PROCEEDINGS OF SCIENCE

Non-perturbative heavy quark action tuning using machine learning

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We present a fully non-perturbative determination of a relativistic heavy quark action's parameters on the CLS $n_f = 2+1$ Wilson-clover ensembles using neural networks. We then further illustrate the applicability of such an approach for lattice NRQCD bottom quarks, and finally investigate some physics quantities under our tuning. In particular, we look at the excited spectrum of bottomonia, a popular $ud\bar{b}\bar{b}$ tetraquark candidate, and the not-yet observed bottom-strange cousins of the exotic $J^P = 0^+$ $D^*_{s0}(2317)$ and $J^P = 1^+$ $D_{s1}(2460)$ mesons.

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1. Introduction

It is becoming more evident that QCD hadrons containing one or more heavy charm or bottom quarks can permit more complicated structures than those predicted simply from the relativistic quark model. Such examples of exotic states in the charm sector are the experimental discoveries of various tetraquarks and pentaquarks [1–3] (see [4] for a recent review). Lattice QCD is in an ideal place to investigate the spectrum of QCD from first principles, and having well-behaved heavy-quark prescriptions are of significant importance.

As of writing, typical dynamical-fermion lattice calculations have inverse lattice spacing of the order of 2 to 3 GeV. This is quite close to the energy scale needed to pair-produce charm quarks, and hence naively a direct fermion prescription of heavy charm quarks will be expected to have sizeable discretisation effects. A way to cope with such discretisation effects is to break the spatial and temporal symmetry in the action with parameters that can help absorb discretisation effects as in the Fermilab approach [5, 6], these are called Relativistic Heavy Quark (RHQ) actions. As it will be our ultimate goal to measure scattering properties via the Lüscher formalism [7, 8] a well-behaved dispersion relation of $c^2 \approx 1$ is particularly desirable and this will be a salient feature of our tuning.

For the bottom quark, lattice non-relativistic QCD (NRQCD) is a reasonable approximation, and there has been a long history of lattice NRQCD studies determining relevant heavy-quark physics. Typically, the use of tree-level coefficients in the action is somewhat common (e.g.[9, 10]), but so is having some coefficients being determined from one-loop lattice perturbation theory [11]. Here, we will want to investigate our fully non-perturbative tuning at fixed order ($(O(v^4))$) of the NRQCD expansion on some states of interest: the excited bottomonium spectrum, the deeply-bound nature of a $ud\bar{b}\bar{b}$ $0(1^+)$ tetraquark candidate, and whether the conjectured-to-be exotic 0^+ and 1^+ B_s mesons lie below their respective BK and B^*K thresholds.

2. Heavy-quark tuning

For all of the work discussed here we will use $n_f = 2 + 1$, $O(a)$-improved Wilson-clover ensembles generated by the CLS consortium [12, 13]. These ensembles have gauge fields with open or periodic temporal boundary conditions.

Generically, the tuning for both subsections discussed below will be based on the expansion of the heavy-heavy dispersion relation:

$$E(p) = M_1 + \frac{p^2}{2M_2} - \frac{(p^2)^2}{8M_4^3} - \frac{a^3 W_4}{6} \sum_i p_i^4 + \dots, \quad (1)$$

In the charm tuning we will demand that the prescription is fully-relativistic i.e. $M_1 = M_2 = M_4 \dots$ to all orders, and hence $c^2 = 1$. In the lattice NRQCD tuning M_1 is irrelevant due to the additive mass renormalisation and instead the kinetic mass M_2 is tuned to the physical spin-average of the η_b and υ mesons. We will work with partially-twisted boundary conditions [14, 15] along the direction (θ, θ, θ), which minimises the rotational-symmetry breaking contributions multiplied by W_4.

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2.1 Relativistic heavy-quark tuning for charm

The RHQ action we will use for our charm-quarks is the "Tsukuba" action [16],

$$
\begin{aligned}
D_{xy} = \delta_{xy} - \kappa_c &\left[\sum_i (r_s - \nu\gamma_i) U_i(x)\delta_{x+i,y} + (r_s + \nu\gamma_i) U_i^\dagger(x)\delta_{x,y+i} \right] \\
&- \kappa_c \left[(r_t - \gamma_t) U_t(x)\delta_{x+t,y} + (r_t + \gamma_t) U_t^\dagger(x)\delta_{x,y+t} \right] \\
&- \kappa_c \left[c_B \sum_{i,j} \sigma_{ij} F_{ij}(x) + c_E \sum_i \sigma_{it} F_{it}(x) \right] \delta_{xy}.
\end{aligned} \tag{2}
$$

This action has 5 tuneable parameters κ_c, r_s, ν, c_E, and c_B, and we set $r_t = 1$ as it is argued to be redundant in the literature.

Our tuning strategy [17] is as follows:

- Randomly draw RHQ parameters, and measure simple quark-line connected S-wave and P-wave ground-state spectrum and $(\eta_c - J/\psi)$ spin-averaged effective speed of light squared
- Train a small neural network on the relation between charmonium spectrum and RHQ parameters
- Use Particle Data Group (PDG) [18] values for the ground-state spectrum and $c^2 = 1$ to obtain optimal action parameters predicted by the network

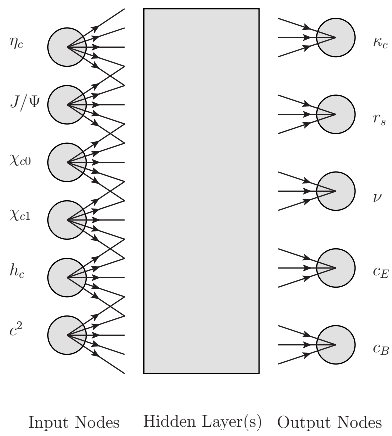

Figure 1: Neural network tuning picture for charm

The ability for our tuning to reproduce the simple ground-state spectrum of charmonium is illustrated in Fig.4 of [17].

2.2 Non-relativistic heavy-quark tuning for bottom

We will consider the typical $(O(v^4))$ [19] tadpole-improved NRQCD action (here we will use stability parameter $n = 4$ for all ensembles considered here)

$$
\begin{aligned}
H_0 &= -\frac{1}{2aM_0}\Delta^2, \\
H_I &= \left(-c_1 \frac{1}{8(aM_0)^2} - c_6 \frac{1}{16n(aM_0)^2}\right)\left(\Delta^2\right)^2 + c_2 \frac{i}{8(aM_0)^2}(\tilde{\Delta}\cdot\tilde{E} - \tilde{E}\cdot\tilde{\Delta}) + c_5 \frac{\Delta^4}{24(aM_0)} \\
H_D &= -c_3 \frac{1}{8(aM_0)^2}\sigma\cdot\left(\tilde{\Delta}\times\tilde{E} - \tilde{E}\times\tilde{\Delta}\right) - c_4 \frac{1}{8(aM_0)}\sigma\cdot\tilde{B} \\
\delta H &= H_I + H_D.
\end{aligned} \tag{3}
$$

Here we have broken-up the spin dependent and independent terms for clarity. Tildes indicate some form of higher-order lattice discretisation improvement. It is expected that the coefficients of this Hamiltonian are of order 1, and the choice of setting them all to 1 is tree-level NRQCD tuning.

Where propagators "G" are generated through applications of the symmetric evolution equation

$$G(x,t+1) = \left(1 - \frac{\delta H}{2}\right)\left(1 - \frac{H_0}{2n}\right)^n \tilde{U}_t(x,t_0)^\dagger \left(1 - \frac{H_0}{2n}\right)^n \left(1 - \frac{\delta H}{2}\right) G(x,t). \tag{4}$$

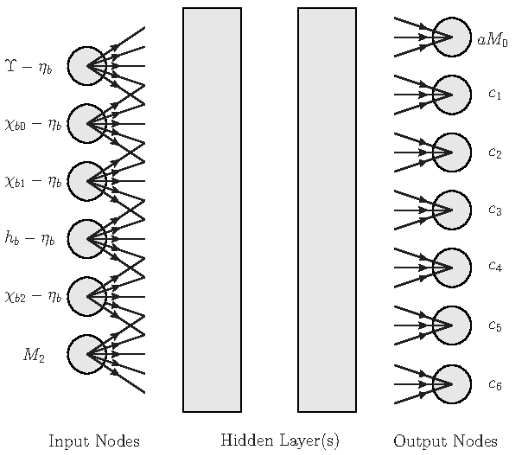

Figure 2: Schematic picture of our NRQCD setup

Our non-perturbative NRQCD tuning is similar to that of the RHQ charm action:

- due to additive mass we must only consider splittings with respect to some reference mass, we choose to subtract the η_B as this reference
- we perform tuning only at the $\mathrm{SU}(3)_f$-symmetric point as the pion-mass dependence is likely small
- use Coulomb gauge-fixed wall sources for all our correlators
- need extended derivative type operators [20] for the P-wave states

3. Results

The *preliminary* heavy-light results shown below in this section will all be taken from the "1" lattice spacing $a = 0.0864(1)$ fm, as this collection of ensembles is expected to have reasonably small NRQCD artifacts. Our investigation of the pure, excited bottomonia spectrum will feature four $\mathrm{SU}(3)_f$-symmetric ensembles with lattice spacing ranging from $a \approx 0.0498$ to 0.0993 fm that we have directly used in our tuning.

3.1 Excited states of bottomonia

We form a 4×4 symmetric GEVP of simple quark-line connected meson correlators to determine the first few P- and S-wave states of bottomonium. The GEVP is built from 4 different

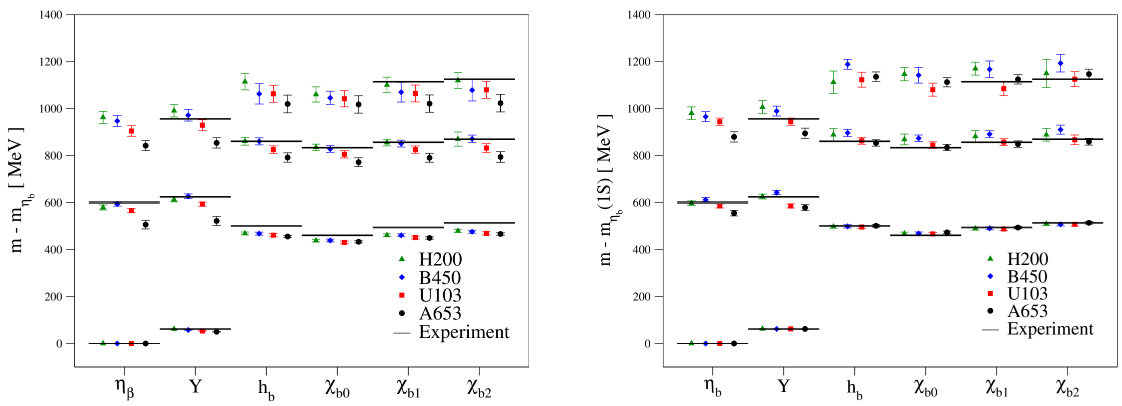

Figure 3: *Preliminary* (left) excited states below the $B\bar{B}$ threshold for the tree-level NRQCD tuning. (right) similarly for the neural-network tuning.

Gaussian smearing radii at the source and sink.

Fig.3 shows *preliminary* excited states of bottomonia (with respect to our η_b) for tree-level parameters and our neural-network tuning. The tree-level tuning does a poor job of getting the P-wave-η_b splittings correct, and although it is difficult to see here the $\Upsilon(1S) - \eta_b(1S)$ splitting is also poor. As these are parts of our tuning for the neural-network they will be well represented if the tuning works. For the $\Upsilon(2S) - \eta_b(1S)$ splitting larger discretisation effects are visible for the tree-level tuning.

3.2 $ud\bar{b}\bar{b}$ tetraquark

For this state we follow [21] and create 4×4 GEVP of the following operators,

$$\begin{aligned} D(x) &= ({u_a}^T C\gamma_5 d_b)(\bar{b}_a C\gamma_i \bar{b}_b^T)(x), \\ E(x) &= ({u_a}^T C\gamma_t\gamma_5 d_b)(\bar{b}_a C\gamma_i\gamma_t \bar{b}_b^T)(x), \\ M(x) &= (\bar{b}_a\gamma_5 u_a)(\bar{b}_b\gamma_i d_b)(x) - [u \leftrightarrow d], \\ N(x) &= (\bar{b}_a I u_a)(\bar{b}_b\gamma_5\gamma_i d_b)(x) - [u \leftrightarrow d]. \end{aligned}$$

We use gauge-fixed wall sources and Gaussian-smeared sinks for both the light and bottom quarks, so the GEVP is not symmetric. We use a diagonalisation strategy using the left and right eigenvectors to determine our principle correlators [22–24].

Fig. 4 illustrates the "binding energy" of this tetraquark candidate where we have subtracted the measured BB^* threshold at a fixed lattice spacing. It is clear that the neural-network tuned bottom quarks or the tree-level bottom-quark prescriptions are consistent and that most of the non-perturbative tuning dependence appears to cancel when forming this binding energy quantity. Much like in previous studies [24–27] as the light-quark mass decreases the binding gets deeper.

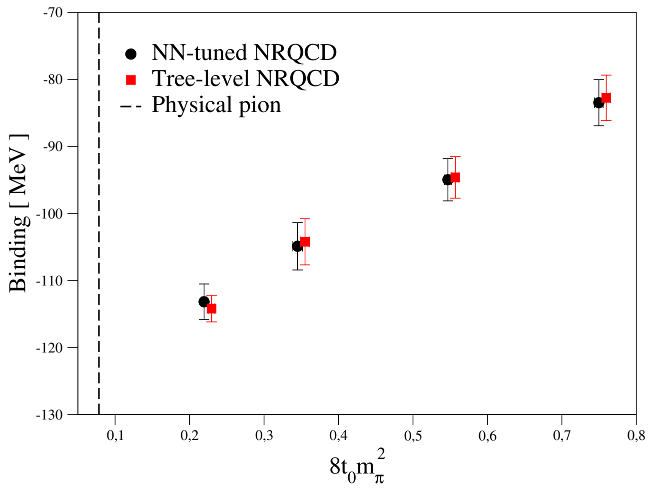

Figure 4: *Preliminary* $ud\bar{b}\bar{b}$ tetraquark with neural-network tuned (black circles) and tree-level (red squares) NRQCD tunings. NRQCD results have been shifted for clarity.

3.3 Exotic B_s mesons

Finally we consider scalar and axial-vector exotic B_s mesons, which have been predicted to lie below their respective BK and B^*K thresholds from the lattice in [28] and phenomenologically in e.g. [29–31]. However, some theoretical calculations have stated these lie at or above threshold e.g. [32, 33] as have some lattice studies [11, 34].

Here, we will just consider the simple single-meson operators:

$$O_{B_{s0}} = (\bar{b}Is), \qquad O_{B_{s1}} = (\bar{b}\gamma_i\gamma_5 s). \tag{5}$$

The *preliminary* data of Fig. 5 illustrates that all of our measured exotic B_s mesons lie below their expected two-meson thresholds.

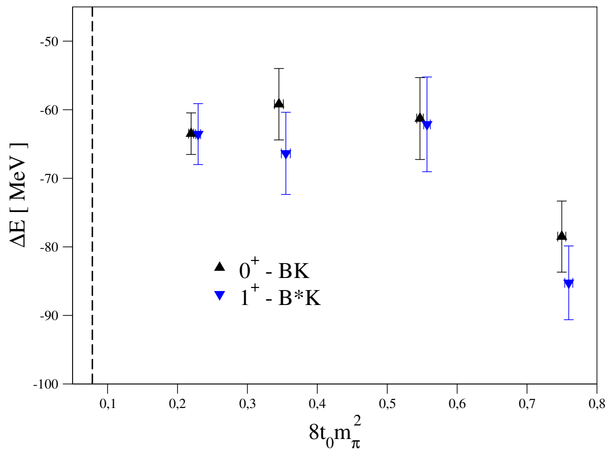

Figure 5: *preliminary* determination of the energies of the B_{s0} and B_{s1} mesons below threshold.

4. Conclusions

We have illustrated two ways to tune heavy quark actions non-perturbatively; the first was for an RHQ action for charm quarks, for which we were able to obtain to a reasonable precision a relativistic dispersion relation $c^2 = 1$. This will help facilitate our future studies into D-meson - pion scattering. Scattering studies with the RHQ action and tuning presented here are underway and we expect that having a relativistic dispersion relation will help avoid systematics that exist in other investigations of heavy-light systems including charm quarks.

Our second tuning strategy tunes the kinetic mass of lattice NRQCD as well as the v^4 parameters $c_1 \rightarrow c_5$ to obtain a well-behaved ground and excited-state bottomonium spectrum. We have shown that although we get a better bottomonium spectrum using the neural network tuning, for heavy-light quantities with NRQCD b-quarks there is little difference to results obtained with the tree-level action. Either for the $ud\bar{b}\bar{b}$ tetraquark binding or the B_s exotics considered here. It is possible that once we subtract the expected thresholds we cancel a lot of the benefits from the neural-network tuning, or that these particular heavy-light quantities are mostly insensitive to what prescription we use for the heavy quarks. As our tuning is based on pure bottomonia it is unclear what benefits, if any, will extend to the heavy-light sector.

Work is ongoing to investigate finite volume and lattice-spacing effects for the $ud\bar{b}\bar{b}$ tetraquark and the exotic B_s mesons in order to provide an accurate determination with good control over systematics.

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