Exploring free-form smearing for bottomonium and B meson spectroscopy

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Motivation

To study a particular hadronic state, it would be ideal to have an operator that couples only to that state. An operator with the correct angular momentum quantum numbers is necessary but not sufficient. The spatial structure of the operator (shape) helps to distinguish states with different principal quantum numbers.

Free-form smearing was designed as a way to implement source operators of any desired shape [G. M. von Hippel, B. Jäger, T. D. Rae and H. Wittig, JHEP1309, 014 (2013)] and a variation of the method has been introduced that reduces the computational cost by reducing the number of link multiplications to its absolute minimum [M. Wurtz, R. Lewis and R. M. Woloshyn, arXiv:1505.04410].

A practical implementation of the new method is provided here, and the practical utility of the algorithm is demonstrated through calculations of bottomonium and B_c, B_s and B meson masses.

Free-form smearing

Though free-form smearing can be applied to a quark propagator in any context, consider for definiteness a meson operator defined at a lattice site x. Let $\chi(x)$ represent the antiquark field and let $\tilde{\tilde{\psi}}(x)$ represent the free-form smeared quark field. The meson operator is then

$$\chi(x)\tilde{\tilde{\psi}}(x) = \chi(x)\sum_y \Omega(x-y)\frac{\tilde{\psi}_x(y)}{\left\langle\left|\left|\tilde{\psi}_x(y)\right|\right|\right\rangle}$$

where $\Omega(x-y)$ is chosen by the user to define the desired shape and quantum numbers of the operator. The denominator is the ensemble average of a color+Dirac trace

$$\left\langle\left|\left|\tilde{\psi}_x(y)\right|\right|\right\rangle = \sqrt{\mathrm{Tr}\left(\tilde{\psi}_x^\dagger(y)\tilde{\psi}_x(y)\right)}$$

and its purpose is to divide out spatial variations in the quark field $\tilde{\psi}_x(y)$ so the interpretation of $\Omega(x-y)$ is as transparent as possible.

The original implementation of free-form smearing defined $\tilde{\psi}$ through standard Gaussian smearing, but a more efficient definition is the minimal-path definition, where no paths are duplicated in the calculation:

$$\tilde{\psi}_x(y) = \sum_{\text{shortest paths}} U(x\to y)\psi(y)$$

The link variables in $U(x\to y)$ can be thin or thick; our examples use stout links [C. Morningstar and M. J. Peardon, Phys. Rev. D69, 054501 (2004)].

The minimal-path algorithm to compute $\tilde{\psi}_x(y)$

sitevisited = false
linkvisited = false ▷ Initialize all sites and links as having not been visited.
$\tilde{\psi} = 0$
$\tilde{\psi}(x) = 1$ ▷ Initialize the field to unity at the origin and zero everywhere else.
sitevisited(x) = true ▷ Mark the origin, x, as having been visited.
$y_{\text{frontier}}(1) = x$ ▷ Mark the origin, x, as on the frontier.
$n = 1$ ▷ Initially there is only one point on the frontier.
while $n > 0$ **do** ▷ Loop until all sites have been visited, *i.e.* the frontier contains no points ($n = 0$).
  $n_{\text{new}} = 0$ ▷ Initialize the number of points on the new frontier to zero.
  for $i = 1, n$ **do** ▷ Visit all of the points on the frontier.
    $y = y_{\text{frontier}}(i)$
    for $\mu = 1, 3$ **do**
      Forward direction
      if linkvisited(μ, y) = false **then** ▷ If the link $U_\mu(y)$ has not been visited.
        $\tilde{\psi}(y+\mu) = \tilde{\psi}(y+\mu) + U_\mu^\dagger(y)\tilde{\psi}(y)$ ▷ Multiply the new link to $\tilde{\psi}$ at the old frontier and add it to $\tilde{\psi}$ at the new frontier.
        linkvisited(μ, y) = true ▷ Mark this link as visited.
        if sitevisited$(y+\mu)$ = false **then** ▷ If this site has not been visited before.
          sitevisited$(y+\mu)$ = true ▷ Mark this site as visited and add it to the new frontier.
          $n_{\text{new}} = n_{\text{new}} + 1$
          $y_{\text{newfrontier}}(n_{\text{new}}) = y + \mu$
        end if
      end if
      Backward direction, essentially $\mu \to -\mu$
      if linkvisited(μ, y) = false **then** ▷ If the link $U_\mu(y-\mu)$ has not been visited.
        $\tilde{\psi}(y-\mu) = \tilde{\psi}(y-\mu) + U_\mu(y-\mu)\tilde{\psi}(y)$ ▷ Multiply the new link to $\tilde{\psi}$ at the old frontier and add it to $\tilde{\psi}$ at the new frontier.
        linkvisited(μ, y) = true ▷ Mark this link as visited.
        if sitevisited$(y-\mu)$ = false **then** ▷ If this site has not been visited before.
          sitevisited$(y-\mu)$ = true ▷ Mark this site as visited and add it to the new frontier.
          $n_{\text{new}} = n_{\text{new}} + 1$
          $y_{\text{newfrontier}}(n_{\text{new}}) = y - \mu$
        end if
      end if
    end for
  end for
  $n = n_{\text{new}}$ ▷ Sites in the new frontier become sites in the old frontier.
  $y_{\text{frontier}} = y_{\text{newfrontier}}$
end while

Sample smearing shapes

To smear a bottom quark for use in bottomonium or a bottom-flavored meson, we choose $\Omega(x-y)$ to have a Coulomb wave function shape (familiar from the quantum mechanics of hydrogen) as well as the requisite J^P quantum numbers. All of the $\Omega(x-y)$ functions from S wave to G wave are listed in the preprint [arXiv:1505.04410] so only the first few are displayed here:

	${}^1S_0$	${}^3S_1$	${}^1P_1$	${}^3P_0$	…
0th radial	e^{-r/a_0}	$e^{-r/a_0}\sigma_i$	$e^{-r/a_0}\sin(2\pi(x_i-y_i)/L)$	$e^{-r/a_0}\sum_{i=1,2,3}\sigma_i\sin(2\pi(x_i-y_i)/L)$	
1st radial	$(r-b)e^{-r/a_0}$	$(r-b)e^{-r/a_0}\sigma_i$	$(r-b)e^{-r/a_0}\sin(2\pi(x_i-y_i)/L)$	$(r-b)e^{-r/a_0}\sum_{i=1,2,3}\sigma_i\sin(2\pi(x_i-y_i)/L)$	
2nd radial	$(r-c)(r-b)e^{-r/a_0}$	$(r-c)(r-b)e^{-r/a_0}\sigma_i$			

The radius and nodal parameters (a_0, b, c) are tuned for each hadron to optimize the signal, and in all of the studies reported here they satisfy $0.5 \le a_0 \le 7.0$ and $2.1 < b \le 6.2$ and $c = 6.0$ in lattice units. The argument r of $\Omega(r)$ is defined by

$$r = \sqrt{(x_1-y_1)^2_{\min} + (x_2-y_2)^2_{\min} + (x_3-y_3)^2_{\min}}.$$

Simulation details

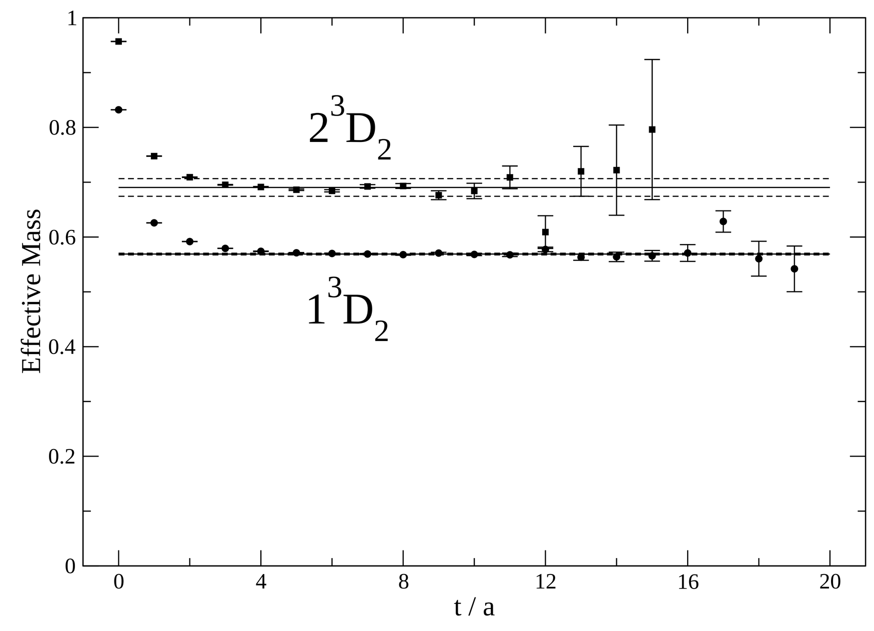
The spectrum calculations presented here use an ensemble of 198 configurations produced by the PACS-CS collaboration [S. Aoki et al., Phys. Rev. D79, 034503 (2009)]. Bottom quark propagators are computed with $O(v^4)$ tadpole-improved lattice NRQCD; all other quark propagators are clover-improved Wilson computed using the sap_gcr solver from DD-HMC [M. Lüscher, Comput. Phys. Commun. 165, 199 (2005)]. Parameters for the charm quark, following the Fermilab interpretation, are from C. B. Lang, L. Leskovec, D. Mohler, S. Prelovsek and R. M. Woloshyn, Phys. Rev. D90, 034510 (2014).

Several methods were used to increase statistical precision:

- A random U(1) wall source was used, with support from 4^3 evenly spaced free-form smeared lattice sites.
- The source was moved to every time step (for bottomonium) or every second time step (for bottom mesons).
- NRQCD propagators are calculated forward and backward in time.

A first verification

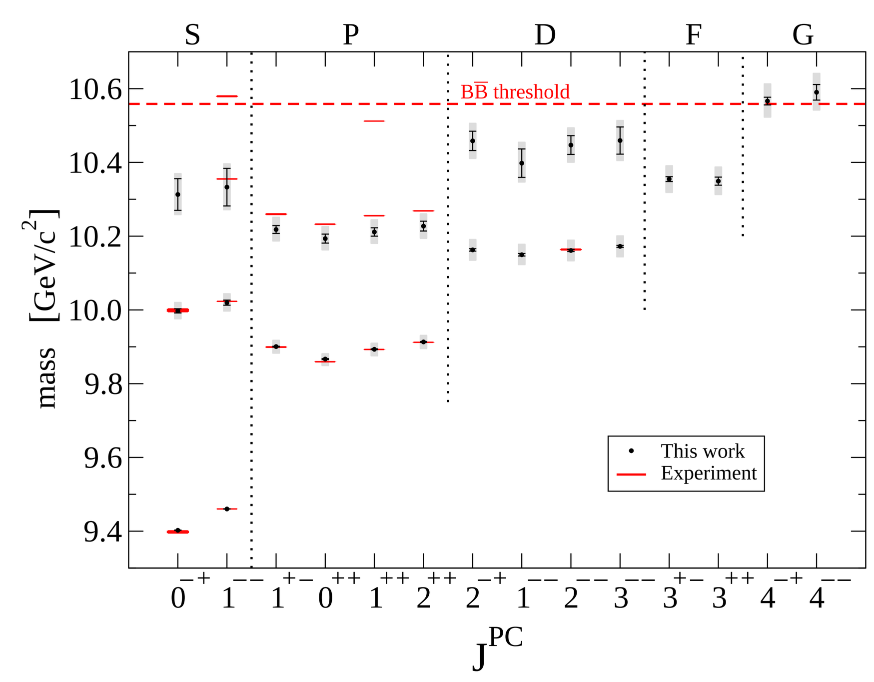
To verify orthogonality based on operator shape, here are the correlation functions from the 0th and 1st radial D-wave bottomonium operators.



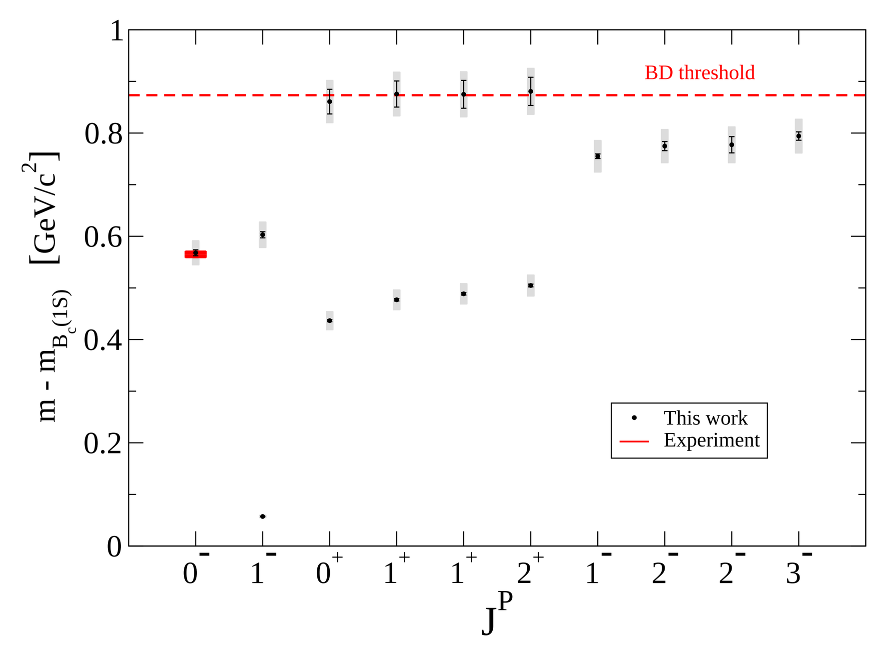
Note that the n=2 result shows no contamination from the lighter n=1 meson.

To determine the complete spectrum, several operators were used for each J^{PC} channel and a simultaneous fit was performed. Summary plots are shown below. For further details, please consult arXiv:1505.04410.

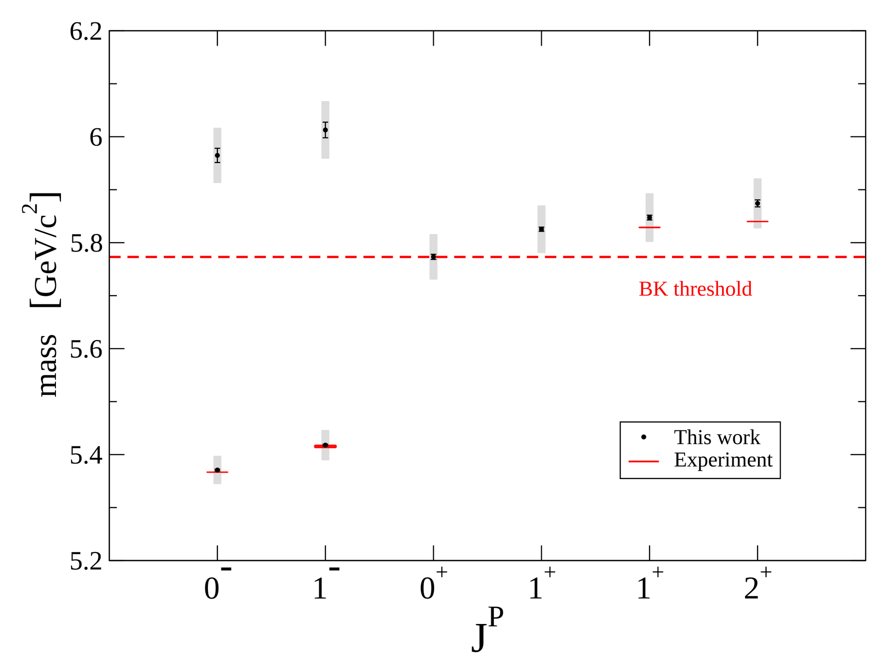
bottomonium spectrum



B_c meson spectrum



B_s meson spectrum



B meson spectrum