Charmonium spectrum from quenched QCD with overlap fermions

χQCD Collaboration

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Abstract

We present the first study of the charmonium spectrum using overlap fermions, on quenched configurations. Simulations are performed on $16^3 \times 72$ lattices, with Wilson gauge action at $\beta = 6.3345$. We demonstrate that we have discretization errors, as indicated by the dispersion relation, at about 5%. We obtain 88(4) MeV for the $1S$ hyperfine splitting using the $r_0$ scale, and 121(6) MeV using the $(1\bar{P} - 1\bar{S})$ scale. This Letter should encourage the pursuit of using the same chiral fermions for both heavy and light quarks on the same lattice.

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1. Introduction

Over the last few years, numerical simulations of chiral fermions have matured. The stage of testing has passed for simulating valence chiral fermions, and physically relevant results have been reported in lattice simulations. All the studies so far have concentrated on simulating light quarks. This is natural, as chiral symmetry plays an important role for small quark masses. However, the use of overlap fermions to simulate heavy as well as light quarks has been suggested in [1]. In this Letter we want to make the point that overlap fermions can also alleviate some problems related to simulating heavy quarks. Here we present the first quantitative study of a heavy quark system using overlap fermions. This opens the door for the simulation of experimentally more interesting heavy-light systems. Using the unequal mass Gell-Mann–Oakes–Renner relation as the renormalization condition, the renormalization factor in the heavy-light current can be determined non-perturbatively to a high precision for overlap fermions [1]. This is important for the computation of heavy-light decay constants.

Here we demonstrate the value of overlap fermions to simulate heavy quarks, by studying hyperfine splitting in the charmonium system. It is known that with staggered quarks there is an ambiguity about Nambu–Goldstone (NG) and non-NG modes for the $\eta_c$, resulting in widely different estimates of hyperfine splitting—51(6) MeV (non-NG) and 404(4) MeV (NG) [2]. NRQCD converges only slowly for charm [3]. Including $O(v^6)$ terms changed the result from 96(2) MeV to 55(5) MeV. Wilson fermions have $O(a)$ errors. With Sheikholeslami–Wohlert action, this error can be reduced to $O(a^2)$ provided the coefficient of the correction term, $c_{SW}$, is determined non-perturbatively. Hyperfine splitting is very sensitive to the coefficient of the correction term, $c_{SW}$. There are many studies [4–6] using Wilson type valence quarks, including...
some with non-perturbative $c_{SW}$, and with continuum extrapolation. The quenched clover estimate of hyperfine splitting has stabilized around 72–77 MeV using the $r_0$ scale [5–7], and a higher number of about 85 MeV using the $(1P - 1S)$ scale [5]. Results from a $2+1$ dynamical simulation using tree-level $c_{SW}$, still fall short of the experimental value of 117 MeV by about 20% [8].

Although costly to simulate, overlap fermions [9] have the following desirable features:

- Exact chiral symmetry on the lattice;
- No additive quark mass renormalization;
- No flavor symmetry breaking;
- No $O(a)$ error;
- The $O(m^2a^2)$ and $O(\Lambda_{QCD}ma^2)$ errors are also small, from dispersion relation and renormalization constants. Ref. [20] indicates that discretization errors are small for overlap fermions.

The first two features are especially significant for light quarks. Many exciting results at low quark masses have been reported using overlap fermions [10]. The last three features are more important for computing charmonium hyperfine splitting using overlap fermions. The last feature, demonstrated in [1], is an unexpected bonus in this regard. The key observation is that the discretization errors are only about 5% all the way up to $ma \approx 0.5$. In Fig. 1, we reproduce (from Ref. [1]) a plot of the speed of light as a function of $ma$, obtained from the pseudoscalar meson dispersion relation. This is obtained using a $16^3 \times 28$ lattice at a spacing of 0.20 fm. It is harder to study the dispersion relation on the configurations we use for this Letter, because on the small volume lattice box we use, one unit of momentum corresponds to about 1.6 GeV. This is a huge momentum, and as a result, the data is noisier. The effective energies for 0, 1 and 2 units of lattice momentum are shown in Fig. 2. There is no clean plateau already for 2 units of momentum. This results in a large error bar for the energy corresponding to that momentum. Fig. 2 corresponds to $ma = 0.35$. For smaller values of $ma$, the data is even more noisy, and it is hard to obtain the speed of light reliably for smaller masses.

![Fig. 1. This is a plot of the speed of light, $c$, obtained from the dispersion relation. It can be seen that the discretization errors are only a few percent till $ma \approx 0.5$. This data comes from a $16^3 \times 28$ lattice at a spacing of 0.20 fm.](image1)

![Fig. 2. Effective energies for pseudoscalar mesons, for 0, 1 and 2 units of lattice momentum, from the $16^3 \times 72$ lattice, at $ma = 0.350$. The effective energy for 2 units of momentum is very noisy, as explained in text.](image2)

![Fig. 3. Percent deviation of the speed of light from unity, as a function of $ma$. This serves as an estimate of the relative discretization error. Near our charm mass, the discretization errors are about 5%. However, it is expected that the deviation of speed of light from 1 is larger for higher values of $ma$. Fig. 3 shows percent deviation of the speed of light from unity, obtained from a fit to the dispersion relation as a function of quark mass using the equation

\[
(E(p)a)^2 = c^2(pa)^2 + (E(0)a)^2.
\]

This figure indicates that we have discretization errors at about the 5–7% level near the charm mass, which is near $ma \approx 0.35$.](image3)

2. Simulation details

Our simulations are performed on $16^3 \times 72$ isotropic lattices. We present results on 100 configurations. The Wilson gauge action is used at $\beta = 6.3345$. We use a multi-mass inverter to obtain propagators for 26 masses ranging from 0.020–0.85 in lattice units. Only five of these masses in the range 0.25–0.50 are used for this study.

In this section, we elaborate on some technical details regarding overlap inversions required for this Letter. This section can be skipped without loss of continuity. Numerical details of our overlap simulations are given in Ref. [11]. The interested reader may also refer to [12] for background on practical aspects of simulating overlap quarks.
Since overlap simulations are computationally expensive, it is important to choose the required residuals carefully—blindly requiring extremely precise inversions is not the optimal use of computing resources. We use the standard 2-norm residual with the source normalized to unity, i.e. \( \|MX - b\|/\|b\| \). For overlap simulations, there are three relevant numbers: residual for eigenvectors projected out to reduce the condition number of the matrix to be inverted in the inner loop, the residual for inner loop which computes the overlap operator, and the residual for the outer loop which actually computes the quark propagators. For the lattices we use, we only need to project out about 15 eigenvectors, so we simply demand a very small residual, \( \times 10^{-10} \) for this step. Unlike this step, however, the inner and outer loop residuals demanded affect the computational cost substantially. To determine what residual is good enough, we repeat the quark propagator inversion for one spin, one color and one configuration, and compare the “pseudoscalar” two-point function for various quark masses. This is not a physical quantity since no trace over spin and color is performed, and no configuration average is taken—we are simply studying precision issues here. Comparing results for an inner loop residual of \( \times 10^{-6} \) with those from an inner loop residual of \( \times 10^{-3} \), we find no change for small quark masses. However for heavy quarks, the two-point function falls through many orders of magnitude, and becomes very small at the center of the lattice. To get this precisely, we find we need a small inner loop residual—\( \times 10^{-6} \) is not sufficient. In Fig. 4 we show the effect of inner loop residual on “pseudoscalar” propagators for heavy quarks. The curves are slightly shifted for clarity. For \( ma = 0.450 \), even an inner loop residual of \( \times 10^{-6} \) appears to be good enough. However, for a larger \( ma = 0.630 \), this residual is not good enough for \( t > 30 \). For our production runs, we choose an inner loop residual of \( \times 10^{-8} \) and an outer loop residual of \( \times 10^{-5} \). We have tested an outer loop residual of \( \times 10^{-7} \), two orders of magnitude better. This affects results at less than half percent level, so we deem an outer loop residual of \( \times 10^{-5} \) to be sufficient. This residual of \( \times 10^{-5} \) is demanded for the lightest quark mass. Near the charm mass, the residual obtained through the multi-mass inversion algorithm is \( \approx 2 \times 10^{-9} \).

3. Analysis

In this Letter, we study five charmonium states shown in Table 1—\( \eta_c(1S_0) \), \( J/\Psi(1S_1) \), \( h_c(1P_0) \), \( \chi_c(1P_1) \) and \( \chi_c(3P_1) \). For the \( P \) states, there are two possible operators—one (denoted by \( \Gamma \)) simply with appropriate \( \gamma \) matrices and the other (denoted by \( \Delta \)) with a derivative as well as \( \gamma \) matrices. We always use a \( \Gamma \) operator for the source, because using a \( \Delta \) operator for the source would require additional costly inversions. (It is for this reason we do not study \( \chi_c^+ \). This state has no \( \Gamma \) operator.) Using a \( \Delta \) sink does not cost additional inversions. Thus for our \( P \) state analysis, we have three possibilities—\( \Gamma \), \( \Delta \) or \( \Gamma \Delta \). The last one is our notation for a simultaneous fit to both \( \Gamma \) and \( \Delta \) sink correlators.

The effective mass plots for the pseudoscalar and the vector states are shown in Fig. 5. The lower half of this figure shows the effective hyperfine splitting from the ratio of vector to pseudoscalar correlators. These show a long plateau to justify a single exponential fit. For the \( P \) states, the effective masses are shown in Fig. 6. These have much larger error bars, but they are still flat. The data gets noisy beyond \( t = 30 \) and precision problems cannot be excluded for channels other than the pseudoscalar meson. We do not use time-slices beyond 30 in our fits.

We use two ways to set the scale—from the \( r_0 \) (using 0.5 fm) and from the \( (1P - 1S) \) splitting in the charmonium system. The singlet \( P \) mass \( m_h \) is used for \( P \), and \( (3m_{J/\Psi} + m_h) / 4 \) for the \( \bar{S} \) mass. The \( (1P - 1S) \) scale analysis has three sub-cases, depending on which of the \( \Gamma \), \( \Delta \) or \( \Gamma \Delta \) fits is used for \( h_c \).

We present the \( r_0 \) results first. The lattice spacing for the \( \beta \) we use is 0.0561 fm [13]. The experimental \( m_{J/\Psi} \) is used to

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Table 1

| charmonium states. For the \( P \) states, there are two possible interpolating fields, denoted by \( \Gamma \) and \( \Delta \). Experimental masses in GeV are shown |
|---|---|---|---|---|---|
| \( \eta_c \) | \( 1S_0 \) | \( 0^{++} \) | \( \psi \gamma S \psi \) | \( \psi \gamma S \psi \) | 2.979 |
| \( J/\Psi \) | \( 3S_1 \) | \( 1^{--} \) | \( \psi \gamma S \psi \) | \( \psi \gamma S \psi \) | 3.097 |
| \( h_c \) | \( 1P_0 \) | \( 1^{++} \) | \( \psi \gamma S \psi \) | \( \psi \gamma S \psi \) | 3.526 |
| \( \chi_c \) | \( 3P_0 \) | \( 0^{++} \) | \( \psi \gamma S \psi \) | \( \psi \gamma S \psi \) | 3.517 |
| \( \chi_c \) | \( 3P_1 \) | \( 1^{++} \) | \( \psi \gamma S \psi \) | \( \psi \gamma S \psi \) | 3.511 |

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Fig. 4. Effect of inner loop precision on pseudoscalar propagators for heavy quarks. We study the output of one spin and one color for a single configuration for this illustration. The curves are slightly shifted horizontally for clarity.

Fig. 5. Effective masses for the pseudoscalar and vector correlators. The plateau for the ratio of vector to pseudoscalar correlator is also shown. We use this ratio to obtain our results for hyperfine splitting. These plots are for \( ma = 0.35 \).
set $m_c$ (in lattice units). Interpolation for $m_{J/\psi}$ as a function of $ma$ is shown in Fig. 7. A straight line fit is used. Interpolation for the hyperfine splitting is shown in Fig. 8. The fit form used is $(m_{J/\psi} - m_{\eta_c})a = A/\sqrt{ma} + B/ma$ [15]. Knowing the charm mass and the scale, the hyperfine splitting in MeV can be determined. Our result for the hyperfine splitting using the $r_0$ scale is 88(4) MeV. Recent quenched results from Wilson-type fermions are 77(2)(6) MeV [6], 71.8(20) MeV [7] and 72.6(0.9)(+1.2)(−3.8) [5]. Since our result is for a single lattice spacing, a direct comparison is not possible. However, a scaling study of overlap fermions [20] suggests that our errors due to finite lattice spacing may be small. The spectrum obtained using $r_0$ scale is shown in Fig. 9. The corresponding results can be found in Table 2.

The $(1\bar{P}−1\bar{S})$ scale has the advantage that it is set within the charmonium system, using masses of physical particles, so it is expected to be more relevant for this system, and that it is model independent. However, we have large errors on the $P$ states. Consequently, the scale set from $(1\bar{P}−1\bar{S})$ splitting itself will have about 12% error, which is not included in the direct statistical errors on various masses quoted below. Furthermore, we caution the reader about possible systematic errors associated with our small spatial extent of 0.8–0.9 fm, since our lattice is close to the deconfinement transition [14].

The interpolation for the $\Gamma \Delta$ fit for $m_{hc}$ is shown in Fig. 7, along with the interpolations for $m_{J/\psi}$ and $m_{\eta_c}$. We also show $m_{hc}$ obtained using $\Gamma$ and $\Delta$ fits on the same plot. It is clear from this plot that $m_{hc}$ obtained from the three fits completely agree within error bars. However, the slight difference in $m_{hc}$ in the three cases changes the scale, the charm mass and the hyperfine splitting values considerably.

In the case of the spin splitting scale, the determination of $a$ and $m_c a$ is entangled. The procedure we follow to disentangle these is as follows. As shown in Fig. 7, all hadron masses in lattice units are fitted to a straight line, $m_h a = A_h ma + B_h$.

![Fig. 6. Effective masses for the $P$ states. The filled circles correspond to $\Gamma$ operator and the open circles to $\Delta$ operator. The plots for different $P$ states are shifted along the y-axis. These effective masses are rather noisy, and we use conservative error bars on our fitted results. Again, the plots are for $ma = 0.35$.](image1)

![Fig. 7. We fit the meson masses linearly in quark mass. Fits are shown for $\eta_c$, $J/\psi$ and $h_c$ masses. All masses are in lattice units. $h_c$ masses obtained using $\Gamma$ and $\Delta$ operators are also shown, but the fit line is shown only for the $\Gamma \Delta$ fit.](image2)

![Fig. 8. Hyperfine splitting as a function of quark mass, with interpolation shown at $m_c a$.](image3)

![Fig. 9. Charmonium spectrum in physical units. Results from both the $r_0$ and the $(1\bar{P}−1\bar{S})$ scales are shown. Note, for the latter scale, a linear combination of $h_c$ and $\eta_c$ masses, along with the $J/\psi$ mass, is used for input.](image4)

<table>
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<tr>
<th>Parameter</th>
<th>$(1\bar{P}−1\bar{S})$</th>
<th>$(1\bar{P}−1\bar{S})$</th>
<th>$\eta_c$</th>
<th>$J/\psi$</th>
<th>$h_c$</th>
<th>$X_c0$</th>
<th>$X_c1$</th>
<th>$m_{\eta_c}$</th>
<th>$m_{J/\psi}$</th>
<th>$m_{h_c} a$</th>
<th>$a (\text{fm})$</th>
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<td>2.977(6)</td>
<td>2.967(7)</td>
<td>2.943(9)</td>
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<td>0.121(6)</td>
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<td>$h_c$</td>
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<td>3.53(8)</td>
<td>3.49(9)</td>
<td>3.47(12)</td>
<td>3.526</td>
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<td>3.39(10)</td>
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<td>3.41(7)</td>
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<td>$m_{J/\psi}$</td>
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<td>1.30</td>
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<td>0.0480</td>
<td>0.0460</td>
<td>0.0416</td>
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Expt.
Lattice spacing $a$ and bare charm quark mass $m_c a$ are two unknowns; $m_{1/2}$ and $m(1\bar P - 1\bar S)$ in physical units are the two inputs. We solve for $a$ and $m_c a$ to obtain the values shown in Table 2. The charm masses obtained are indicated in Fig. 7. We would like to point out that while $m_c a$ in lattice units differs considerably in the three sub-cases of $(1\bar P - 1\bar S)$ analyses, values for unrenormalized $m_c$ in GeV, tabulated in Table 2, cluster much tighter.

The value we obtain for the hyperfine splitting in MeV is extremely sensitive to the value used for the lattice spacing $a$. For a slightly smaller $a$, the hyperfine splitting in lattice units is considerably larger, since it falls rapidly with increasing $a$, as seen in Fig. 8. Converting this to physical units further increases the value. As a result, our results from the three sub-cases of $(1\bar P - 1\bar S)$ analysis look quite different—113(5) MeV using $\Gamma_s$, 121(6) MeV using $\Gamma_s\Delta$ and 144(9) MeV using $\Delta$. We would like to emphasize here that the errors quoted are only direct statistical errors, and the errors on $a$ are large enough to bring these results into statistical agreement with each other.

Fig. 9 shows the charmonium spectrum obtained from both $r_0$ and $(1\bar P - 1\bar S)$ analysis. Agreement with the experimental values is much better for the $(1\bar P - 1\bar S)$ scale. The agreement with experimental numbers for all the particles studied is very reasonable, indicating that the discretization errors must indeed be small for overlap fermions. This is because the different mass differences are supposed to measure differently defined quark masses $M_2$, $M_E$, etc. [16]. The inequality of these quark masses implies discretization errors. If all the mass differences come out right, it would imply that $M_{1s} \approx M_{2s} \approx M_E$, and that the discretization errors are small.

Finally, we summarize the results in Table 2. The errors quoted are only statistical; the error on $a$ is not included. All masses are in GeV. Our value for the hyperfine splitting, using the $(1\bar P - 1\bar S)$ scale and simultaneous fits to $\Gamma_s$ and $\Delta$ correlators, actually agrees with experiment. This is fortuitous, because the contribution from dynamical fermions is not included, and may be significant. However, there is no real contradiction here, because we have substantial statistical and systematic errors, as detailed below:

1. Direct statistical errors: these are quoted in Table 2.
2. Statistical error on $a$: in the $(1\bar P - 1\bar S)$ scale, this is primarily due to the error on the $h_c$ mass, which is about 53 MeV. This is about 12% of the physical $(1\bar P - 1\bar S)$ mass difference of 458 MeV. Note, this error is absent when the scale is set using $r_0$. On the other hand, $r_0$ is a model-dependent scale, and it can have comparable errors. It has been pointed out that 0.45 fm may be a better value to use for $r_0$ than 0.50 fm [17]. Using this value brings our $r_0$ results closer to the $(1\bar P - 1\bar S)$ results.
3. Discretization errors: as explained in Section 1, these are estimated at about 5%, from the dispersion relation. Results from Ref. [20], in particular the Aoki plot, demonstrate that discretization errors are small for overlap fermions. Since the lattice spacing used in this study, 0.056 fm, is much smaller than the lattice spacings used in Ref. [20], 0.17 fm and 0.20 fm, we expect that we have very small discretization errors.
4. Finite volume errors: our simulations are performed on a box size of only 0.8–0.9 fm, hence it is not inconceivable that the $P$ states have some finite volume errors. However, even this small box should be large enough for the $S$ state particles—$J/\Psi$ and $\eta_c$. A finite volume study using the $r_0$ scale [6] finds a reduced hyperfine splitting on their smallest volume, with a spatial extent of 0.75 fm.
5. Quenched approximation: dynamical fermions are expected to increase the value of hyperfine splitting. This increase is about 20 MeV for the Wilson-type fermions [8]. On the other hand, a study with NRQCD [18] does not find a significant contribution from dynamical fermions.
6. Exclusion of OZI-suppressed diagrams: while a contribution of about 20 MeV cannot be ruled out, the contribution due to these appears to be small in the charm quark region [19]. Lattice calculations with smaller statistical and systematic errors are needed to settle this issue.

4. Summary

We have presented the first study of the charmonium spectrum using overlap fermions. We get a better agreement with the experimental spectrum using the $(1\bar P - 1\bar S)$ scale rather than the $r_0$ scale. Our value for the hyperfine splitting is 121(6) MeV and 88(4) MeV using the $(1\bar P - 1\bar S)$ and $r_0$ scales, respectively. We observe that, for our lattice spacing of about 0.056 fm, overlap fermions increase the hyperfine splitting compared to the continuum results from Wilson-type fermions, and it is now important to repeat the overlap study at a different lattice spacing and a larger volume. We have indications, from dispersion relation and scaling study [20], that our discretization errors for this fine lattice spacing should be small. Unquenched overlap results with more statistics and somewhat larger box size may very well settle the charmonium hyperfine splitting issue. With smaller discretization errors, the overlap fermion may be suitable for studying heavy-light quark systems on the same lattice.

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