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Simon Catterall
Syracuse University

F. R. Devlin
University of Cambridge

I. T. Drummond
University of Cambridge

R. R. Horgan
University of Cambridge

A. D. Simpson
The University of Edinburgh

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Non-relativistic QCD for Heavy Quark Systems

UKQCD Collaboration

S.M. Catterall, F.R. Devlin, I.T. Drummond, R.R. Horgan

DAMTP, Silver St., University of Cambridge, Cambridge CB3 9EW, UK

A.D. Simpson

Department of Physics, The University of Edinburgh, Edinburgh EH9 3JZ,
Scotland

Abstract

We employ a nonrelativistic version of QCD (NRQCD) to study heavy $q\bar{q}$ -bound states in the lowest approximation without fine structure. We use gluon configurations on a $16^3 \times 48$ -lattice at $\beta = 6.2$ from the UKQCD collaboration. For a bare quark mass near that of the b-quark ($Ma = 1.6$) we obtain the bound state masses for the S , P and both types of D -waves. We also detect signals for two types of hybrids ($q\bar{q}g$ -states). The results are sufficiently accurate to confirm that the values of the D -wave mass from both D -waves coincide thus indicating that the cubical invariance of the lattice is restored to full rotational invariance to a good approximation.

We also study S and P -wave masses for values of the range of bare quark mass $Ma = 1.0, 1.3, 1.6$ & 1.9 . The results confirm the idea that the S/P -splitting is relatively insensitive to the value of the bare quark mass.

1 Introduction

Heavy quark bound states (J/ψ , Υ) are not only intrinsically interesting but because of the nearly non-relativistic motion of the constituent quarks, offer the prospect of numerical calculations considerably more tractable than the standard calculations for light quarks [1, 2, 3, 4, 5]. Several theoretical proposals have been made [6] and a number of numerical calculations carried out [7, 8].

For quark masses $M \gg \Lambda_{QCD}$, the quark velocity $v \ll 1$, so that its dynamics are well modelled by an effective field theory, nonrelativistic QCD (NRQCD), in which the kinetic energy term is nonrelativistic [3, 6]. Clearly this approximation will only be valid for momenta very much less than some cut-off $\Lambda = a^{-1}$ (a is the lattice spacing) of the order of the heavy quark mass M . Furthermore the effective action will contain correction terms which serve both to implement relativistic effects such as the hyperfine structure splitting and to compensate for the effects of the high momentum states which have been removed from the theory. These may be reorganised into a power series in the characteristic quark velocity determined by the dynamics. In practice this series is truncated at some finite order in the quark velocity and the couplings tuned so as to reproduce the low energy behaviour of full QCD.

These systems serve as an important testing ground for lattice QCD since finite volume effects are expected to be much less important than for light quark states. Furthermore the NRQCD approach avoids the problem of fermion doubling and allows a rapid calculation of the quark propagator as an initial value problem (since it is determined by a lattice difference equation which is first order in time) [3, 6]. Issues to be decided concern the appropriate size of lattice and the optimum values for the couplings and masses in the “non-relativistic” hamiltonian in order to best describe the bound state.

In this letter we extend the numerical study of heavy quark bound states in QCD to a higher value of the coupling constant $\beta = 6.2$, using QCD gauge field configurations on $16^3 \times 48$ -lattice from the UKQCD collaboration. We have employed the lowest order approximation in which we retain only the kinetic energy term in the effective action and studied correlation functions corresponding to the ground state (S -wave) and angular excitations (P & D) of the $q\bar{q}$ -system. We have also looked for hybrid $q\bar{q}g$ -states and obtained a clear though still noisy signal. We have examined the S & P -waves for other

(lower) bare masses for the quarks and detected trends in the bound state energies and level splittings consistent with the results of Davis and Thacker [8].

The important problem of fine structure of the energy levels we have not tackled in this paper partly because of restrictions in computational facilities. We intend to explore these and other questions in future work.

2 Propagators and Operators

The evolution equation for the heavy quark propagator takes the form

$$G(x, t+1) = U_t^\dagger(x, t) \left(\left(1 - \frac{H_0}{n}\right)^n G(x, t) \right) + \delta(x) \delta(t) \quad (1)$$

where x labels the spatial position and $G(t) = 0$ for $t \leq 0$ and n is the order of the update as discussed by Thacker and Davies [7]. The modified update is necessary for stability at certain values of the bare quark mass. We have used $n = 2$ & 3 , as appropriate. In fact there appeared to be little sensitivity to the value of n in the results when sufficient stability was present. The kinetic operator H_0 is defined as

$$H_0 = \frac{-1}{2Ma} \sum_{i=1}^3 \Delta_i^+ \Delta_i^- \quad (2)$$

The covariant finite differences Δ^+ , Δ^- are given by their usual expressions (we have suppressed all colour and spin indices)

$$\Delta_i^+ G(x, t) = U_i(x, t) G(x+i, t) - G(x) \quad (3)$$

$$\Delta_i^- G(x, t) = G(x, t) - U_i^\dagger(x-i, t) G(x-i, t) \quad (4)$$

The correlation functions that we have considered are of the form

$$g_i(x, t) = \langle O_i(x, t) O_i^\dagger(0, 0) \rangle \quad (5)$$

where the index i runs over the different lattice operators corresponding to the S , P , D and hybrid states. For the S wave $O_S(x, t)$ with quantum numbers $J^{PC} = 0^{-+}$

$$O_S(x, t) = \chi^\dagger(x, t) \psi(x, t) \quad (6)$$

The fields $\psi(x, t)$ and $\chi(x, t)$ represent the quark and antiquark with propagators $G(x, t)$ and $G^\dagger(x, t)$ respectively. In the current approximation these are spin independent. The higher angular momentum states involve the correlations of two displaced quarks, the P operator with $J^{PC} = 1^{+-}$ being

$$O_P(x, t) = \frac{1}{2} \chi^\dagger(x, t) \overleftrightarrow{\Delta}_i \psi(x, t) \quad (7)$$

$$= \frac{1}{2} \left(\chi^\dagger(x, t) (\Delta_i \psi(x, t)) - (\Delta \chi(x, t))^\dagger \psi(x, t) \right) \quad (8)$$

The choice of $\overleftrightarrow{\Delta}$ (with Δ now a forward derivative) ensures that the state is orthogonal to the S state and yields a correlation function that is entirely real. The continuum D state splits into two states under the lattice group, call them D_1 and D_2 . These correspond to the operators

$$O_{D_1}(x, t) = \frac{1}{4} \chi^\dagger(x, t) \left\{ \overleftrightarrow{\Delta}_i \overleftrightarrow{\Delta}_j \right\} \psi(x, t) \quad (9)$$

$$O_{D_2}(x, t) = \frac{1}{4} \chi^\dagger(x, t) \left(\overleftrightarrow{\Delta}_i^2 - \overleftrightarrow{\Delta}_j^2 \right) \psi(x, t) \quad (10)$$

The indices i and j correspond to two (distinct) spatial directions and the curly braces in D_1 indicate a symmetrised combination is to be taken. The hybrid states we investigate fit conveniently into the same computational framework. They correspond to taking *commutators* of the lattice covariant derivatives and therefore are only non-trivial in the presence of a gauge field configuration. We have

$$O_{H_1}(x, t) = \frac{1}{2} \chi^\dagger(x, t) \left(\left[\overrightarrow{\Delta}_i, \overrightarrow{\Delta}_j \right] + \left[\overleftarrow{\Delta}_i, \overleftarrow{\Delta}_j \right] \right) \psi(x, t) \quad (11)$$

$$O_{H_2}(x, t) = \frac{1}{2} \chi^\dagger(x, t) \left(\left[\overrightarrow{\Delta}_i, \overrightarrow{\Delta}_j \right] - \left[\overleftarrow{\Delta}_i, \overleftarrow{\Delta}_j \right] \right) \psi(x, t) \quad (12)$$

These states possess quantum numbers J^{PC} equal to 1^{-+} and 1^{--} respectively. Because we have not included fine structure splitting in our hamiltonian the 1^{--} state does not mix with the $q\bar{q}$ -state with the same quantum numbers. An application of Wick's theorem then allows all the correlation functions to be built up out of sums of (gauge invariant) loops on the lattice constructed from the quark propagators and appropriate link matrices.

3 Results

Our results are obtained from ten uncorrelated configurations on a $16^3 \times 48$ quenched lattice at $\beta = 6.2$. They were used to generate the NRQCD correlation functions with bare quark masses $Ma = 1.0, 1.3, 1.6$ & 1.9 . The configurations were obtained using the 64 i860-node Meiko Computing Surface at Edinburgh. The update consisted of a cycle of 1 three-subgroup Cabibbo-Marinari heat-bath sweep followed by 5 over-relaxed sweeps.

In order to extract the maximum information from each configuration we used three starting timeslices spaced by 16 units in the temporal direction and evolved the propagators from 4^3 evenly spaced spatial starting points within each of these slices. In addition we performed an average over spatial directions for the higher angular momentum states. It was found that each of these procedures contributed to a reduction in the raggedness of the results from a particular configuration. Indeed the ground state S -wave correlation function computed from a single configuration was already rather smooth even out to 48 time slices. The higher waves of course required more data. A total of 6 quark propagators were needed to reconstruct all the correlators of interest. The errors were assessed by treating the data from each configuration as statistically independent.

To extract estimates for the masses of the states we utilised a two exponential fit with four parameters to the zero spatial momentum correlator for times $t \leq 24$.

$$G(t) = Ae^{-M_0t} (1 + Be^{-M_1t}) \quad . \quad (13)$$

The basis for the fit was a simple least squares procedure based on the statistical errors estimated from the data. The fitting procedure was carried out for a sequence of initial time slices. The numbers quoted are those obtained from the best fit consistent within one standard deviation with those from succeeding initial time slices. We further checked that fits to a single exponential at large times gave statistically consistent results.

For the case $Ma = 1.6$ we used all 10 gauge field configurations. If we use a value for the lattice spacing extracted from string tension measurements, $a^{-1} = 2.7$ Gev, to convert masses to physical units this corresponds to $M = 4.32$, roughly the b-quark mass. The procedure worked well particularly for S and P -waves. The fits are shown in Fig. 1. Clearly for these states we are in good quantitative control of both the statistical and systematic errors. As a further check we fitted the S -wave data out to 48 timeslices and found a stable plateau in the ground state mass. Figs. 2a & 2b show the results for the two D states. Here we used the two exponential fit only for $t < 20$ since this yielded a more stable mass estimate. As we can see from Table 1. the two D -state masses are equal to within the errors which is an indication of the restoration of full rotational invariance at large distance.

The data and fits for the hybrid states are plotted in Figs. 3a & 3b . Clearly our data is much noisier for these states and we attempted only a

rough single exponential fit for an intermediate range of time-slices. This yielded estimates for the masses in the vicinity of the D -wave mass for both hybrids (see Table 1.). Although the results are very much provisional, it is nevertheless encouraging to see a signal at this stage. Hybrids are of particular interest because they can only exist as a result of propagation effects in the gauge fields and cannot be realised directly in a simple quark potential model. We hope in the future to achieve better results for these and the more conventional states. This will require both higher statistics and the use of improved operators with a stronger overlap on the physical states.

On converting our lattice value for the S/P -splitting to physical units we obtain $\Delta E_{SP} = 0.35(2)$ Gev which is quite close to the experimental number of 0.4 for the splitting between triplet S and P -states of the Υ -system. It is also close to the implied physical value for the splitting found in ref [8]. This supports the physical ideas underlying the method. We have further strengthened the basis for the calculation by investigating the dependence of S/P -splitting on the bare quark mass with results at $Ma = 1.0, 1.3, 1.6$ & 1.9 summarised in Table 2. These confirm the approximate independence of this quantity on the bare quark mass. It should be noted however that these results which were obtained for reasons of computational economy from only 3 configurations, required the use of a third order update method in order to encompass the lowest mass $Ma = 1$. These new results for $Ma = 1.6$ using a third order update are consistent with the original results using a second order method at this value of the bare quark mass.

Finally in Figs. 4a & 4b, we show effective mass plots for the S and P -waves at $Ma = 1.6$ and in Figs. 5a & 5b the same for $Ma = 1.0$. In both cases the effective mass for the S -wave shows a very convincing plateau. The P -wave at $Ma = 1.6$ is rather convincing also while the P -wave at $Ma = 1.0$ is much noisier. It is a matter of judgement whether these results can be taken as exhibiting the oscillations for the effective mass encountered by Davies and Thacker [8]. It should be noted however that our computed errors are somewhat larger than those claimed in ref [8]. The greater noise in the results at the lower mass is we suspect, due to the fact that with a third order update the limit of stability is roughly $Ma = 1.0$ [7]. This potential instability underlines the need for using higher order updates. It is therefore encouraging that when there is stability ($Ma = 1.3, 1.6$ & 1.9) the results appear to be insensitive to the order of the update. This is an important

point that should be more thoroughly checked.

4 Conclusions

We have investigated the application of the NRQCD method in a numerical simulation of the lowest order kinetic energy hamiltonian, thus neglecting fine structure splitting for the purposes of this paper. We found that the S/P splitting was roughly independent of *a)* the bare mass of the quark and *b)* the order of the time update used to compute the quark Green's functions. This encourages belief in the physical meaning of the method. At the highest mass value we obtained results sufficiently accurate to confirm that the two versions of the D -wave were degenerate. This was true not only of the D -wave masses themselves but also of the additional parameters in the two exponential fit that mimic the higher mass states that obviously affect the form of the Green's function at small time separation. The S/D -split is approximately twice that of the S/P -wave split.

Hybrid states in the quark model have long been of interest [9]. It is encouraging therefore that we were able to obtain a signal for hybrid $q\bar{q}g$ -states. Although the signal was noisy it suggests that they exist at a mass comparable to that of the D -wave. This implies an excitation energy above the ground state of $\sim .8$ Gev, a value rather less than but not grossly out of line with that suggested by excited static potential calculations applied to the Υ system [10, 11].

Calculations to check the dependence of physical results on the bare quark mass suggests that this is weak as is the dependence on the order of the update. The absolute values of the energies of the states investigated do depend on the value of the bare quark mass. We note a trend of *decreasing* S -wave mass with *increasing* quark mass revealed in Table 2. In fact our results suggest that M_S^{-1} is approximately linear in the bare quark mass M as one might intuitively expect. This is consistent with the results of ref [8]. However we have not explored the effects of mass renormalization in this context, important though that issue is.

We believe that we have obtained encouraging results for the NRQCD method and that it is possible to extract good results from only a few configurations. We intend to extend our calculations to other sizes of lattice and other values of the coupling constant. This is particularly important since

the lattice value of $\sim .13$ for the S/P -splitting suggests Υ radii of $\sim 6 - 8$ lattice units at $\beta = 6.2$. This is consistent with the wavefunction radius measured in ref[8] and predicted in other calculations [12]. In order to ensure that finite size effects do not influence our results at this value of β it is important to repeat our calculations on a larger lattice. However because we see reasonable agreement with the results of ref[8] obtained with $\beta = 6.0$ on our size of lattice we do not expect there to be a strong effect. Further improvements in extracting data from QCD configurations can be envisaged such as better statistical treatment of the data and the use of better wave functions in the measurement of the more difficult states as well as higher statistics from more configurations.

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Table Captions

1. Masses for the states measured with $Ma = 1.6$ using the second order update.
2. The M_S, M_P & S/P -splitting at various masses using the third order update.

Figure Captions

Fig. 1 S and P wave correlation functions at $Ma = 1.6$ with solid line fit (two exponential).

Fig. 2a D_1 wave correlation functions at $Ma = 1.6$ with solid line fit (two exponential).

Fig. 2b D_2 wave correlation functions at $Ma = 1.6$ with solid line fit (two exponential).

Fig. 3a H_1 hybrid correlation functions at $Ma = 1.6$ with solid line fit (single exponential).

Fig. 3b H_2 hybrid correlation functions at $Ma = 1.6$ with solid line fit (single exponential).

Fig. 4a Effective mass plot for S -wave at $Ma = 1.6$.

Fig. 4b Effective mass plot for P -wave at $Ma = 1.6$.

Fig. 5a Effective mass plot for S -wave at $Ma = 1.0$.

Fig. 5b Effective mass plot for P -wave at $Ma = 1.0$.

Tables

Table 1.

State	M_0a	M_1a
S	1.098(2)	0.32(3)
P	1.230(10)	0.29(4)
$D1$	1.442(19)	0.66(22)
$D2$	1.415(31)	0.68(22)
$H1$	1.42(11)	-
$H2$	1.37(8)	-

Table 2.

Ma	M_{Sa}	M_{Pa}	S/P -split
1.0	1.38(1)	1.51(6)	0.13(7)
1.3	1.20(1)	1.32(2)	0.12(3)
1.6	1.086(9)	1.22(3)	0.14(4)
1.9	1.003(8)	1.14(2)	0.14(2)