The charmed double bottom baryon

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Abstract: The aim of this project is to calculate the wavefunction and energy of the ground state of the Ω^0_{cbb} baryon, which is made up of 2 *bottom* and 1 *charm* quarks. Such a particle has not been found yet, but recent observation of the doubly charmed baryon Ξ^{++}_{cc} (ucc) indicates that a baryon with three heavy quarks may be found in the near future. In this work, we will use the fundamental representation of the $SU(3)$ group to compute the interaction between the quarks, then we will follow the Born-Oppenheimer approximation to find the effective potential generated by the motion of the c quark, which will allow us to solve the Schrödinger equation for the bb system. The total spatial wavefunction we are looking for results from the product of the wavefunctions of the two components (c and bb). Finally, we will discuss the possible states taking into account the spin and color wavefunctions.

I. INTRODUCTION

In July 2017, the LHCb experiment at CERN reported the observation of the Ξ^{++}_{cc} baryon [1], indicating that, sooner rather than later, baryons made up of three heavy quarks will be found.

In this project we are going to study the specific case of the charmed double bottom Omega baryon Ω^0_{cbb}, whose mass and properties have not been established yet. The fact that we are dealing with three heavy quarks implies that, at first approximation, the QCD potential is Coulomb-like, which allows us to use the well-known techniques of atomic and molecular physics, accessible at the Bachelor's degree level.

We will study the strong interactions using the fundamental representation of the $SU(3)$ group, and we will apply the Born-Oppenheimer approximation to calculate the possible wavefunctions of the 3-body system.

In order to do so, we will split the problem into two parts, which is a good path to follow thanks to the mass difference between the bottom and charm quarks, being the former much heavier than the latter. First, we will suppose that the b's are fixed and at a relative distance R, and we will use the variational principle to find the ground state energy of the c quark for each possible value of R, which will act as a potential energy to the bb system. To do this more accurately, we must find a charge factor function $k(R)$ using numerical methods, as it will appear to be the solution to a transcendental equation.

Then, we will solve the Schrödinger equation for the motion of the bb system numerically, running a code on Mathematica, letting the total potential be the sum of the energy of the fundamental state of the c quark and the QCD potential between the bb pair.

Finally, we will discuss the possible states of the total wavefunction taking into account the color and spin of the constituent particles and the *Pauli Exclusion Principle*.

II. THE STRONG INTERACTION

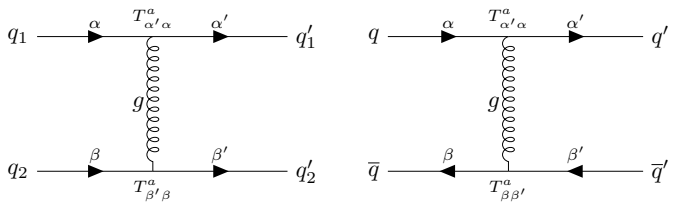
The interaction between quarks is explained by Quantum Chromodynamics (QCD), which is a gauge theory based on the $SU(3)$ symmetry group. At short distances, where the confinement term is negligible, the interaction potential between two heavy quarks is Coulomb-like because it approximately corresponds to the exchange of a single gluon. It is given, in natural units, by

$$V(r) = \frac{\#\alpha_s}{r}, \tag{1}$$

where α_s is the strong interaction coupling constant and $\#$ is the *color factor*, which depends on the representation of the two quarks. The value of $\#$ is found using the properties of the fundamental representation of the $SU(N)$ Lie algebra. This properties are:

- Antisymmetric structure constants: $[T^a, T^b] = if^{abc}T^c$
- Traceless: $Tr(T^a) = 0$
- Normalization: $Tr(T^aT^b) = \frac{1}{2}\delta_{ab}$
- Symmetric structure constants: $\{T^a, T^b\} = \frac{1}{N}\delta_{ab} + d^{abc}T^c$
- Projection operator: $T^a_{ij}T^a_{kl} = \frac{1}{2}\left(\delta_{il}\delta_{jk} - \frac{1}{N}\delta_{ij}\delta_{kl}\right)$

The Feynman diagram for the quark-quark and the quark-antiquark interactions are the following



being α and β the color of the ingoing quarks (antiquarks) and α' and β' the color of the outgoing quarks (antiquarks). The Feynman rule for a vertex involving two quarks and a gluon is $-ig_s\gamma^\mu_{ij}T^a_{\alpha'\alpha}$. We are interested in the product $T^a_{\alpha'\alpha}T^a_{\beta'\beta}$, which will yield the suitable color factor when we multiply it by $\epsilon_{\alpha\beta\gamma}$, connecting the indexes of the ingoing quarks so the resulting particle has zero net color charge. We have

$$T^a_{\alpha'\alpha}T^a_{\beta'\beta}\epsilon_{\alpha\beta\gamma} = \frac{1}{2}\left(\delta_{\alpha'\beta}\delta_{\beta'\alpha} - \frac{1}{N}\delta_{\alpha'\alpha}\delta_{\beta'\beta}\right)\epsilon_{\alpha\beta\gamma} = \\ = \frac{1}{2}\left(\epsilon_{\beta'\alpha'\gamma} - \frac{1}{N}\epsilon_{\alpha'\beta'\gamma}\right) = -\frac{N+1}{2N}\epsilon_{\alpha'\beta'\gamma}$$

showing that $\#_{qq} = -\frac{N+1}{2N} \overset{N=3}{=} -\frac{2}{3}$.
For the quark-antiquark interaction we are interested in the product $T^a_{\alpha'\alpha}T^a_{\beta\beta'}$ multiplied by δ^β_α, so the net charge of the resulting meson is zero.

$$T^a_{\alpha'\alpha}T^a_{\beta\beta'}\delta_{\alpha\beta} = \frac{1}{2}\left(\delta_{\alpha\beta}\delta_{\beta'\alpha'} - \frac{1}{N}\delta_{\beta'\beta}\delta_{\alpha'\alpha}\right)\delta_{\alpha\beta} = \\ = \frac{1}{2}\left(\delta_{\alpha\alpha}\delta_{\beta'\alpha'} - \frac{1}{N}\delta_{\beta'\alpha}\delta_{\alpha\alpha'}\right) = \\ = \frac{1}{2}\left(N\delta_{\beta'\alpha'} - \frac{1}{N}\delta_{\beta'\alpha'}\right) = \frac{N^2-1}{2N}\delta_{\beta'\alpha'}$$

thus, the color factor is $C_F = \#_{q\bar{q}} = \frac{N^2-1}{2N} \overset{N=3}{=} -\frac{4}{3}$.

A. Running coupling

The α_s coupling is a function of a renormalization scale μ. When μ is taken close to the scale of momentum transfer Q in a given process, then $\alpha_s(\mu^2 \simeq Q^2)$ is indicative of the effective strength of the strong interaction in that process. The coupling satisfies the following renormalization equation

$$\mu^2\frac{d\alpha_s}{d\mu^2} = -(b_0\alpha_s^2 + b_1\alpha_s^3 + \cdots) \tag{2}$$

with $b_0 = (33-2n_f)/12\pi$, $b_1 = (153-19n_f)/(24\pi^2)$ as found in [4], and $n_f = 3$ the number of active quark flavors at our energy scale.
We need to calculate this value at two different scales: the center-of-mass (C.o.M) of the bc system (for the motion of c) and the C.o.M energy of the bb system (for the interaction of the b's). We use the experimental values of the *charmonium* ($c\bar{c}$) mass and a solution of equation (2) at second order to solve the self-consistent system

$$M_{exp}(c\bar{c}) = 2m_c - \left(C_F\alpha_s^{(c\bar{c})}\right)^2\frac{m_c}{2}$$
$$\alpha_s^{(c\bar{c})} \simeq \frac{1}{b_0 t}\left(1 - \frac{b_1}{b_0^2}\frac{\ln t}{t}\right) \quad \text{with} \quad t \equiv \ln\frac{\mu^2}{\Lambda^2} = \ln\frac{m_c^2c_F^2\alpha_s^2}{4\Lambda^2} \tag{3}$$

to find suitable values for $\alpha_s^{(c\bar{c})}$ and m_c. We took $\Lambda \equiv \Lambda_{\overline{MS}} = 332 \pm 17$MeV (a constant of integration whose value is indicative of the energy range where non-perturbative dynamics dominates) from eq. (24.d) in [4], corresponding to $n_f = 3$, and $M_{exp}(c\bar{c})$ from [5]. The solution is $\alpha_s^{(c\bar{c})} = 0.624$ and $m_c = 1.86\,\text{GeV}$. Repeating this calculation for the b's using experimental values of the *bottomium* ($b\bar{b}$) we get $\alpha_s^{(b\bar{b})} = 0.373$ and $m_b = 5.03\,\text{GeV}$.
Now that we have the masses m_b and m_c, we are able to calculate the coupling at the scales we are interested in, namely the C.o.M of bc and that of bb. We will do it by solving (3) with the right expressions for t:

$$t = \ln\left[\left(\frac{m_bm_c}{m_b+m_c}\right)^2\frac{\#_{qq}^2\alpha_s^2}{\Lambda^2}\right] \longrightarrow \alpha_s^{(bc)} = 0.762$$
$$t = \ln\left[\left(\frac{m_b}{2}\right)^2\frac{\#_{qq}^2\alpha_s^2}{\Lambda^2}\right] \longrightarrow \alpha_s^{(bb)} = 0.524.$$

III. THE BORN-OPPENHEIMER APPROXIMATION

The Born-Oppenheimer approximation in molecular physics consists in the assumption that the motion of atomic nuclei and electrons in a molecule can be separated due to the difference in the velocity of the protons (slow) and the electrons (fast). In mathematical terms, it allows the wavefunction of a molecule to be broken into its electronic and nuclear components.
A similar assumption can be made regarding the motion of our baryon, breaking down the system in two components: the bb pair, which will act as the nucleus, and the c quark. It is possible to do so thanks to the mass difference between the quarks, $2m_b >> m_c$, which allows us to treat each component separately.
Let's take the Hamiltonian of our system:

$$\hat{H} = -\frac{\hbar^2\nabla^2_{b_1}}{2m_b} - \frac{\hbar^2\nabla^2_{b_2}}{2m_b} - \frac{\hbar^2\nabla^2_c}{2m_c} - \\ - \frac{N+1}{2N}\hbar c\left(\frac{\alpha_s^{(bb)}}{|r_{b_1}-r_{b_2}|} + \frac{\alpha_s^{(bc)}}{|r_{b_1}-r_c|} + \frac{\alpha_s^{(bc)}}{|r_{b_2}-r_c|}\right) \tag{4}$$

where b_1, b_2 and c subscripts refer to the two b and c quarks respectively. The wavefunctions and energies of this system are obtained from the Schrödinger equation

$$\hat{H}\psi(q_{b_1}, q_{b_2}, q_c) = E\psi(q_{b_1}, q_{b_2}, q_c) \tag{5}$$

where the q's denote the coordinates of the quarks. The key remains on the fact that c is much lighter than the bb pair. Thus, it will move much faster than the "nucleus", and, in good approximation, we can consider the bb fixed while c moves around. Classically speaking, during one cycle of c, the change in the bb configuration is negligible. This way, if we consider the separation of the b's at a fixed

distance, say $R = |r_{b_1} - r_{b_2}|$, we can omit the kinetic energy terms of equation (4) to obtain the equation of motion for c:

$$(\hat{H}_c + V_{bb})\psi_c = U\psi_c \tag{6}$$

with

$$\hat{H}_c = -\frac{\hbar^2\nabla_c^2}{2m_c} - \frac{N+1}{2N}\hbar c\left(\frac{\alpha_s^{(bc)}}{|r_{b_1} - r_c|} + \frac{\alpha_s^{(bc)}}{|r_{b_2} - r_c|}\right) \tag{7}$$

and

$$V_{bb} = -\frac{N+1}{2N}\frac{\hbar c\alpha_s^{(bb)}}{R}. \tag{8}$$

The energy U in equation (6) is the energy of c including the attraction between bb, which is constant for a given value of R. Of course, there are infinite possible configurations for bb, and for each of them we can solve the Schrödinger equation (6) to find a set of wavefunctions and their corresponding energies for c. This way, the wavefunctions and energies depend parametrically of the bb configuration:

$$\psi_c = \psi_c(q_c, R) \quad \text{and} \quad U = U(R).$$

As V_{bb} is constant for a given configuration, omitting this term in the Hamiltonian does not affect the wavefunctions and only changes the eigenvalues of the energy by V_{bb}. We obtain

$$\hat{H}_c\psi_c = E_c\psi_c$$

where the energy E_c (that depends parametrically on the configuration of bb) is related to U by

$$U = E_c + V_{bb}. \tag{9}$$

Thus, if we get to find E_c for a particular configuration of the bb pair, we will be able to calculate U from equation (9), where V_{bb} is easily found from (8).

A. Variational principle

From now on, we will work with a generalization of atomic units, wich defines length and energy units as follows:

$$a_0 = \frac{\hbar}{m_c c\alpha_s^{(bc)}\frac{N+1}{2N}} = 0.209\,\text{fm}$$
$$E = \left(\frac{N+1}{2N}\right)^2 {\alpha_s^{(bc)}}^2 m_c c^2 = 0.478\,\text{GeV},$$

and also $\hbar = m_c = 1$. This way, our Hamiltonian,

$$\hat{H}_c = -\frac{1}{2}\nabla_c^2 - \frac{1}{|r_{b_1} - r_c|} - \frac{1}{|r_{b_2} - r_c|}, \tag{10}$$

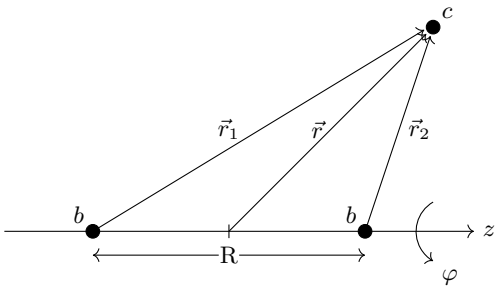


FIG. 1: Coordinates

looks like the one for the hydrogen molecule H_2^+, which greatly simplifies our work. Also, we will take coordinates as shown in Fig. 1, with the origin on the middle point between the b's.

Now we are in the position to use the Variational Principle. Consider, in first place, that the distance between both b's is very large, so c is close to one of them, say b_1. Essentially, we have a hydrogen atom with origin on b_1 whose fundamental wavefunction is

$$1s_1 = \pi^{-1/2}e^{-r_1}, \tag{11}$$

and we can do the same for b_2. These considerations suggest that we can test as variational function

$$c_1\pi^{-1/2}e^{-r_1} + c_2\pi^{-1/2}e^{-r_2} \tag{12}$$

where c_1 and c_2 are variational parameters. When c is close to b_1 the first term predominates, yielding a function such as (11), as expected.

Prior to solving the secular equation, we can improve our test function. Consider the limit of the wavefunction when R goes to 0. Then, our H_2^+ wavefunction becomes the ion He^+, whose wavefunction in the ground state is (taking $Z = 2$ in the hydrogen-like function)

$$2^{3/2}\pi^{-1/2}e^{-2r}. \tag{13}$$

As we see in Fig. 1, when R goes to 0, r_a and r_b go to r, so the test function goes to $(c_1 + c_2)\pi^{-1/2}e^{-r}$. Clearly, it does not behave well in the limit $R = 0$, as it tends to e^{-r} instead of e^{-2r}. We can solve this by adding a variational parameter $k = k(R)$, that will act as a charge factor, such that $k(0) = 2$ and $k(\infty) = 1$ for the ground state. So our test function looks like

$$c_1 1s_1 + c_2 1s_2 = c_1 k^{3/2}\pi^{-1/2}e^{-kr_1} + c_2 k^{3/2}\pi^{-1/2}e^{-kr_2},$$

with the factor $k^{3/2}$ normalizing the function.

It can be seen in Chapter 13 of [3] that this test function leads to:

$$\varphi_+ = \frac{1s_1 + 1s_2}{\sqrt{2(1+S_{12})}} \quad \text{and} \quad \varphi_- = \frac{1s_1 - 1s_2}{\sqrt{2(1-S_{12})}}$$

where $S_{12} = e^{-kr}(1+kR+k^2R^2/3)$, with the corresponding energies

$$W_\pm = t^2F_\pm(t) + tG_\pm(t) \tag{14}$$

with

$$F_\pm = -\frac{1}{2} + \frac{1 \pm (1+t)e^{-t}}{1 \pm e^{-t}(1+t+t^2/3)}, \tag{15}$$

$$G_\pm = \frac{\frac{t+1}{t}(e^{-2t}-1) \mp 2(1+t)e^{-t}}{1 \pm e^{-t}(1+t+t^2/3)}, \tag{16}$$

and $t \equiv kR$, which are the ground and first excited states (as we will see later, φ_+ corresponds to the ground state).

B. Finding k

The relation $k(R)$ (for each W) is found by minimizing W as a function of k, and the condition $\partial W/\partial k = 0$ leads to

$$k = -\frac{G(t) + tG'(t)}{2F(t) + tF'(t)}. \tag{17}$$

This allows us to find k for a given value of t, and then we use $R = t/k$ to find the value of R corresponding to each value of k. Using *Mathematica*, we generate a large number of values of t and then we plot k *vs* R. Here we can see both $k(R)$ curves, corresponding to W_+ and W_-.

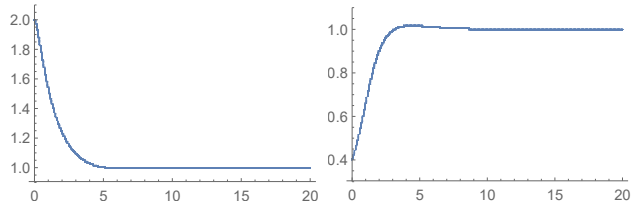


FIG. 2: Numerical data for $k_+(R)$ and $k_-(R)$

As we see, the first one ($k_+(R)$) is almost monotonically decreasing from $k(0) = 2$ to $k(\infty) = 1$, as expected, and the other one increases from $k(0) = 0.4$ to $k(\infty) = 1$. As neither of them is greater than 2, it is easy to see using (14), (15) and (16) that $W_+ < W_-$, so the ground state energy corresponds to $W_+ \equiv W$. From now on we will stick to it, since our approximations are not valid for the excited states.

Now, we try adjusting our plot with functions of the type $k(R) = \frac{2+aR+bR^2}{1+cR+bR^2}$ and $k(R) = \frac{2+aR^2}{1+aR^2}$ (which behave as wanted at $R = 0$ and $R \to \infty$) using the built-in **NonLinearModel** function (*Mathematica*). The adjusted functions are shown in red and the plotted points in blue, in Figures 3 and 4.

We can see in Fig. 3 that the first function is a better adjustment for $k(R)$. Now we can express $W = (kR)^2 F(kR) + (kR)\, G(kR)$ as a function of just R.

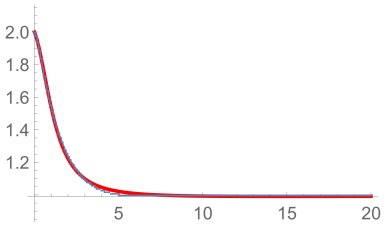


FIG. 3: $k(R) = \frac{2-0.04485R+0.5196R^2}{1+0.09218R+0.5196R^2}$

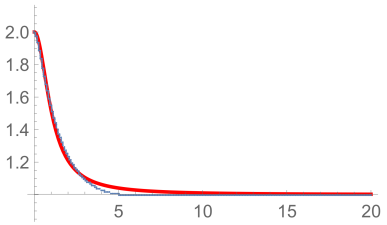


FIG. 4: $k(R) = \frac{2+0.9391R^2}{1+0.9391R^2}$

C. The Schrödinger equation

Now that we have solved the motion of c with the bb pair fixed at a distance R, we are able to use the code on [6] to solve the Schrödinger equation for the motion of the b's, whose Hamiltonian is, explicitly

$$\hat{H}_{bb} = -\frac{\nabla^2_{b_1}}{2m_b/m_c} - \frac{\nabla^2_{b_2}}{2m_b/m_c} + U(R)$$

with the potential $U(R)$ given by (9), using

$$E_c = W(R) \quad \text{and} \quad V_{bb} = -\frac{\alpha_s^{(bb)}/\alpha_s^{(bc)}}{R} = -\frac{0.687}{R}$$

and the mass $m_b/m_c = 2.713$. Note that everything is given in units of m_c for consistency. The resulting energy for the ground state ($n = 1$, $l = 0$) of bb is $E_g = -1.71 = -0.816\,\text{GeV}$ and the normalized radial wavefunction $\mathcal{R}_{10}(R)$ is shown in Fig. 5.

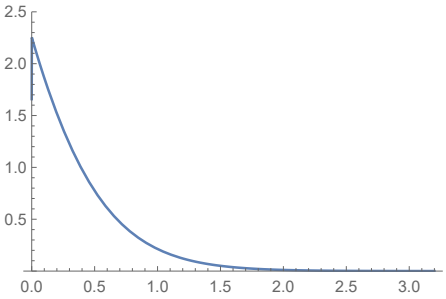


FIG. 5: Normalized radial wavefunction as a function of R.

The angular component is the $l = m = 0$ spherical harmonic $Y_{00}(\theta, \phi) = \sqrt{\frac{1}{4\pi}}$.

IV. CONCLUSIONS

- The c quark wavefunction is

$$\psi_c = \varphi_+(r_1, r_2) = \frac{1s_1 + 1s_2}{\sqrt{2(1+S_{12})}}$$

which corresponds to $\sigma_g 1s$ in the notation of H_2^+ wavefunctions. It has $L_c = 0$ angular momentum and is symmetric under the interchange of the b's.

The wavefunction of the bb is

$$\psi_{bb} = \mathcal{R}_{10}(R)Y_{00}(\theta, \phi),$$

and has $L_{bb} = 0$ so it is also symmetric. Thus, the total spatial wavefunction $\psi_{spatial} = \psi_c\psi_{bb}$ is symmetric under the interchange $b_1 \leftrightarrow b_2$.

Now, the total wavefunction of our baryon is made up of three components: $\psi_{spatial}$, ξ_{color} and χ_{spin}. We have already seen that $\psi_{spatial}$ is symmetric, and the color wavefunction is antisymmetric because it must correspond to the color singlet state

$$\xi_{color} = \frac{1}{\sqrt{6}}(rgb - rbg + gbr - grb + brg - bgr)$$

due to confinement, being r, g, b the three color states of the quarks.

Since the *Pauli Exclusion Principle* must hold for our particle, the total wavefunction must be antisymmetric, which implies that the spin component χ_{spin} is symmetric in the interchange of the b's. This implies that the bb pair must have spin 1, corresponding to parallel quark spins and symmetric wavefunction. Adding the spin of the third quark gives $J = S = \frac{1}{2}, \frac{3}{2}$, so we should expect our particle to be in a degenerate energy state with both values of J. Observing the light baryons, though, we see that those with $J = \frac{1}{2}$ tend to be lighter, mainly due to the spin-spin interaction [7], but for heavy quarks this is not clear since this interaction is proportional to m^{-1}.

The parity of the baryon is

$$P = P_c P_b P_b (-1)^{L_c} (-1)^{L_{bb}} = 1$$

as the intrinsic parity of each quark is 1. In conclusion, our baryon is expected to have $J^P = \frac{1}{2}^+, \frac{3}{2}^+$.

- The final mass $M_{\Omega^0_{cbb}}$ of the baryon corresponds to the sum of the masses of each quark and the binding energy of the whole system, E_g. In addition, we need to estimate the error made in (1), where additional terms depending on powers of α_s, which correspond to the exchange of more than one gluon, should be accounted for. A simple (and gross) way to do this is to multiply the binding energy by α_s. In our case, we will use $\alpha_s^{(bc)}$ since it is an upper bound for all the couplings.

$$\begin{aligned} M_{\Omega^0_{cbb}} =& 2m_b + m_c + E_g(1 \pm \alpha_s^{(bc)}) = \\ =& 11.10 \pm 0.62\,\text{GeV}. \end{aligned}$$

It might be possible to reduce the level of error by analyzing the contribution of each α_s in the final result, and also by noting that α_s always appears multiplied by the color factor $\#_{qq} = \frac{2}{3}$.

V. APPENDIX

- Hydrogen-like wavefunctions:

  $\psi_{nlm}(r, \theta, \phi) = \mathcal{R}_{nl}(r)Y_{lm}(\theta, \phi)$.

  - Radial wavefunctions:
    $\mathcal{R}_{10}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} \exp(\frac{-Zr}{a_0})$.
  - Spherical harmonics:
    $Y_{00}(\theta, \phi) = \sqrt{1/4\pi}$.

Acknowledgments

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