Precision Υ Spectroscopy and Fundamental Parameters From NRQCD

The NRQCD Collaboration

We present results from a high precision NRQCD simulation of the quenched Υ system at $\beta = 6$. We demonstrate a variety of important lattice techniques, including the perturbative improvement of actions, tadpole improvement, and multicorrelated fits for extracting the spectrum of excited states. We present new determinations of $\alpha_s(M_Z)$ and $M_b$, two fundamental parameters of the Standard Model.

1. Introduction

In this paper we report new results from an accurate numerical simulation of the spectrum of the Υ family of mesons. (Results for the $J/\psi$ family are presented in [1].) Our simulation uses the NRQCD action for the quarks, including all relativistic effects through $O(M_b v^4)$ where $M_b$ is the $b$-quark's mass and $v$ its average velocity. We demonstrate a variety of important lattice techniques, including the perturbative improvement of actions, tadpole improvement, and multicorrelated fits for extracting the spectrum of excited states. Furthermore, the high statistics and small systematic errors of our results allow us to extract accurate values for two of the fundamental parameters of the Standard Model: the mass of the $b$-quark, and the strong coupling constant $\alpha_{\overline{MS}}(M_Z)$.

The $b$-quarks in Υ’s are quite nonrelativistic ($v^2$ is about 0.1). We exploit this in NRQCD by replacing the Dirac action for the quarks with a Schrödinger action. The Schrödinger theory is computationally much easier to solve because it can be treated as an initial-value problem, rather than a boundary-value problem. Relativistic effects are systematically introduced, order-by-order in $v^2$, as corrections to the nonrelativistic action [2,3]. These terms are quite similar in form to the corrections that remove finite-lattice-spacing errors. We include both types of correction in our simulations. Consequently the dominant source of systematic error in our results is the gluon action—we use configurations produced with the standard Wilson action, and no light-quark vacuum polarization. (Finite volume errors are negligible since Υ’s are much smaller than ordinary mesons.)

A complication in using improved actions such as ours is that each of the correction terms has its own coupling constant. These new coupling constants must be computed somehow. In principle they can be computed using weak-coupling perturbation theory [2,3]. Our simulations demonstrate that this is also the case in practice, provided tadpole-improved perturbation theory is employed. Indeed (tadpole-improved) tree-level perturbation theory seems quite sufficient for most aspects of Υ physics, at least at $\beta = 6$; and work has begun on the first-order corrections [4].

This perturbative control over the effective action means that there are really only two parameters in the quark action, the mass and the charge, just as in the continuum theory. Thus our simulations are truly calculations from first principles, unlike calculations based upon a QCD-motivated phenomenological model like the quark potential model.

In what follows, we first summarize the details of the simulation and fitting procedures. We then focus upon results for the spectrum, $a^{-1}$, $M_b$, and $\alpha_{\overline{MS}}(M_Z)$. Finally we comment upon the implications of our work concerning improved actions and simulations on coarse grids.

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2. The Simulation

The NRQCD quark lagrangian we used in our simulations was

$$\psi^\dagger \left(1 - \frac{aH_0}{2n}\right)^n U^\dagger \left(1 - \frac{aH_0}{2n}\right)^n (1-a\delta H) \psi,$$  \hspace{1cm} (1)

where $n = 2$, $H_0$ is the nonrelativistic kinetic energy operator,

$$H_0 = -\frac{\Delta^{(2)}}{2M_b^0},$$  \hspace{1cm} (2)

and $\delta H$ is the leading relativistic and finite-lattice-spacing correction,

$$\delta H = -\frac{(\Delta^{(2)})^2}{8(M_b^0)^2} \left(1 + \frac{aM_b^0}{2n}\right) + \frac{a^2\Delta^{(4)}}{24M_b^0}$$

$$- \frac{g}{2M_b^0} \sigma \cdot B + \frac{ig}{8(M_b^0)^2} (\Delta \cdot E - E \cdot \Delta)$$

$$- \frac{g}{8(M_b^0)^2} \sigma \cdot (\Delta \times E - E \times \Delta).$$ \hspace{1cm} (3)

Here $\Delta$ and $\Delta^{(2)}$ are the simple gauge-covariant lattice derivative and laplacian, while $\Delta^{(4)}$ is a lattice version of the continuum operator $\sum D^2_k$. We used the standard cloverleaf operators for the chromo-electric and magnetic fields, $E$ and $B$.

The entire action was tadpole improved by dividing every link operator $U_\mu$ by $u_0 \equiv (\frac{4}{3} \text{Tr} U_{\text{plaq}})^{1/4}$. Potential models indicate that corrections beyond $\delta H$ contribute only of order 5–10 MeV to $\Upsilon$ energies.

The only parameter in the NRQCD action is the bare mass of the quark, $M_b^0$. We did a complete simulation for each of three masses: $2/a$, $1.8/a$, and $1.71/a$. Our analysis indicates that the last of these is the closest to the real mass (see below). However the statistical analysis for this mass is not yet complete and so most of the results we quote are for $aM_b^0 = 1.8$. Except where noted otherwise, the difference has negligible effect.

Note that meson energies in NRQCD are non-relativistic energies and do not include the rest mass energy. To obtain the rest mass of the $\Upsilon$, for example, we measured the momentum dependence of its energy, fitting it to a form

$$E_\Upsilon(p) = E_{\text{NR}}(\Upsilon) + \frac{p^2}{2M_{\text{kin}}(\Upsilon)} + \cdots$$ \hspace{1cm} (4)

where the kinetic mass $M_{\text{kin}}$ is the physical mass of the meson (see below).

Our quark propagators were computed using an ensemble of quenched configurations obtained from the Staggered Collaboration. This ensemble contains 105 $16^3 \times 24$ configurations, generated with an unimproved Wilson action at $\beta = 6.0$ and gauge fixed to Coulomb gauge. Potential models indicate that the errors due to quenching and to finite-$a$ errors in the gluon action could be order 40 MeV in $\Upsilon$ energies, making these the most important systematic errors.

We performed all of our measurements from 8 different origins separated by $L/2$ in the initial time slice, and treated the propagators at these origins as statistically independent. At each value of the bare mass, our spectrum measurements required a total of 17 heavy quark propagators, each with 3 spin-color components at the source and 6 at the sink, using about 17 GFlops-hour of CPU time, i.e. about 800 inversions per GFlops-hour.

When measuring meson propagators, we used gauge non-invariant smearing at both source and sink. With fast fourier transforms, all source-sink combinations can be measured at a computational cost of one quark-propagator inversion per source smearing function. We used 1S, 2S, 3S, 1P, and 2P wavefunctions computed in the quark potential model (with the Richardson potential) as our smearing functions. In addition we used local sources for both $S$ and $P$ states. We also created smearing functions for $S$-states with small, nonzero momenta. For each allowed set of quantum numbers, all source-sink combinations were measured, resulting in a $4 \times 4$ matrix of correlation functions for $S$ states, $3 \times 3$ for $P$ states, and $2 \times 2$ for momentum states.

3. Fitting

We used a variety of fitting strategies to obtain the spectrum from our meson propagators. For the spectrum of spin-averaged $S$ and $P$ states we tried two sorts of multieponential fit to multiple propagators. In the first we fit multiple exponentials to the set of propagators with smeared sources and a local sink: for example, the ground and first excited state of the $\Upsilon$ were determined.
by simultaneously fitting three exponentials to
the 1l and 2l propagators, where 1l indicates
1S smearing at the source and local smearing
at the sink, and 2l indicates 2S smearing at the
source and local smearing at the sink. We dis-
carded results from the highest energy state in
such fits, since this is the most susceptible to bi-
asing due to higher states. These are the propa-
gators for which our statistics are the best; how-
ever, the statistical quality of the results degrades
markedly for the excited states.

The second approach we used for spin-averaged
spectra was to fit the full matrix of propagators
formed by taking every combination of nonlo-
cal smearing function at the source and at the
sink: for example, the Υ and its first two ex-
cited states were determined by simultaneously
fitting three exponentials to the 11, 12, 13, 21,
22, 23, 31, 32, and 33 propagators formed us-

ing quark-model wavefunctions for the first three
S-states as smearing functions. The statistics
were poorer for these smeared-smeared propaga-
tors compared with the smeared-local propagators
discussed above; but the fitting is highly
overdetermined, and consequently significantly
more robust. This approach gave the best results
for highly excited states; it also avoids spurious
plateaus |

For splittings between two highly correlated
states we found that the best method is to fit
a single exponential to the jackknifed ratio of the
two propagators for the two states. This approach
is useful for computing spin splittings and the ki-
netic mass of the Υ.

Statistical uncertainties for the fitting param-
eters were estimated by varying the parameters
until $\delta \chi^2 = 1$. In several cases we checked this
estimate using a bootstrap analysis. The two esti-
mates agreed in each case tested, suggesting that
the statistical fluctuations in our propagators are
at least approximately gaussian.

Our fitting protocol follows closely the tech-
niques discussed in |, including the use of sin-
gular value decomposition to allow the inversion
of the variance matrix with finite precision arith-
metric. In general, we had very few problems in
obtaining successful fits, even for the second ex-
cited Υ state. This is due to the high statistics

in our data set, and to our simultaneous fits us-
using many smearing functions. In particular, it
was important to include a smearing function for
every state we were attempting to fit.

4. The Spectrum and $a^{-1}$

In Figure 1 we present our simulation results
for the $^3S_1$ and $^1P_1$ spectra, together with the
corresponding experimental values from |. We
use $a^{-1} = 2.4$ GeV and Monte Carlo data with
$aM_0^b = 1.8$. Because the $h_b$ has not been ob-
served, the experimental values quoted for the
$^1P_1$ states are actually the spin averages of the $\chi_b$
states; strong theoretical arguments, supported
by our measurements, indicate that the two are
the same.

In Figure 2, we present our results for the spin
Figure 2. Simulation results for the spin structure of the lowest lying $P$-state in the $\Upsilon$ family. The dashed lines are the experimental values for the triplet states, and the experimental spin average of all states for the singlet ($h_b$).

The error bars are only for statistical errors. We expect systematic errors in the $P$-state energies of order 5 MeV, which is comparable to the statistical errors shown.

We determined the inverse lattice spacing by fitting the simulated spectrum to the experimentally determined spectrum. Rather than choosing $a^{-1}$ to make, say, the $\chi_b(1P) - \Upsilon(1S)$ splitting correct, we used a bootstrap analysis to perform a correlated fit for $a^{-1}$ to the whole spectrum. Specifically, treating the 840 origins in our ensemble as statistically independent, we generated 20 bootstrap ensembles, each containing the meson propagators from 840 origins (with repetition). We then extracted the spectrum from each of these ensembles, giving us an ensemble of 20 spectra. Choosing various states for inclusion in the fit, we did a 1-parameter correlated fit of our spectra to the experimental spectrum to determine $a^{-1}$. This procedure was carried out twice, i.e. with two different sets of 20 bootstrap ensembles.

| Splittings         | $a^{-1}$ | Q  |
|--------------------|----------|----|
| $2S-1S, 1P-1S$     | 2.37(9)  | .21|
| $2S-1S, 1P-1S, 2P-1S$ | 2.41(10) | .42|
| $2S-1S, 1P-1S, 2P-1S$ | 2.42(7)  | .27|
| $2S-1S, 1P-1S$     | 2.39(10) | .43|
| spin-splittings    | 2.32(6)  | .15|
|                    | 2.35(9)  | .31|

Table 1
Bootstrap results for $a^{-1}$.

The results of our $a^{-1}$ fits for different groups of states are summarized in Table 1. The splittings for $S$-states are between $^3S_1$ states, while spin averages are used for the $P$-states. The spin-splittings used are for the lowest lying $P$-state. For each set of states fit, we tabulate the values of $a^{-1}$ and the associated goodness of fit $Q$ for both sets of 20 spectra. ($Q$ typically lies between 0.1 and 0.9 for a good fit.) These fits indicate that

$$a^{-1} = 2.4(1) \text{ GeV.}$$

(5)

Because of quenching, our $a^{-1}$ should not agree with those obtained by matching simulation results for observables that are more infrared, like the string tension, to experiment; we expect such determinations to yield smaller values of $a^{-1}$.

The success of our global fits of the $\Upsilon$ spectrum show that our simulation is accurately modeling the general features of the $\Upsilon$ physics. There are certainly systematic errors in our simulation results, but these do not degrade the fits because they are generally smaller than the statistical errors. Only a small improvement in statistics is needed before these systematic effects will become apparent. Indeed there is already a slight indication ($2\sigma$) that the $2S-1S$ and $1P-1S$ splittings are inconsistent, the first being too large and the second too small. This is precisely the effect expected due to quenching of the gauge fields. Such discrepancies will be useful when comparable simulations with unquenched configurations are begun. Similar effects are expected in the spin splittings, particularly for $S$-states.
5. $M_b$ Determination

The $b$-quark’s mass $M_b$ is an important fundamental parameter of the Standard Model. Our simulation results lead to two independent determinations of this mass (i.e., of the pole mass)\textsuperscript{[12]}. These are among the most accurate and reliable determinations of this mass (i.e., of the pole mass)\textsuperscript{[12]}. These could be 10–20% of $M_b$. Our second procedure for determining $M_b$ is to tune the bare quark mass $M_b^0$ until the kinetic mass of the $\Upsilon$, as computed in the simulation (Eq. (\textsuperscript{[4]})), agrees with the measured mass of the $\Upsilon$. Then the pole mass of the quark is $M_b = Z_m M_b^0$ where renormalization constant $Z_m$ is computed using perturbation theory\textsuperscript{[4]}:

$$Z_m = 1 + b_m a_V (q_m) + \mathcal{O}(a_V^2)$$ \textsuperscript{(8)}

where scale $q_m \sim 1/a$. To reduce the sensitivity of the result to the value of the lattice spacing and to the bare quark mass, we rewrite the expression for the pole mass as

$$M_b = Z_m M_T \frac{a M_b^0}{a M_{\text{kin}}(\Upsilon)}$$ \textsuperscript{(9)}

where $M_T = 9.46$ GeV is the $\Upsilon$’s experimental mass, while $M_{\text{kin}}(\Upsilon)$ is its mass as determined from our simulation with bare mass $M_b^0$. Our results are summarized in Table 3. These indicate that our best estimate for bare quark mass is $M_b^0 = 1.7(1)/a$, and therefore the pole mass is again $M_b = 4.7(1)$ GeV. Here the main source of uncertainty is again perturbative: the two-loop corrections to $Z_m$ could shift $M_b$ by 2–3%. Uncertainties due to $a^{-1}$, tuning the bare mass, etc. are of order 1% or less.

Our two determinations of the $b$-quark mass are very different, and yet they both yield a pole mass of $M_b = 4.7(1)$ GeV. The complete agreement between the two methods is a strong indication of the validity of each, and more generally of the lattice QCD techniques upon which they rely.

### Table 2

Simulation and perturbative results used in the first method for determining $M_b$. Values for $M_b$ are in GeV.

| $\beta$ | $a M_b^0$ | $aE_{\text{NR}}(\Upsilon)$ | $a E_0$ | $M_b$ |
|--------|----------|---------------------------|--------|------|
| 6.0    | 1.71     | 0.455(1)                  | 0.21   | 4.69 |
| 1.80   | 0.451(1) | 0.21                      | 4.70   |
| 2.00   | 0.444(1) | 0.22                      | 4.73   |

### Table 3

Simulation and perturbative results used in the second method for determining $M_b$. Values for $M_{\text{kin}}(\Upsilon)$ and $M_b$ are in GeV.

| $\beta$ | $a M_b^0$ | $a M_{\text{kin}}(\Upsilon)$ | $Z_m$ | $M_b$ |
|--------|----------|-------------------------------|------|------|
| 6.0    | 1.71     | 3.95(5)                       | 1.15 | 9.5(4) |
| 1.80   | 4.10(5)  | 1.15                          | 9.8(4) |
| 2.00   | 4.45(5)  | 1.14                          | 10.7(4) |

Here $\alpha_V$ is the strong coupling constant as defined in\textsuperscript{[14]}, and $q_0 \sim 1/a$. In Table \textsuperscript{[2]} we present the simulation results for $E_{\text{NR}}$, and the corresponding $E_0$’s from perturbation theory. From these results we conclude that the pole mass of the $b$-quark is $M_b = 4.7(1)$ GeV. The major source of uncertainty in this determination is from the two-loop corrections to $E_0$. These could be 10–20% of $E_0$, or 1–2% of $M_b$. Uncertainties due to finite lattice spacing, quenching, tuning of the bare quark mass, statistics, and $a^{-1}$ are all less than 1%.

Our second procedure for determining $M_b$ is

$$M_b = \frac{1}{2} \left( M_T - a^{-1} (a E_{\text{NR}}(\Upsilon) - 2 a E_0) \right)$$ \textsuperscript{(6)}

where $M_T = 9.46$ GeV is the experimentally measured mass of the $\Upsilon$, and $E_0$ is the nonrelativistic energy of a $p = 0$ $b$-quark in NRQCD. The quantity $E_{\text{NR}}(\Upsilon) - 2 a E_0$ can be thought of as the effective binding energy of the meson. The quark energy $E_0$ is an ultraviolet divergent quantity and thus it can be computed using weak-coupling perturbation theory\textsuperscript{[3]}:

$$a E_0 = b_0 \alpha_V (q_0) \left( 1 + \mathcal{O}(\alpha_V) \right)$$ \textsuperscript{(7)}

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Our two determinations of the $b$-quark mass are very different, and yet they both yield a pole mass of $M_b = 4.7(1)$ GeV. The complete agreement between the two methods is a strong indication of the validity of each, and more generally of the lattice QCD techniques upon which they rely.

6. $a_M(\xi)$ Determination

The strong coupling constant is completely specified by two lattice quantities: the inverse
The strong coupling constant as determined from Monte Carlo results for various Wilson loops.

| Loop | $\alpha_V(3.41/a)$ |
|------|-------------------|
| $\log W_{11}$ | 0.152 |
| $\log W_{12}$ | 0.152 |
| $\log W_{13}$ | 0.152 |
| $\log W_{22}$ | 0.153 |
| $\log W_{23}$ | 0.154 |
| $\log W_{33}$ | 0.159 |

Table 4

For quarkonium the relevant $q^*$ is the mean momentum-transfer in the potential, which is computed from the expectation value of the potential between wavefunctions for the state of interest:

$$\langle \frac{\alpha_V^{(3)}(q)}{q^2} \rangle \equiv \alpha_V^{(3)}(q^*) \langle \frac{1}{q^2} \rangle.$$  

Quark-model wavefunctions for $1s$, $2s$, and $1p$ states imply $q^*$ is 0.75(25) GeV for $\Upsilon$'s. To correct for the wrong $n_f$, we use the two-loop perturbative beta function to make the connections:

$$\alpha_V^{(0)}(3.41/a) \quad \alpha_V^{(3)}(3\text{ GeV})$$

$$\downarrow \quad \uparrow$$

$$\alpha_V^{(0)}(q^*) \quad = \quad \alpha_V^{(3)}(q^*)$$

The perturbative beta function is probably reliable down to scales of order 0.7–0.8 GeV (see Figure 3). We obtain a value for the unquenched coupling of

$$\alpha_V^{(3)}(3\text{ GeV}) = 0.262(12)$$

where the uncertainty in $q^*$ is the dominant source of error.

It is customary to quote values for the coupling constant in terms of $\alpha_{\overline{MS}}(M_Z)$. The standard $\overline{MS}$ coupling is related to $\alpha_V$ by

$$\alpha_{\overline{MS}}(q) = \alpha_V \left( e^{5/6} q \right) \{ 1 + 2 \alpha_V / \pi + O(\alpha_V^2) \}.$$  

Converting to $\overline{MS}$ and running the scale up to the mass of the $Z$ meson, we obtain finally:

$$\alpha_{\overline{MS}}^{(5)}(M_Z) = 0.112(4),$$

which compares well with other lattice determinations [11], as well as with 0.110–0.125 as obtained from various high-energy experiments. The main sources of error in our result are:

$$n_f = 0 \rightarrow 3 \quad \Rightarrow \quad 0.002$$

$$\alpha_V \rightarrow \alpha_{\overline{MS}} \quad \Rightarrow \quad 0.002$$

$$\alpha_V^{(0)}(3.41/a) \quad \Rightarrow \quad 0.001$$

$$a^{-1} \quad \Rightarrow \quad 0.001$$

All of these errors can be significantly reduced in the immediate future.

7. Perturbative Improvement

The lowest-order (or Schrödinger) NRQCD action accounts for the bulk of $\Upsilon$ and $\psi$ physics.
However high precision results require an improved action. The key ingredients for an improved action are:

- a tree-level perturbative calculation of the leading correction terms in the action (Eq. (4));
- tadpole improvement of the correction terms, where every link is replaced by

$$U_\mu \rightarrow U_\mu/\lambda_0,$$

and $\lambda_0$ is the Monte Carlo value of $(\frac{1}{N} \text{Tr} U_{\text{plaq}})$; this step is essential for avoiding large renormalizations of the tree-level corrections;
- a calculation of $O(\alpha_V(1/\lambda))$ renormalizations of the corrections (if very high precision is needed).

We have implemented the first two of these improvements in our NRQCD simulations, and they have been strikingly successful, as is illustrated by the three examples listed in Table 5.

The first example is the determination of the Y mass from its dispersion relation (Eq. (4)). This is compared with the “exact” result obtained from the relation

$$aM_Y = 2 \left( Z_m aM_0^0 - aE_0 \right) + aE_{\text{NR}}(Y),$$

where renormalizations $Z_m$ and $aE_0$ are computed perturbatively, as discussed above (Eqs. (6) and (8)). Both the addition of correction terms to the action and tadpole improvement are essential for accurate results. The most important correction terms in the action for this quantity are the spin independent $O(\nu^2, a, a^2)$ terms. (Note that the kinetic mass of a composite particle equals the sum of the masses of the constituents in a nonrelativistic theory; the binding energy comes in only with relativistic corrections.)

The second example is the spin-splitting between the $\chi_{b2}$ and $\chi_{b0} P$-state in the Y family. This splitting vanishes in the lowest order theory since that theory is spin independent. Tadpole improvement is essential here since the dominant operator that contributes to this splitting, $\psi^\dagger i \sigma \cdot D \times g E \psi$, involves the cloverleaf operator for the chromoelectric field. Again only the fully corrected theory works well; it gives results in excellent agreement with experiment.

The third example is the spin-splitting between the $\psi$ and $\eta_c$ mesons. The situation here is quite analogous to that for the $P$-state splittings, except that here the dominant operator is $\psi^\dagger i \sigma \cdot g B \psi$. Again correction terms and tadpole improvement are essential. The fully corrected simulation gives an excellent result; the 20% discrepancy between this result and experiment is consistent with the expected size of $\alpha_V$ corrections, uncertainties in the mass, $O(\nu^4)$ operators, and effects due to quenching.
| Quantity | $\delta H = 0$ | $u_0 = 1$ | Corrected | Exact |
|----------|---------------|------------|------------|-------|
| $aM_\Upsilon$ | 3.60(5) | 5.00(5) | 4.15(5) | 4.10(9) |
| $\chi^{3/2} - \chi^{60}$ | 0 | 25(7) | 51(7) | 53 MeV |
| $\psi - \eta_c$ | 0 | 94(1) | | 117 MeV |

Table 5
NRQCD predictions compared with exact results. Simulation results are presented for the theory without $O(a, v)$ corrections ($\delta H = 0$), the theory without tadpole improvement ($u_0 = 1$), and for the fully corrected theory.

These results are compelling evidence that perturbative improvement of actions, when combined with tadpole-improved perturbation theory, is a highly effective procedure.

8. Conclusions

We have presented early results from our continuing program of high-precision analyses of heavy-quark mesons using NRQCD. We have shown that lattice simulations can accurately account for the structure of the $\Upsilon$ spectrum up through the $\Upsilon(3S)$, and including spin structure. And we have used these results to make new determinations of the strong coupling constant and the $b$-quark’s mass.

Our results are possibly the most thorough QCD tests to date of perturbative improvement for lattice actions. They underscore the reliability of perturbation theory, the utility of tree-level improvement, and the critical importance of tadpole improvement (without it, the improvements tend to be much too small). The success of the perturbative improvement for NRQCD strongly suggests that it will work for gluons and light quarks, particularly since the quarkonium states we examine are 3–5 times smaller than light hadrons. (Note that $O(a^2)$ errors for the $\Upsilon$ at $\beta = 6$ are only of order a few percent, even though the meson’s radius is only two lattice spacings.) Simulations of light hadrons with improved actions should permit precision work on lattices that are much coarser than those commonly used today.

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