = E_0 + O(e^{-(E_1 - E_0)t}) \quad \text{obtain } E_0 \text{ at large } t$$

"effective energy"  $E_{\text{eff}}(t)$

if  $\mathcal{O} = \mathcal{O}'$  then  $C(t)$  is positive and convex

$\Rightarrow E_{\text{eff}}(t)$  approaches  $E_0$  monotonically, from above

Example: single isovector meson at zero momentum

$$\text{let } \mathcal{O}(t) = \int d^3x \bar{u}(\vec{x}, t) \Gamma d(\vec{x}, t) \quad \text{e.g. } \Gamma = \gamma_5 \rightarrow \pi \quad J^5 = O^- \\ \Gamma = \gamma_i \rightarrow e \quad I^-$$

$$\Rightarrow \mathcal{O}^+(t) = \int d^3x \bar{d}(\vec{x}, t) \bar{\Gamma} u(\vec{x}, t), \quad \bar{\Gamma} = \gamma_4 \Gamma^\dagger \gamma_4$$

$$C(t) = \langle \mathcal{O}(t) \mathcal{O}^+(0) \rangle$$

$$= \int d^3x d^3y \langle \bar{u}(\vec{x}, t) \Gamma d(\vec{x}, t) \bar{d}(\vec{y}, 0) \bar{\Gamma} u(\vec{y}, 0) \rangle \quad \text{one Wick contraction}$$

$$= \int d^3x d^3y \langle -\text{tr} [\Gamma \bar{D}_d(\vec{x}, t; \vec{y}, 0) \bar{\Gamma} \bar{D}_u(\vec{y}, 0; \vec{x}, t)] \rangle$$

Abuse of notation!  $\langle \mathcal{O}(t) \mathcal{O}^+(0) \rangle$  refers to QCD path integral (over gauge + fermion fields)  
but now  $\langle \dots \rangle$  refers to Monte Carlo integral over gauge fields

how to compute? simplest method: use translation symmetry +  $\gamma_5$ -hermiticity  
with degenerate u and d:

$$C(t) = -L^3 \int d^3\bar{x} \left\langle \text{tr} \left[ \Gamma D^i(\bar{x}, t; \vec{0}, 0) \bar{\Gamma} \gamma_5 D^i(\bar{x}, t; \vec{0}, 0)^+ \gamma_5 \right] \right\rangle$$

↗      ↘  
point-source quark propagator

### Variance of $C(t)$

In general: for estimator  $X$ ,  $\text{var}(X) = \langle X^2 \rangle - \langle X \rangle^2$   
Monte Carlo expectation

Variance depends on how we compute  $C(t)$ .

point-source estimator yields

$$\text{variance} = L^6 \int d^3\bar{x} d^3\bar{y} \left\langle \text{tr} \left[ \Gamma D^i(\bar{x}, t; \vec{0}, 0) \bar{\Gamma} \gamma_5 D^i(\bar{x}, t; \vec{0}, 0)^+ \gamma_5 \right] \times \text{tr} \left[ \Gamma D^i(\bar{y}, t; \vec{0}, 0) \bar{\Gamma} \gamma_5 D^i(\bar{y}, t; \vec{0}, 0)^+ \gamma_5 \right] \right\rangle - C(t)^2$$

$$\sim \langle 0 \begin{array}{c} \xrightarrow{\bar{x}, t} \\ \xrightarrow{\bar{y}, t} \end{array} \rangle - \langle 0 \xrightarrow{\bar{x}, t} \rangle \langle 0 \xrightarrow{\bar{y}, t} \rangle$$

what is this expectation value?

$$\langle (\bar{u} \Gamma d)(\bar{x}, t) (\bar{u}' \Gamma d')(\bar{y}, t) (\bar{d} \bar{\Gamma} u \bar{d}' \bar{\Gamma} u')(\vec{0}, 0) \rangle$$

Need 4 different degenerate valence flavours  $u, d, u', d'$  to produce this diagram  
→ expectation value in partially quenched theory

What states can propagate between 0 and t?

smallest energy: 2 pseudoscalar mesons  $\Rightarrow$  variance  $\sim e^{-2m_\pi t}$

Signal-to-noise ratio  $\frac{C(t)}{\text{variance}} \sim e^{-(E_0 - m_\pi)t}$  good for  $E_0 = m_\pi$   
bad for heavier mesons

problem is severe for many quarks: A nucleon  $\rightarrow \sim e^{-A(m_N - \frac{3}{2}m_\pi)t}$

## Combining multiple operators

let  $\hat{O}_i(t)$ ,  $1 \leq i \leq N$ , be linearly independent interpolating operators with chosen quantum numbers

define the correlator matrix  $C_{ij}(t) \equiv \langle \hat{O}_i(t) \hat{O}_j^\dagger(0) \rangle$   $N \times N$   
 hermitian, positive definite  $\xrightarrow{t \rightarrow \infty} \sum_{n=0}^{\infty} Z_{in} Z_{jn}^* e^{-E_n t}$ ,  $Z_{in} = \langle \Omega | \hat{O}_i | n \rangle$

What do we gain from this?

consider extreme scenario of  $v$  degenerate states:  $E_0 = E_1 = \dots = E_{v-1}$

then correlator has  $\left( \sum_{n=0}^{v-1} Z_{in} Z_{jn}^* \right) e^{-E_0 t} + \text{excited states}$   
 matrix of rank  $\min(N, v)$

for a single correlator ( $N=1$ ) it is impossible to identify degenerate states  
 and very difficult to identify near-degenerate states

if  $N \geq v$  then the states can be identified in principle and in practice

## Variational method

want to find linear combination  $\tilde{O}_n = \sum_{i=1}^N (v_n)_i \hat{O}_i$  s.t.  $\tilde{O}_n^\dagger | \Omega \rangle \approx | n \rangle$

if states  $n \geq N$  can be neglected (only  $N$  states contribute)

then solution satisfies  $\sum_{j=1}^N Z_{jn}^* (v_m)_j = \delta_{nm}$

$v_n$  is a solution to generalized eigenvalue problem (GEVP)  $C(t)v_n = \lambda_n C(t_0)v_n$   
 with eigenvalue  $\lambda_n = e^{-E_n(t-t_0)}$

neglected part of  $C_{ij}(t)$ :  $\sum_{n=N}^{\infty} Z_{in} Z_{jn}^* e^{-E_n t} = O(e^{-E_N t})$

Corrections from neglected states (ALPHA collab. 2009):

let  $E_n^{\text{eff}}(t, t_0) = -\frac{\partial}{\partial t} \log \lambda_n(t, t_0)$

if  $t_0 \geq \frac{t}{2}$  then  $E_n^{\text{eff}}(t, t_0) = E_n + O(e^{-(E_N - E_n)t})$

more operators (increase  $N$ )  $\rightarrow$  larger  $E_N \rightarrow$  faster convergence to  $E_n$

Notes:

\* Proven result is asymptotic behaviour for large  $t$ .

Need to let  $t_0$  depend on  $t$  in some way: e.g.  $t_0 = \frac{t}{2}$  or  $t_0 = t - \delta t$ .

\* Solving GEVP yields set  $\{\lambda_n\}_{n=0}^{N-1}$  but ordering is arbitrary.

For each  $n$ , need to pick  $\lambda_n$  out of this set for each  $t$ , each resample.

If energies well separated  $\rightarrow$  sort by value.

Otherwise consider using eigenvectors to match different  $t$ , different resamps.

\* Alternative approach: for fixed  $(t_0, t_D)$  solve  $C(t_D)v_n = \lambda_n C(t_0)v_n$ ,  
then let  $\bar{C}(t) = v_n^\dagger C(t) v_n$ .

$\bar{C}(t)$  is approximately diagonal; let  $E_n^{\text{eff}}(t) = -\frac{d}{dt} \log \bar{C}_{nn}(t)$ .

Simpler but need to verify stability as  $(t_0, t_D)$  varied.

Downside: lacks proven good asymptotic behaviour.