



INSTITUT FÜR THEORETISCHE PHYSIK

MASTER THESIS

Combining Lattice QCD results and Nonrelativistic Quantum
Mechanics in the Born-Oppenheimer Approximation to study
possibly existing Tetraquarks

Author:
Jonas Scheunert

Supervisor and 1st examiner:
Prof. Marc Wagner

2nd examiner:
Prof. Pedro Bicudo

September 3, 2015

Selbständigkeitserklärung

Gemäß §30 (12) der Ordnung des Fachbereichs Physik an der Johann Wolfgang Goethe-Universität für den Bachelor- und Masterstudiengang Physik vom 24.04.2013 versichere ich, dass ich die vorliegende Arbeit selbständig und ohne Benutzung anderer als der angegebenen Quellen und Hilfsmittel verfasst habe. Ferner erkläre ich, dass diese Arbeit, auch nicht auszugsweise, für eine andere Prüfung oder Studienleistung verwendet worden ist.

Unterschrift

Datum

Abstract

In this work possibly existing tetraquarks consisting of two heavy anti-bottom quarks and two light up/down quarks are studied. Lattice QCD is used to compute effective potentials for the anti-bottom quarks in the Born-Oppenheimer approximation. These potentials are used in a nonrelativistic coupled channel Schrödinger equation that includes effects due to the heavy anti-bottom spin. We discuss solutions to this equation to investigate the existence of a bound state. Indications for a tetraquark state with $I(J^P) = 0(1^+)$ are found.

Contents

1	Introduction	1
2	Heavy spin effects	3
2.1	Fierz transformations	3
2.2	Rearranging operators	5
2.3	Choosing L and S	6
2.4	Coupled Schrödinger equation	9
3	Solving the coupled Schrödinger equation	11
3.1	Block diagonal form	11
3.2	Symmetry of the $\bar{b}b$ wave function	14
3.3	Analytical considerations	15
3.3.1	Boundary conditions	16
3.3.2	Asymptotic behavior	17
3.4	Numerical solution	19
4	Results	21
4.1	Fitting procedure and results	21
4.2	Energy of the four quark system	22
4.3	Further sources of systematic errors	26
5	Conclusion and Outlook	27
A	Gamma matrices	29

Chapter 1

Introduction

According to the current understanding of quantum chromodynamics (QCD) there is no obvious reason why the usual mesons and baryons, the former consisting of a quark-antiquark pair and the latter of three quarks, are the only possible hadrons. However, confirming the existence or non-existence of exotic hadrons has proven to be a very difficult problem.

One possibility for exotic multiquark states are tetraquarks, which are mesons consisting of four valence quarks. There are several hadronic resonances, e.g. the light scalar mesons σ , κ , $f_0(980)$ and $a_0(980)$ [1], which are tetraquark candidates. However these mesons have quantum numbers and masses that are consistent with the two quark picture. This makes it hard to find definitive proof of their tetraquark nature.

The recent tetraquark candidates Z_c^\pm and Z_b^\pm have electrical charge of ± 1 which can be explained by $I = 1$ and masses and decay products that indicate the presence of $c\bar{c}$ and $b\bar{b}$ pairs. While the Z_b^\pm so far has only been claimed by the BELLE collaboration [2], Z_c^\pm has been observed by several other collaborations [3, 4, 5, 6, 7, 8, 9, 10].

It is undoubtedly interesting to get a better theoretical understanding of these results to correctly interpret them and also to guide future investigations. Theoretical studies of tetraquarks however pose a challenging problem: usually they are open to meson-meson decay and are complex relativistic four body systems. Studying tetraquark systems with $b\bar{b}$ pairs as claimed by BELLE with lattice QCD would be very difficult since they couple to several decay channels.

In this thesis we therefore extend the technical simpler studies done in [11, 12]. There, the existence/non-existence of tetraquarks with two heavy \bar{b} quarks in the presence of two lighter quarks was investigated. In this work we will focus on the case where the light quarks are degenerate u/d quarks. We will give a short summary of the aspects of these studies which are relevant for this project.

To avoid technical difficulties, bound states rather than resonances are investigated. Since the \bar{b} quarks are much heavier than the light u/d quarks they are treated nonrelativistic and the Born-Oppenheimer approximation [13] is employed: for the light quarks the \bar{b} quarks are regarded as static color sources. Once the energy of the light quarks is computed using lattice QCD from first principles it is used as an effective potential for the heavy \bar{b} quarks in a nonrelativistic Schrödinger equation.

The energy of the effective potential for the spatial separation $r = |\vec{r}_1 - \vec{r}_2|$ of the \bar{b} quarks is obtained from the exponential decay of the correlation functions

$$C(t, r) = \langle \Omega | \mathcal{O}^\dagger(t, r) \mathcal{O}(0, r) | \Omega \rangle \quad (1.1)$$

of four quark creation operators

$$\mathcal{O}(t, r) = (S)_{\alpha\beta} (L)_{\gamma\delta} \left(\bar{Q}_\alpha(\vec{r}_1) q_\gamma^{(1)}(\vec{r}_1) \right) \left(\bar{Q}_\beta(\vec{r}_2) q_\delta^{(2)}(\vec{r}_2) \right) \quad (1.2)$$

at sufficiently large $t_{\min} \leq t \leq t_{\max}$. Here \bar{Q} denotes a static antiquark operator approximating the \bar{b} quark, $q^{(1)}q^{(2)} \in \{uu, dd, (ud + du)/\sqrt{2}, (ud - du)/\sqrt{2}\}$ depending on isospin and the Greek indices denote spin degrees of freedom. In the static approximation the spin of the heavy quarks are irrelevant, so different choices for the matrix S which couples the heavy spin degrees of freedom lead to the same potential. Therefore the matrix L which couples the light degrees of freedom in spinor space determines spin and parity of the state. For a detailed discussion of the lattice calculations see [14, 15].

The lattice QCD results of course provide the energy of the potentials only for a limited number of discrete separations r . To use them in a Schrödinger equation these results have to be interpolated and extrapolated by an appropriate fit function. Finding such a function necessitates a qualitative understanding of the four quark system.

The pair of heavy antiquarks is immersed in a cloud of two light quarks. For small distances r the diquark interaction of the heavy antiquarks is the main contribution to the potential. The diquark potential has a Coulomb-like $-\alpha/r$ behavior for small separations, whereas for large separations it is linear and confining. In our case, however, at larger separations the interaction is screened by the light quarks. When the antiquarks are separated far enough one is essentially dealing with two bottom mesons. In [11, 12] L was chosen in a way that these bottom mesons are pseudoscalar B and/or vector B^* mesons, which are the lightest mesons containing a \bar{b} quark [1]. In the static limit these mesons are degenerate because the spin interaction between the light and heavy quarks is neglected.

These considerations suggest the following fit function for the $\bar{b}\bar{b}$ potentials:

$$V(r) = -\frac{\alpha}{r} \exp\left(-\left(\frac{r}{d}\right)^p\right) + V_0. \quad (1.3)$$

The exponential function mediates the screening due to the light quarks and V_0 is included to account for two times the mass of the static-light meson.

Using the most attractive potential from [14, 15] in a Schrödinger equation for the \bar{b} quarks results in a bound state with binding energy

$$E_{\text{bind}} = 93_{-47}^{+43} \text{ MeV}. \quad (1.4)$$

As mentioned above already, effects due to heavy spin have been neglected in these considerations. These effects, however, could be of the same order as the binding energy, as one can estimate e.g. by the mass difference of the B and B^* meson, $m_{B^*} - m_B \approx 46 \text{ MeV}$. The aim of this thesis is to extend the strategy that has been outlined in this section to include consequences of heavy spin.

Chapter 2

Incorporating heavy spin effects

In principle effects due to heavy spin could be included by computing corrections to the potentials using lattice QCD. For the standard quark-antiquark potential this has been pioneered in [16, 17]. However, we expect this to be extremely difficult for a four quark system.

Alternatively, to incorporate the mass difference of the B and the B^* mesons due to heavy spin one can add the mass difference in appropriate cases to the asymptotic value V_0 of the fit function (1.3) after the fitting procedure. The advantage of this method is that no new (expensive) lattice calculations have to be made.

In order to accomplish this in a sensible way we need to interpret the meson-meson structure generated by the $qq\bar{Q}\bar{Q}$ potential creation operators. To achieve this, we refine the method that was used to explain the asymptotic behavior of the potentials in [14, 15]. This means we express the $qq\bar{Q}\bar{Q}$ potential creation operators in terms of static-light bilinears. As a mathematical means to this end we introduce Fierz transformations.

2.1 Fierz transformations

We start by defining the sixteen 4×4 matrices

$$\Gamma^S := \mathbb{1}, \Gamma_\mu^V := \gamma_\mu, \Gamma_{\mu\nu}^T := \frac{1}{2} [\gamma_\mu, \gamma_\nu] := \gamma_\mu \gamma_\nu \quad \mu < \nu, \Gamma_\mu^A := \gamma_\mu \gamma_5, \Gamma^P := \gamma_5, \quad (2.1)$$

these matrices are labeled with the numbers one to sixteen in the obvious manner and will be referred to as Γ -matrices from now on. We will show that these matrices form a basis for $\mathbb{C}^{4 \times 4}$.

First, note that these matrices can be seen as representatives for any product of gamma matrices in the following sense: for any $(s_1, s_2, s_3, s_4) \in \mathbb{N}^4$ and $\alpha \in \{\pm 1\}$ there is an $\alpha' \in \{\pm 1\}$ and $a \in \{1, \dots, 16\}$ such that

$$\alpha \prod_{\mu=1}^4 \gamma_\mu^{s_\mu} = \alpha' \Gamma^a, \quad (2.2)$$

this can be seen easily by using the anti-commutation relations of the gamma matrices (cf. equation (A.1)). From this and by using the anti-commutation relations again we can

conclude that ¹

$$(\Gamma^a)^2 = \chi^{aa} \mathbb{1} \text{ where } (\chi^{ab}) := \mathbb{1}_{5 \times 5} \oplus -\mathbb{1}_{10 \times 10} \oplus \mathbb{1}_{1 \times 1}, \quad (2.3)$$

$$\text{tr}(\Gamma^a) = 0 \text{ if } \Gamma^a \neq \Gamma^S = \mathbb{1}, \quad (2.4)$$

and that for every pair $(a, b) \in \{1, \dots, 16\}^2$ there exists a $c \in \{1, \dots, 16\}$ such that one can choose $\alpha \in \{\pm 1\}$ to fulfill

$$\Gamma^a \Gamma^b = \alpha \Gamma^c. \quad (2.5)$$

The Γ -matrices are proportional to their inverses (see equation (2.3)) and pairwise linear independent and therefore

$$\Gamma^a \Gamma^b \neq \alpha \mathbb{1} \quad \forall \alpha \in \mathbb{C} \text{ if } a \neq b. \quad (2.6)$$

Denoting the inverse of Γ^a by Γ_a equation (2.3) implies

$$\Gamma^a = \sum_{b=1}^{16} \chi^{ab} \Gamma_b. \quad (2.7)$$

Taking all this in consideration we now can show that the Γ^a -matrices are linear independent and therefore, since $\dim(\mathbb{C}^{4 \times 4}) = 16$ (as a vector space over \mathbb{C}), form a basis for $\mathbb{C}^{4 \times 4}$. To this end, suppose that

$$\sum_{a=1}^{16} \lambda_a \Gamma^a = 0 \quad (2.8)$$

for some $\lambda_a \in \mathbb{C}$. Multiplying this equation by Γ_b and taking the trace results in

$$\sum_{a=1}^{16} \lambda_a \text{tr}(\Gamma_b \Gamma^a) = 0. \quad (2.9)$$

The trace is equal to four if $\Gamma_b = \Gamma_a = (\Gamma^a)^{-1}$ and zero otherwise due to equations (2.4) to (2.7). So,

$$4 \sum_{a=1}^{16} \lambda_a \delta_b^a = 0 \quad (2.10)$$

$$\Rightarrow \lambda_b = 0, \quad (2.11)$$

which shows the linear independence. This of course implies that any $M \in \mathbb{C}^{4 \times 4}$ can be expanded in terms of the Γ -matrices and the coefficients for this expansion can be computed using the same logic as above:

$$M = \frac{1}{4} \sum_{a=1}^{16} \text{tr}(\Gamma_a M) \Gamma^a, \quad (2.12)$$

or, in components:

$$M_{\alpha\beta} = \frac{1}{4} \sum_{a=1}^{16} \sum_{\gamma,\delta=1}^4 M_{\delta\gamma} (\Gamma_a)_{\gamma\delta} (\Gamma^a)_{\alpha\beta}. \quad (2.13)$$

Looking at the last equation one can see that the Γ -matrices fulfill the following completeness relation:

$$\delta_{\alpha\gamma} \delta_{\beta\delta} = \frac{1}{4} \sum_{a=1}^{16} (\Gamma^a)_{\alpha\beta} (\Gamma_a)_{\delta\gamma}. \quad (2.14)$$

This completeness relation can be used to derive Fierz identities.

¹At the moment, we do *not* use the Einstein summation convention.

2.2 Rearranging operators

If not mentioned otherwise, summation over repeating indices is implied from now on. To relate the $qq\bar{Q}\bar{Q}$ potential to $B^{(*)}B^{(*)}$ creation operators we are interested in a Fierz identity of the following kind:

$$S_{\alpha\beta}L_{\gamma\delta}(\psi_\alpha^1\psi_\gamma^2)(\psi_\beta^3\psi_\delta^4) = \sum_\lambda(\psi^1M_1(\lambda)\psi^2)(\psi^3M_2(\lambda)\psi^4). \quad (2.15)$$

Since our focus is solely on algebraic manipulations in spinor space we are using generic labels for the fermion operators.

To derive the identity, one separates indices by inserting Kronecker deltas and uses the completeness relation (2.14)

$$S_{\alpha\beta}L_{\gamma\delta}(\psi_\alpha^1\psi_\gamma^2)(\psi_\beta^3\psi_\delta^4) = S_{\alpha'\beta}L_{\gamma'\delta}\delta_{\alpha\alpha'}\delta_{\gamma\gamma'}(\psi_\alpha^1\psi_\gamma^2)(\psi_\beta^3\psi_\delta^4) \quad (2.16)$$

$$= \frac{1}{4}S_{\alpha'\beta}L_{\gamma'\delta}(\Gamma^a)_{\alpha\gamma}(\Gamma_a)_{\gamma'\alpha'}(\psi_\alpha^1\psi_\gamma^2)(\psi_\beta^3\psi_\delta^4) \quad (2.17)$$

$$= \frac{1}{4}(\psi_\alpha^1(\Gamma^a)_{\alpha\gamma}\psi_\gamma^2)(\psi_\beta^3(S^T)_{\beta\alpha'}(\Gamma_a^T)_{\alpha'\gamma'}L_{\gamma'\delta}\psi_\delta^4) \quad (2.18)$$

$$= \frac{1}{4}(\psi^1(\Gamma^a)\psi^2)(\psi^3(S^T)(\Gamma_a^T)L\psi^4). \quad (2.19)$$

Deploying again the fact that the Γ -matrices form a basis we can expand:

$$(S^T)(\Gamma_a^T)L = \frac{1}{4}\text{tr}(\Gamma_b(S^T)(\Gamma_a^T)L)\Gamma^b. \quad (2.20)$$

If we now define the matrix

$$\mathbf{G}(S, L)_{ab} = \frac{1}{16}\text{tr}(\Gamma_b(S^T)(\Gamma_a^T)L) \quad (2.21)$$

and the vector

$$\Psi_a^{(ij)} = \psi^i\Gamma^a\psi^j, \quad (2.22)$$

we have the following identities:

$$S_{\alpha\beta}L_{\gamma\delta}(\psi_\alpha^1\psi_\gamma^2)(\psi_\beta^3\psi_\delta^4) = \frac{1}{16}\text{tr}(\Gamma_b(S^T)(\Gamma_a^T)L)(\psi^1(\Gamma^a)\psi^2)(\psi^3(\Gamma^b)\psi^4) \quad (2.23)$$

$$= (\Psi^{(12)})^T \mathbf{G}(S, L)\Psi^{(34)}. \quad (2.24)$$

Using the defining property of the charge conjugation matrix equation (A.5) one can show that

$$(\Gamma^a)^T = \xi_b^a \mathcal{C}\Gamma^b\mathcal{C}^{-1} \text{ where } (\xi_b^a) := \mathbf{1}_{1\times 1} \oplus -\mathbf{1}_{10\times 10} \oplus \mathbf{1}_{5\times 5}. \quad (2.25)$$

Defining

$$\omega_{ac} := \chi_{ab}\xi_c^b \quad (2.26)$$

and writing

$$L =: \mathcal{C}\tilde{L}, \quad (2.27)$$

$$S^T =: \tilde{S}\mathcal{C}^{-1}, \quad (2.28)$$

we eventually arrive at the following expression for \mathbb{G} :

$$\mathbb{G}(S, L)_{ab} = \frac{1}{16} \omega_{ac} \chi_{bd} \operatorname{tr} \left(\Gamma^d \tilde{S} \Gamma^c \tilde{L} \right) \quad (2.29)$$

$$= \pm \frac{1}{16} \operatorname{tr} \left(\Gamma^b \tilde{S} \Gamma^a \tilde{L} \right) \quad (2.30)$$

2.3 Choosing L and S

As mentioned in chapter 1 the matrix L couples the light spin degrees of freedom in the $qq\bar{Q}\bar{Q}$ potential creation operators and therefore completely determines to which potential the superposition of meson-meson operators in equation (2.23) corresponds to. The different possibilities for L . Besides the restriction for S that

$$\operatorname{tr} \left(S \left(\frac{\mathbb{1} + \gamma_4}{2} \right) S \left(\frac{\mathbb{1} + \gamma_4}{2} \right) \right) \neq 0 \quad (2.31)$$

must be fulfilled (otherwise the corresponding correlator vanishes [18]), it does not influence the potential. The matrix S *does* however affect the interpretation of the meson content of the static potential creation operators.² We are now interested in the possible choices for S and L such that the meson operators correspond to the pseudoscalar/vector mesons B or B^* .

Formulating this aim in the notation of the preceding section we are interested in the possible choices for S and L such that

$$\mathbb{G}(S, L)_{ab} = 0 \text{ if } a \in K \text{ or } b \in K, \quad (2.32)$$

and

$$\mathbb{G}(S, L)_{ab} \neq 0 \text{ for at least one } (a, b) \in A^2 \quad (2.33)$$

with the sets

$$K := \{1, 5, 6, 7, 9, 12, 13, 14\}, \quad (2.34)$$

and

$$A := \{1, \dots, 16\} \setminus K. \quad (2.35)$$

To facilitate the discussion we introduce the projectors

$$\mathbb{P}_{\pm} := \frac{\mathbb{1} \pm \gamma_4}{2} = \frac{\mathbb{1} \pm \gamma_4}{2}, \quad (2.36)$$

it is easy to check (and thereby justify calling them projectors) that

$$\mathbb{P}_{\pm}^2 = \mathbb{P}_{\pm}, \quad (2.37)$$

$$\mathbb{P}_{\pm} \mathbb{P}_{\mp} = 0, \quad (2.38)$$

$$\mathbb{P}_{+} + \mathbb{P}_{-} = \mathbb{1}. \quad (2.39)$$

This enables us to write $\mathbb{C}^{4 \times 4}$ as the direct sum of the \mathbb{P}_{\pm} -invariant subspaces $P_{\pm} := \mathbb{P}_{\pm} \mathbb{C}^{4 \times 4}$:

$$\mathbb{C}^{4 \times 4} = P_{+} \oplus P_{-}. \quad (2.40)$$

²Different choices of S of course only lead to changes which vanish in the static limit, e.g. B to B^*

Now note that

$$P_{\pm} = \mathbb{P}_{\pm} \text{span} \left(\{\Gamma_a\}_{a \in A \cup K} \right) = \text{span} \left(\{\mathbb{P}_{\pm} \Gamma_a\}_{a \in A \cup K} \right), \quad (2.41)$$

of course $\{\mathbb{P}_{\pm} \Gamma_a\}_{a \in A \cup K}$ is no basis, since the elements are not linear independent. A basis can be obtained by removing linear dependent matrices. By direct calculation one can show that for any $a \in K$ there is a unique $b \in K \setminus \{a\}$ such that $\mathbb{P}_{\pm} \Gamma_a$ is linear dependent on $\mathbb{P}_{\pm} \Gamma_b$. An analogous statement can be made for A . Therefore both subspaces have same dimension and can both be split into two four dimensional subspaces:

$$P_{\pm} = P_{\pm}^+ \oplus P_{\pm}^-, \quad (2.42)$$

$$\mathbb{C}^{4 \times 4} = P_+^+ \oplus P_+^- \oplus P_-^+ \oplus P_-^-, \quad (2.43)$$

$$P_+^+ = \text{span} \left(\{\mathbb{P}_+ \Gamma_a\}_{a \in K} \right), \quad (2.44)$$

$$P_+^- = \text{span} \left(\{\mathbb{P}_+ \Gamma_a\}_{a \in A} \right), \quad (2.45)$$

$$P_-^+ = \text{span} \left(\{\mathbb{P}_- \Gamma_a\}_{a \in A} \right), \quad (2.46)$$

$$P_-^- = \text{span} \left(\{\mathbb{P}_- \Gamma_a\}_{a \in K} \right). \quad (2.47)$$

The main property of these subspace that we will utilize is that

$$v_{\pm}^+ \in P_{\pm}^+ \Rightarrow v_{\pm}^+ = \mathbb{P}_{\pm} v_{\pm}^+ = v_{\pm}^+ \mathbb{P}_{\pm} \quad (2.48)$$

and

$$v_{\pm}^- \in P_{\pm}^- \Rightarrow v_{\pm}^- = \mathbb{P}_{\pm} v_{\pm}^- = v_{\pm}^- \mathbb{P}_{\pm}, \quad (2.49)$$

which can easily be understood from the fact that

$$a \in A \Rightarrow \mathbb{P}_{\pm} \Gamma^a = \Gamma^a \mathbb{P}_{\mp} \quad (2.50)$$

and

$$b \in K \Rightarrow \mathbb{P}_{\pm} \Gamma^b = \Gamma^b \mathbb{P}_{\pm}. \quad (2.51)$$

We can now analyze the condition imposed on S by (2.31), which can be rewritten as

$$\text{tr} (S \mathbb{P}_+ S \mathbb{P}_+) \neq 0. \quad (2.52)$$

S will be given in the form of equation (2.28), using equation (A.1) for \mathcal{C} one can show that

$$\mathbb{P}_{\pm}^T = \mathcal{C} \mathbb{P}_{\mp} \mathcal{C}^{-1} \quad (2.53)$$

and therefore \tilde{S} must fulfill

$$\text{tr} \left(\tilde{S} \mathbb{P}_- \mathcal{C}^{-1} \tilde{S} \mathbb{P}_- \mathcal{C}^{-1} \right) \neq 0. \quad (2.54)$$

For $s_{\pm}^+ \in P_{\pm}^+$ we have that

$$s_{\pm}^+ \mathbb{P}_- = \mathbb{P}_{\pm} s_{\pm}^+ \mathbb{P}_- \quad (2.55)$$

$$= s_{\pm}^+ \mathbb{P}_+ \mathbb{P}_- \quad (2.56)$$

$$= 0. \quad (2.57)$$

This means that for $\tilde{S} = s_{\pm}^{\pm}$ condition (2.54) is not fulfilled.

In the chiral representation $\mathbb{P}_- \mathcal{C}^{-1} \in P_{\pm}^+$ and therefore for $s_{\pm}^{\pm} \in P_{\pm}^{\pm}$:

$$\mathbb{P}_- \mathcal{C}^{-1} s_{\pm}^{\pm} = \mathbb{P}_- \mathcal{C}^{-1} \mathbb{P}_- s_{\pm}^{\pm} \quad (2.58)$$

$$= \mathcal{C}^{-1} \mathbb{P}_+ \mathbb{P}_- s_{\pm}^{\pm} \quad (2.59)$$

$$= 0. \quad (2.60)$$

So setting $\tilde{S} = s_{\pm}^{\pm}$ must also be avoided in the representation we are using (cf. Appendix A). In conclusion we restrict ourself to $\tilde{S} \in P_{\pm}^-$.

Similar arguments can be made for \tilde{L} (which is related to L via equation (2.27)) by demanding that equations (2.32) and (2.33) are fulfilled. Let $s_{\pm}^- \in P_{\pm}^-$, then

$$l_{+}^{+} \in P_{+}^{+} \Rightarrow \text{tr} \left(\Gamma^b s_{+}^{-} \Gamma^a l_{+}^{+} \right) = 0 \text{ if } b \in A, \quad (2.61)$$

$$l_{-}^{-} \in P_{-}^{-} \Rightarrow \text{tr} \left(\Gamma^b s_{+}^{-} \Gamma^a l_{-}^{-} \right) = 0 \text{ if } a \in A, \quad (2.62)$$

$$l_{-}^{+} \in P_{-}^{+} \Rightarrow \text{tr} \left(\Gamma^b s_{+}^{-} \Gamma^a l_{-}^{+} \right) = 0 \text{ if } a \in A \text{ or } b \in A, \quad (2.63)$$

in contradiction to equation (2.33). In contrast, for $l_{+}^{-} \in P_{+}^{-}$

$$\text{tr} \left(\Gamma^b s_{+}^{-} \Gamma^a l_{+}^{-} \right) = 0 \text{ if } a \in K \text{ or } b \in K. \quad (2.64)$$

Therefore equation (2.32) is fulfilled in this case and equation (2.33) is also true because the left hand side of equation (2.23) is not zero. Hence both \tilde{S} and \tilde{L} will be chosen such that they are elements of P_{\pm}^- . Consequently we give a possible basis \mathbb{B} for this subspace (by using equation (2.45)):

$$\mathbb{B} = \{ (\mathbb{1} + \gamma_4) \gamma_1, (\mathbb{1} + \gamma_4) \gamma_2, (\mathbb{1} + \gamma_4) \gamma_3, (\mathbb{1} + \gamma_4) \gamma_5 \}. \quad (2.65)$$

For $\tilde{L} \in \mathbb{B}$ the corresponding potentials have been computed in [14, 15], by evaluating³ equation (2.23) for $\tilde{L}, \tilde{S} \in \mathbb{B}$ we are now able to interpret their $B^{(*)} B^{(*)}$ content. Introducing the following abbreviations:

$$\underline{S}_{\alpha\beta} := \begin{pmatrix} [(\mathbb{1} + \gamma_4) \gamma_5 \mathcal{C}^{-1}]_{\alpha\beta}^T \\ [(\mathbb{1} + \gamma_4) \gamma_1 \mathcal{C}^{-1}]_{\alpha\beta}^T \\ [(\mathbb{1} + \gamma_4) \gamma_2 \mathcal{C}^{-1}]_{\alpha\beta}^T \\ [(\mathbb{1} + \gamma_4) \gamma_3 \mathcal{C}^{-1}]_{\alpha\beta}^T \end{pmatrix}, \quad (2.66)$$

$$\underline{B}^{(i)}(\vec{r}) := \begin{pmatrix} B^{(i)}(\vec{r}) \\ B_x^{*,(i)}(\vec{r}) \\ B_y^{*,(i)}(\vec{r}) \\ B_z^{*,(i)}(\vec{r}) \end{pmatrix} := \begin{pmatrix} \bar{Q}(\vec{r}) (\mathbb{1} + \gamma_4) \gamma_5 q^{(i)}(\vec{r}) \\ \bar{Q}(\vec{r}) (\mathbb{1} + \gamma_4) \gamma_1 q^{(i)}(\vec{r}) \\ \bar{Q}(\vec{r}) (\mathbb{1} + \gamma_4) \gamma_2 q^{(i)}(\vec{r}) \\ \bar{Q}(\vec{r}) (\mathbb{1} + \gamma_4) \gamma_3 q^{(i)}(\vec{r}) \end{pmatrix} \quad (2.67)$$

³this can be efficiently done by using a CAS like Maxima [19]

and

$$T := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \end{pmatrix} \quad (2.68)$$

we get the result

$$\begin{pmatrix} \underline{S}_{\alpha\beta} [\mathcal{C} (\mathbf{1} + \gamma_4) \gamma_5]_{\gamma\delta} \left(\bar{Q}_\alpha (\vec{r}_1) q_\gamma^1 (\vec{r}_1) \right) \left(\bar{Q}_\beta (\vec{r}_2) q_\delta^{(2)} (\vec{r}_2) \right) \\ \underline{S}_{\alpha\beta} [\mathcal{C} (\mathbf{1} + \gamma_4) \gamma_1]_{\gamma\delta} \left(\bar{Q}_\alpha (\vec{r}_1) q_\gamma^1 (\vec{r}_1) \right) \left(\bar{Q}_\beta (\vec{r}_2) q_\delta^{(2)} (\vec{r}_2) \right) \\ \underline{S}_{\alpha\beta} [\mathcal{C} (\mathbf{1} + \gamma_4) \gamma_2]_{\gamma\delta} \left(\bar{Q}_\alpha (\vec{r}_1) q_\gamma^1 (\vec{r}_1) \right) \left(\bar{Q}_\beta (\vec{r}_2) q_\delta^{(2)} (\vec{r}_2) \right) \\ \underline{S}_{\alpha\beta} [\mathcal{C} (\mathbf{1} + \gamma_4) \gamma_3]_{\gamma\delta} \left(\bar{Q}_\alpha (\vec{r}_1) q_\gamma^1 (\vec{r}_1) \right) \left(\bar{Q}_\beta (\vec{r}_2) q_\delta^{(2)} (\vec{r}_2) \right) \end{pmatrix} = T \begin{pmatrix} B^{(1)} (\vec{r}_1) \underline{B}^{(2)} (\vec{r}_2) \\ B_x^{*(1)} (\vec{r}_1) \underline{B}^{(2)} (\vec{r}_2) \\ B_y^{*(1)} (\vec{r}_1) \underline{B}^{(2)} (\vec{r}_2) \\ B_z^{*(1)} (\vec{r}_1) \underline{B}^{(2)} (\vec{r}_2) \end{pmatrix} \quad (2.69)$$

The operators in (2.67) excite states that for large t correspond to $B^{(*)}$ mesons.

2.4 The coupled channel Schrödinger equation

The lattice potentials are spherically symmetric and parametrized by the fit function (1.3), where $r = |\vec{r}_2 - \vec{r}_1|$ and \vec{r}_1 and \vec{r}_2 are the positions of the \bar{b} quarks. For details about the fitting procedure see section 4.1. There are two different potentials, V_5 for $L = \mathcal{C} (\mathbf{1} + \gamma_4) \gamma_5$ and V_j for $L = \mathcal{C} (\mathbf{1} + \gamma_4) \gamma_j$, $j = 1, 2, 3$. These potentials can be thought of as the potentials between two \bar{b} quarks in the presence of two light u/d quarks.

We now want to use these potentials in a Schrödinger equation for the two heavy \bar{b} quarks

$$H\Psi(\vec{r}_1, \vec{r}_2) = E\Psi(\vec{r}_1, \vec{r}_2), \quad (2.70)$$

that includes the mass difference of B and B^* due to heavy spin, to see if they form a bound state.

We start by setting $V_0 = 0$ since we will include the asymptotic value according to equation (2.69).

The wave function Ψ has sixteen components which correspond to the meson operators on the right hand side of equation (2.69). The Hamiltonian can be split in a free and an interacting part, $H = H_0 + H_{int}$. The free part of the Hamiltonian contains the masses of the $B^{(*)}$ mesons (as replacement for V_0) and the kinetic energy of the \bar{b} quarks:

$$H_0 = M \otimes \mathbb{1}_{4 \times 4} + \mathbb{1}_{4 \times 4} \otimes M + \frac{\vec{p}_1^2}{2m_b} \mathbb{1}_{16 \times 16} + \frac{\vec{p}_2^2}{2m_b} \mathbb{1}_{16 \times 16}, \quad (2.71)$$

where

$$M = \text{diag} (m_B, m_{B^*}, m_{B^*}, m_{B^*}). \quad (2.72)$$

For the masses the following values were used: $m_B = 5279$ MeV, $m_{B^*} = 5325$ MeV [1] and $m_b = 4977$ (as used in quark models [20])

The interacting part consists of the potential matrix

$$V = \text{diag} (V_5, V_j, V_j, V_j) \otimes \mathbb{1}_{4 \times 4} \quad (2.73)$$

and relates it to the components of the wave function via the matrix T (equation (2.68)) in analogy to equation (2.69):

$$H_{\text{int}} = T^{-1} V T. \quad (2.74)$$

The aim of the next section will be to solve equation (2.70).

Chapter 3

Solving the coupled Schrödinger equation

In the first section of this chapter we bring the Schrödinger equation (2.70) to a block-diagonal form by rearranging its components according to total spin J . The advantage of this form is twofold: on the one hand, the maximal block size in this form is 2×2 and therefore simplifies the solution of the equation. On the other hand, it also allows for an implementation of the correct symmetrization of the $\bar{b}b$ Wave function, which was neglected so far due to the usage of static quarks for the lattice computation.

Eventually we derive boundary conditions a physically sensible solution should have and present our method to numerically solve the equation.

3.1 Block diagonal form

We now use the following notation: the first component of the wave function will be denoted BB , the second by BB^* and so on analogous to the meson operators in equation (2.69). Furthermore we define the abbreviation

$$\vec{B}^* = \begin{pmatrix} B_x^* \\ B_y^* \\ B_z^* \end{pmatrix}. \quad (3.1)$$

We also define the 16×16 matrix

$$(a \leftrightarrow b)_{ij} := \delta_{ij} - \delta_{ai}\delta_{aj} - \delta_{bi}\delta_{bj} + \delta_{ai}\delta_{bj} + \delta_{bi}\delta_{aj}, \quad (3.2)$$

which, when applied to a vector, switches the a^{th} element with the b^{th} element of the vector, i.e.

$$(1 \leftrightarrow 2) \begin{pmatrix} BB \\ BB_x^* \\ \vdots \end{pmatrix} = \begin{pmatrix} BB_x^* \\ BB \\ \vdots \end{pmatrix} \quad (3.3)$$

Our first step in order to introduce a change of basis according to total spin J consists of defining the following matrix

$$R = (7 \leftrightarrow 8)(8 \leftrightarrow 9)(9 \leftrightarrow 10)(10 \leftrightarrow 11)(11 \leftrightarrow 12)(12 \leftrightarrow 13)(6 \leftrightarrow 7)(7 \leftrightarrow 8)(8 \leftrightarrow 9), \quad (3.4)$$

which introduces row switches which have the following effect

$$U \begin{pmatrix} \underline{BB} \\ B_x^* \underline{B} \\ B_y^* \underline{B} \\ B_z^* \underline{B} \end{pmatrix} = \begin{pmatrix} BB \\ B\vec{B}^* \\ \vec{B}^* B \\ B_x^* \vec{B}^* \\ B_y^* \vec{B}^* \\ B_z^* \vec{B}^* \end{pmatrix}. \quad (3.5)$$

Next, we define a transformation so that the individual mesons are eigenvalues of the z-component of their spin operator. Denoting $B_j^{j_z}$ the meson with spin j and spin projection quantum number along z-axis j_z one has

$$\begin{pmatrix} B_0^0 \\ B_1^1 \\ B_1^0 \\ B_1^{-1} \end{pmatrix} = \begin{pmatrix} B \\ 2\sqrt{\frac{\pi}{3}}Y_1^{-1}(B_x^*, B_y^*, B_z^*) \\ 2\sqrt{\frac{\pi}{3}}Y_1^0(B_x^*, B_y^*, B_z^*) \\ 2\sqrt{\frac{\pi}{3}}Y_1^1(B_x^*, B_y^*, B_z^*) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} B \\ \vec{B}^* \end{pmatrix} =: \begin{pmatrix} 1 & \\ & z \end{pmatrix} \begin{pmatrix} B \\ \vec{B}^* \end{pmatrix}, \quad (3.6)$$

where we have defined the 3×3 matrix z and $Y_j^{j_z}$ denotes a spherical harmonic in Cartesian coordinates at $r = 1$ employing the Condon-Shortley phase [21]. Therefore the transformation acting on the sixteen component wave function is

$$Z := \begin{pmatrix} 1 & & & \\ & z & & \\ & & z & \\ & & & z \otimes z \end{pmatrix}, \quad (3.7)$$

with the effect

$$Z \begin{pmatrix} BB \\ B\vec{B}^* \\ \vec{B}^* B \\ B_x^* \vec{B}^* \\ B_y^* \vec{B}^* \\ B_z^* \vec{B}^* \end{pmatrix} = \begin{pmatrix} BB \\ B\vec{B}_1 \\ \vec{B}_1 B \\ B_1^1 \vec{B}_1 \\ B_1^0 \vec{B}_1 \\ B_1^{-1} \vec{B}_1 \end{pmatrix}, \quad (3.8)$$

where

$$\vec{B}_1 = \begin{pmatrix} B_1^1 \\ B_1^0 \\ B_1^{-1} \end{pmatrix}. \quad (3.9)$$

In the next step we introduce the 9×9 matrix c which makes the decomposition $1 \otimes 1 \cong 0 \oplus 1 \oplus 2$ of $SU(2)$ representations explicit, i.e. it contains the appropriate Clebsch-Gordan coefficients. In the CAS Maxima [19] this matrix can be computed by the commands

```
load("clebsch_gordan");
c_list: [];
for J in [0,1,2] do (
  c_list: append(c_list,reverse(makelist(flatten(
    reverse((makelist(reverse(makelist(
      clebsch_gordan(1,1,m1,m2,J,M),m2,-1,1)),m1,-1,1))))),M,-J,J)));
c_matrix:apply('matrix,c_list);
```

which leads to

$$c := \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{3}} & 0 & -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{\sqrt{2}}{\sqrt{3}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (3.10)$$

Defining

$$C := \begin{pmatrix} \mathbb{1}_{7 \times 7} \\ c \end{pmatrix} \quad (3.11)$$

the desired change of basis is

$$S := CZR. \quad (3.12)$$

The transformed Hamiltonian $\tilde{H} = SHS^{-1}$ leads to independent simpler coupled channel equations corresponding to definite total spin J :

- a single 2×2 coupled channel equation corresponding to $J = 0$ with the Hamiltonian

$$\tilde{H}_{0,J=0} = \begin{pmatrix} 2m_B & 0 \\ 0 & 2m_{B^*} \end{pmatrix} + \left(\frac{\vec{p}_1^2}{2m_b} + \frac{\vec{p}_2^2}{2m_b} \right) \mathbb{1}_{2 \times 2}, \quad (3.13a)$$

$$\tilde{H}_{\text{int},J=0} = \frac{1}{4} \begin{pmatrix} V_5(r) + 3V_j(r) & \sqrt{3}(V_5(r) - V_j(r)) \\ \sqrt{3}(V_5(r) - V_j(r)) & 3V_5(r) + V_j(r) \end{pmatrix}, \quad (3.13b)$$

the wave function is related to the original wave function via

$$\tilde{\Psi}_{J=0} = \begin{pmatrix} BB \\ (1/\sqrt{3})\vec{B}^2 \end{pmatrix}; \quad (3.14)$$

- five identical 1×1 equations corresponding to $J = 2$ (degeneracy due to $j_z = -2, 1, 0, 1, 2$) with the Hamiltonian

$$\tilde{H}_{2,J=2} = 2m_{B^*} + \frac{\vec{p}_1^2}{2m_b} + \frac{\vec{p}_2^2}{2m_b}, \quad (3.15)$$

and the wave functions

$$\tilde{\Psi}_{J=2}^{j_z} = 2\sqrt{\frac{2\pi}{15}} Y_2^{j_z}(B_x^*, B_y^*, B_z^*); \quad (3.16)$$

- three identical (degeneracy due to $j_z = -1, 0, 1$) 3×3 coupled channel equations corresponding to $J = 1$ with the Hamiltonian

$$\tilde{H}_{0,J=1} = \begin{pmatrix} m^* + m & 0 & 0 \\ 0 & m^* + m & 0 \\ 0 & 0 & 2m^* \end{pmatrix} + \left(\frac{\vec{p}_1^2}{2m_b} + \frac{\vec{p}_2^2}{2m_b} \right) \mathbb{1}_{3 \times 3} \quad (3.17)$$

$$\tilde{H}_{\text{int},J=1} = \frac{1}{4} \begin{pmatrix} V_5(r) + 3V_j(r) & V_j(r) - V_5(r) & \sqrt{2}(V_5(r) - V_j(r)) \\ V_j(r) - V_5(r) & V_5(r) + 3V_j(r) & \sqrt{2}(V_j(r) - V_5(r)) \\ \sqrt{2}(V_5(r) - V_j(r)) & \sqrt{2}(V_j(r) - V_5(r)) & 2(V_5(r) + V_j(r)) \end{pmatrix} \quad (3.18)$$

and the wave functions

$$\tilde{\Psi}_{J=1}^{j_z} = \begin{pmatrix} BB_1^{j_z} \\ B_1^{j_z} B \\ -\sqrt{2}/2 (\vec{B}_1 \times \vec{B}_1)_{j_z} \end{pmatrix}. \quad (3.19)$$

Symmetrization of the first and anti-symmetrization of the second component

$$\begin{pmatrix} BB_1^{j_z} \\ B_1^{j_z} B \\ -\sqrt{2}/2 (\vec{B}_1 \times \vec{B}_1)_{j_z} \end{pmatrix} \rightarrow \begin{pmatrix} B_1^{j_z} B + BB_1^{j_z} \\ B_1^{j_z} B - BB_1^{j_z} \\ -\sqrt{2}/2 (\vec{B}_1 \times \vec{B}_1)_{j_z} \end{pmatrix}, \quad (3.20)$$

leads to further simplifications: $\tilde{H}_{\text{int},J=1}$ is split into

- a 1×1 matrix (corresponding to the symmetric part)

$$H'_{\text{int},J=1,1 \times 1} = V_j(r) \quad (3.21)$$

and

- a 2×2 matrix (corresponding to the anti-symmetric part)

$$H'_{\text{int},J=1,2 \times 2} = \frac{1}{2} \begin{pmatrix} V_5(r) + V_j(r) & V_j(r) - V_5(r) \\ V_j(r) - V_5(r) & V_5(r) + V_j(r) \end{pmatrix}. \quad (3.22)$$

3.2 Symmetry of the $\bar{b}\bar{b}$ wave function

So far we have not specified if we are using potentials from the isosinglet ($I = 0$) or isotriplet channel ($I = 1$), i.e. if we are using $q^1 q^2 = ud - du$ or $q^1 q^2 \in \{uu, dd, ud + du\}$ in equation (1.2). As it will turn out, the four Hamiltonians (3.13), (3.15), (3.21) and (3.22) are physically sensible only for specific isospin respectively.

This has to do with the fact that the \bar{b} quarks are fermions and therefore their wave function must be anti-symmetric under exchange, which leads to the Pauli-Principle. This has been neglected in the lattice computations since the \bar{b} quarks are treated as spinless color sources which can be distinguished by their position.

We expect that in the ground state the \bar{b} quarks form a spatially symmetric s-wave, as well as the light quarks. Now assume that the light quarks are antisymmetric in flavor space, i.e. $I = 0$. According to the decomposition $3 \otimes 3 \cong \bar{3} \oplus 6$ of $SU(3)$ -representations they are either in the antisymmetric $\bar{3}$ or the symmetric 6 representation in color space. Assuming $\bar{3}$ they must be antisymmetric in spin space due to the Pauli-Principle, which means they have spin 0. The four quark system must form a color singlet, so in this case the \bar{b} quarks must be in the antisymmetric 3 representation in color space. Since $\bar{b}\bar{b}$ can only be symmetric in flavor space this means they have spin 1, so the four quark system has spin 1. Applying this logic to all possible combinations of quantum numbers leads to Table 3.1.

Combination one and two in Table 3.1 both have total spin 1 and therefore correspond to the 2×2 Hamiltonian (3.22). Combination four leads to total spin 0, 1 and 2. Therefore combination four together with combination three are associated to the 2×2 Hamiltonian

	qq			$\bar{b}\bar{b}$		
combination	flavor	spin	color	color	flavor	spin
1	asym ($I = 0$)	asym (0)	asym ($\bar{3}$)	asym (3)	sym	sym (1)
2	asym ($I = 0$)	sym (1)	sym (6)	sym ($\bar{6}$)	sym	asym (0)
3	sym ($I = 1$)	asym (0)	sym (6)	sym ($\bar{6}$)	sym	asym (0)
4	sym ($I = 1$)	sym (1)	asym ($\bar{3}$)	asym (3)	sym	sym (1)

Table 3.1: Possible combinations of quantum numbers / representations and the associated symmetries of the wave function

(3.13) and the two 1×1 Hamiltonians (3.21) and (3.15) are both related to combination four.

For $I = 1$ the potential V_j is attractive, however in similar studies it has proven to be too weak to generate a bound state [12]. Since V_5 is repulsive for $I = 1$ we do not expect to find any bound states in this case.

In the case of $I = 0$ V_j is (weakly) repulsive and V_5 is attractive enough to generate a bound state when heavy spin effects are neglected [12, 11]. We therefore study for the rest of this thesis the $I = 0$ and $J = 1$ coupled channel equation. Since both B and B^* have negative parity the four quark system has positive parity.

3.3 Analytical considerations

Defining

$$W_1(r) := V_5(r) + V_j(r) + m_B + m_{B^*}, \quad (3.23)$$

$$W_1^*(r) := W_1(r) + m_{B^*} - m_B \quad (3.24)$$

and

$$W_2(r) := V_j(r) - V_5(r), \quad (3.25)$$

the $I = 0$ and $J = 1$ coupled channel equation can be written as

$$\left(-\frac{\hbar^2}{2m_b} (\Delta_1 + \Delta_2) \mathbb{1}_{2 \times 2} + \begin{pmatrix} W_1(r) & W_2(r) \\ W_2(r) & W_1^*(r) \end{pmatrix} \right) \tilde{\Psi}_{J=1,2 \times 2} = E \tilde{\Psi}_{J=1,2 \times 2}. \quad (3.26)$$

Ultimately, this equation will be solved numerically. It is, however, beneficial to get some analytical insights before attempting to do so. This is done by employing (and generalizing to the 2×2 case if necessary) some well known results from ordinary quantum mechanics [22, 23].

At first, we introduce center of mass and relative coordinates

$$\vec{r}_{CM} = \frac{m_b}{2} (\vec{r}_1 + \vec{r}_2), \quad (3.27)$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2. \quad (3.28)$$

This splits equation (3.26) into two independent equations. The eigenstates of the center of mass equation are simply free-particle eigenstates and do not influence the binding energy. The equation for the relative coordinates reads

$$\left(-\frac{\hbar^2}{2\mu} \Delta \mathbb{1}_{2 \times 2} + \begin{pmatrix} W_1(r) & W_2(r) \\ W_2(r) & W_1^*(r) \end{pmatrix} \right) \psi(\vec{r}) = E\psi(\vec{r}), \quad (3.29)$$

where $\mu = m_b/2$ denotes the reduced mass.

Utilizing spherical symmetry of the potentials we make the ansatz

$$\psi(\vec{r}) = \frac{\chi(r)}{r} = \frac{1}{r} \begin{pmatrix} \chi_1(r) \\ \chi_2(r) \end{pmatrix}, \quad (3.30)$$

for the ground state. This leads to the following ordinary differential equation for χ :

$$D\chi = E\chi, \quad (3.31)$$

where

$$D = \begin{pmatrix} -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + W_1(r) & W_2(r) \\ W_2(r) & -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + W_1^*(r) \end{pmatrix}. \quad (3.32)$$

3.3.1 Boundary conditions

Note that for a solution χ with real E the complex conjugate χ^* also is a solution with the same eigenvalue because

- the derivative commutes with complex conjugation,
- equation (3.31) is linear and
- the entries in D which are no differential operators are real.

If χ has both complex and imaginary part, χ and χ^* are linear independent and one can obtain two real, linear independent solutions with the same eigenvalue by

$$\tilde{\chi}^1 = \chi + \chi^*, \quad \tilde{\chi}^2 = i(\chi - \chi^*). \quad (3.33)$$

Furthermore, if χ is purely imaginary, then

$$\tilde{\chi} = -i\chi \quad (3.34)$$

is a real solution with the same eigenvalue. Therefore, one can restrict the solution space to purely real functions without loss of generality, which we will do henceforth.

Furthermore, we demand that D is hermitian with respect to the functions of the solution space.¹ This means that for two solutions $u = (u_1, u_2)$ and $v = (v_1, v_2)$ the following equation must hold:

$$\int_0^\infty \langle u, Dv \rangle dr = \int_0^\infty \langle Du, v \rangle dr, \quad (3.35)$$

¹We ignore some mathematical subtleties here, namely that there is an important distinction between a self-adjoint operator and a hermitian operator

where $\langle \cdot, \cdot \rangle$ denotes the usual scalar product on \mathbb{R}^2 .

Ignoring the differential operators in D the matrix is symmetric and therefore equation (3.35) implies (using partial integration):

$$(u_1 v_1' + u_2 v_2')|_0^\infty = (v_1 u_1' + v_2 u_2')|_0^\infty. \quad (3.36)$$

For the wave function to be normalizable the solutions will vanish for $r \rightarrow \infty$ so the condition we are left with is

$$u_1(0)v_1'(0) + u_2(0)v_2'(0) = v_1(0)u_1'(0) + v_2(0)u_2'(0). \quad (3.37)$$

To ensure this for arbitrary functions in the solution space we have to impose the following property on functions χ of the solution space:

$$(\chi_1(0) = 0 \vee \chi_1'(0) = 0) \wedge (\chi_2(0) = 0 \vee \chi_2'(0) = 0). \quad (3.38)$$

Now, if $\chi_1'(0) = 0$ and $\chi_1(0) = c \neq 0$ the asymptotic behaviour of χ_1 as $r \rightarrow 0$ is

$$\chi_1 \sim c. \quad (3.39)$$

This means that the first component of ψ behaves as

$$\psi_1 \sim \frac{c}{r} \quad (3.40)$$

which will result in a component proportional to $\delta(r)$ when Δ is applied. Since none of the potentials in equation (3.29) contains a delta function and the argumentation applies to χ_2 analogously the boundary conditions for χ are

$$\chi(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \chi(\infty) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (3.41)$$

3.3.2 Asymptotic behavior

Since $\chi(0) = 0$ it is not necessary for $\chi'(0)$ to be zero in order to fulfill equation (3.38). With a bit more work however, we can also derive values for $\chi'(0)$ or, in other words, the asymptotic behavior of solutions as $r \rightarrow 0$.

Note that equation (3.31) is an ODE with analytic coefficients that have a singularity for $r = 0$, we therefore make the ansatz

$$\chi_1(r) = r^{s_1} \sum_{k=0}^{\infty} a_k r^k, \quad a_0 \neq 0 \quad (3.42)$$

$$\chi_2(r) = r^{s_2} \sum_{k=0}^{\infty} b_k r^k, \quad b_0 \neq 0. \quad (3.43)$$

The potentials can be expanded in the following way:

$$\frac{2\mu}{\hbar} \cdot W_i^{(*)}(r) = r^{-1} \sum_{k=0}^{\infty} w_{i,k}^{(*)} r^k, \quad w_{i,0}^{(*)} \neq 0. \quad (3.44)$$

² $w_{1,k}^* = w_{1,k}$ for $k \neq 1$ and $w_{1,1}^* = w_{1,1} + m_{B^*} - m_B$ due to equation (3.24)

Inserting this into equation (3.31) leads to the equations

$$\begin{aligned}
 0 &= s_1 (s_1 - 1) a_0 r^{s_1-2} + \left(s_1^2 a_1 + a_0 w_{1,0} \right) r^{s_1-1} \\
 &+ r^{s_1} \sum_{k=0}^{\infty} \left\{ [k(k + s_1 + 3) + s_1(s_1 + 1) + 2] a_{k+2} - \sum_{n=0}^{k+1} a_n w_{1,k+1-n} + \varepsilon a_k \right\} r^k \\
 &+ r^{s_2-1} \sum_{k=0}^{\infty} \left(\sum_{n=0}^k b_n w_{2,k-n} \right) r^k,
 \end{aligned} \tag{3.45}$$

$$\begin{aligned}
 0 &= s_2 (s_2 - 1) b_0 r^{s_2-2} + \left(s_2^2 b_1 + b_0 w_{1,0}^* \right) r^{s_2-1} \\
 &+ r^{s_2} \sum_{k=0}^{\infty} \left\{ [k(k + s_2 + 3) + s_2(s_2 + 1) + 2] b_{k+2} - \sum_{n=0}^{k+1} b_n w_{1,k+1-n}^* + \varepsilon b_k \right\} r^k \\
 &+ r^{s_1-1} \sum_{k=0}^{\infty} \left(\sum_{n=0}^k a_n w_{2,k-n} \right) r^k,
 \end{aligned} \tag{3.46}$$

where $\varepsilon = \frac{2\mu}{\hbar} E$. These equations must be fulfilled simultaneously for all $r \in (0, \infty)$. There are now several possibilities:

1. $s_1 - 2 = s_2 + a$, where $a \in \{-1, 0\} \cup \mathbb{N}$,
2. case one with the roles of s_1 and s_2 interchanged and
3. none of the above.

In the first case, one has $s_2 = s_1 - 2 - a$ and equation (3.46) reads

$$\begin{aligned}
 0 &= (s_1 - 2 - a) (s_1 - 3 - a) b_0 r^{s_1-4-a} + \left((s_1 - 2 - a)^2 b_1 + b_0 w_{1,0}^* \right) r^{s_1-3-a} \\
 &+ r^{s_1-2-a} \sum_{k=0}^{\infty} \left\{ [k(k + s_1 + 1 - a) + (s_1 - 2 - a)(s_1 - 1 - a) + 2] b_{k+2} \right. \\
 &- \left. \sum_{n=0}^{k+1} b_n w_{1,k+1-n}^* + \varepsilon b_k \right\} r^k \\
 &+ r^{s_1-1} \sum_{k=0}^{\infty} \left(\sum_{n=0}^k a_n w_{2,k-n} \right) r^k.
 \end{aligned} \tag{3.47}$$

Since $4 + a \geq 3$ and the coefficients multiplied by different powers of r must vanish independently we can infer that $s_1 = 2 + a$ or $s_1 = 3 + a$ in this case (note that $b_0 \neq 0$). The former means $s_2 = 0$, which is against the boundary conditions. One therefore is left with

$s_1 = 3 + a$ and $s_2 = 1$. Inserting this into equation (3.45) results in

$$\begin{aligned}
 0 = & \sum_{k=0}^{2+a} \left(\sum_{n=0}^k b_n w_{2,k-n} \right) r^k \\
 & + (3+a)(2+a) a_0 r^{1+a} + \left((3+a)^2 a_1 + a_0 w_{1,0} \right) r^{2+a} \\
 & + r^{3+a} \sum_{k=0}^{\infty} \left\{ [k(k+6+a) + (3+a)(4+a) + 2] a_{k+2} - \sum_{n=0}^{k+1} a_n w_{1,k+1-n} + \varepsilon a_k \right\} r^k \\
 & + r^{3+a} \sum_{k=0}^{\infty} \left(\sum_{n=0}^{k+3+a} b_n w_{2,k+3+a-n} \right) r^k,
 \end{aligned} \tag{3.48}$$

which implies that if $1 + a > 0$ then $b_0 = 0$, because $w_{2,0} \neq 0$. Since $b_0 \neq 0$ by construction, we are left with the possibility that $a = -1$. Looking at equation (3.48) this means that $b_0 w_{2,0} + 2a_0 = 0$. This implies that b_0 is determined by a_0 and hence that there are not enough parameters to enforce the boundary conditions for *both* χ_1 and χ_2 as $r \rightarrow \infty$. Therefore we can conclude that case 1 is not possible and case 2 can be disregarded using the same argumentation. Case 3 directly implies that $s_1 = s_2 = 1$ ($s_i = 0$ violates the boundary conditions) and therefore the solutions behave linear approaching 0:

$$\chi(r) \sim \begin{pmatrix} Ar \\ Br \end{pmatrix} \text{ as } r \rightarrow 0. \tag{3.49}$$

3.4 Numerical solution

One possibility to solve equation (3.31) numerically is to employ the shooting method. To this end, one integrates equation (3.31) using e.g. the Runge-Kutta-Fehlberg method starting with the correct asymptotic behavior (3.49) at tiny $r = \varepsilon > 0$ ³ to $r = r_{\max}$ with sufficiently large $r_{\max} \gtrsim 10 fm$. This integration is used as an input for a multidimensional root solver to find parameters A/B ⁴ and E such that also $\chi_1(r_{\max}) = \chi_2(r_{\max}) = 0$ is fulfilled. Multidimensional root finding is in general much harder than the one dimensional case, where global convergence can be ensured. In fact, all multidimensional root finding algorithms from [24] fail to converge for our problem even when very good initial guesses are provided. We therefore present a method which reduces the problem of finding the energy E to a one dimensional problem.⁵

To this end, let χ^1 and χ^2 denote the solutions to equation (3.31) with the asymptotic behavior (note that one cannot expect these solutions to fulfill the boundary conditions at

³The potentials have a singularity for $r = 0$.

⁴Normalization can be ensured afterwards.

⁵It will be apparent that this method does not only work for the two dimensional case but also for arbitrary dimensions. To minimize notational clutter we concentrate on the two dimensional case. Also, the method described in the next section to determine A and B *only* works in the two dimensional case.

r_{max}):

$$\chi^1(r) \sim \begin{pmatrix} r \\ 0 \end{pmatrix} \text{ as } r \rightarrow 0 \text{ and} \quad (3.50)$$

$$\chi^2(r) \sim \begin{pmatrix} 0 \\ r \end{pmatrix} \text{ as } r \rightarrow 0. \quad (3.51)$$

Due to the linearity of the Schrödinger equation $\chi := A\chi^1 + B\chi^2$ also solves equation (3.31). This solution has the asymptotic behavior

$$\chi(r) \sim \begin{pmatrix} Ar \\ Br \end{pmatrix} \text{ as } r \rightarrow 0. \quad (3.52)$$

We are interested in energies such that A and B can be chosen to ensure $\chi(r_{max}) = 0$, or, in other words that

$$\chi(r_{max}) = A\chi^1(r_{max}) + B\chi^2(r_{max}) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (3.53)$$

has a nontrivial solution. This is possible if and only if

$$\det(\chi^1(r_{max}), \chi^2(r_{max})) = 0. \quad (3.54)$$

Therefore, it is enough to vary only E until equation (3.54) is fulfilled in order to find eigenvalues for equation (3.31). To determine A/B one then solves the homogeneous linear system equation (3.53).

Numerical Caveats

Even when E is determined to very high precision ($\Delta E \lesssim 10^{-9}$) χ^1 and χ^2 become so unstable beyond the classical turning point that equation (3.54) is never actually fulfilled even approximately. Therefore, in practice, A/B can not be determined by solving a linear system.

To circumvent this, after determining E one uses one dimensional root finding to find A/B such that $\chi_1(r_{max}) = 0$ is fulfilled and repeats the same procedure for χ_2 .⁶ If E has been determined with sufficient precision the two values for A/B obtained using this method are the same within error margins.

⁶Note that the lower indices mean we are talking about the first and second component of χ and not about the solutions with the asymptotic behavior (3.50)

Chapter 4

Results

4.1 Fitting procedure and results

To describe the lattice potentials $V^{\text{lat}}(r)$ by continuous functions we use the strategy explained in [11], details on this method to estimate the statistical error can be found in [25]. We perform uncorrelated χ^2 minimizing fits of equation (1.3). To this end we minimize

$$\chi^2 = \sum_{r=r_{\min}, \dots, r_{\max}} \left(\frac{V(r) - V^{\text{lat}}(r)}{\Delta V^{\text{lat}}(r)} \right)^2 \quad (4.1)$$

with respect to the parameters α , d , and V_0 while keeping $p = 2$ fixed. Since V_0 is discarded afterwards (see section 2.4) we will ignore it for the rest of the discussion. ΔV^{lat} denote the statistical errors obtained by the Jackknife resampling process described in [12].

These fits are performed only for V_5 in the isosinglet channel. The channel for V_j is strongly screened and consistent with $V^{\text{lat}} = 0$ for $r > 2a$. Therefore it is not possible to perform a stable fit for V_j . We will discuss in 4.2 how to deal with this problem.

To estimate the systematic errors for V_5 we perform a large number of fits where the following parameters are varied:

- The range of the temporal separations $t_{\min} \leq t \leq t_{\max}$ that are included when $V^{\text{lat}}(r)$ is obtained from $C(t, r)$. They are varied over the parameter area $4a \leq t_{\min} < t_{\max} \leq 9a$. If t_{\min} is chosen small this might lead to a contamination by excited states, for large t_{\min} and t_{\max} the statistical error increase significantly.
- The minimal and maximal distances between the \bar{b} quarks r_{\max} that are included for the χ^2 minimizing fit. We choose $r_{\min} \in \{2a, 3a\}$ and $r_{\max} \in \{8a, 9a, 10a\}$. Smaller separation than $2a$ are avoided since $V^{\text{lat}}(r)$ are expected to suffer from substantial lattice discretization errors for $r < 2a$.

By weighting each of the resulting fit parameters α_5 and d_5 by $\exp(-\chi^2/\text{dof})$ a distribution for these values is constructed. The central values for α_5 and d_5 are then defined as the medians of the distributions and the difference of the 16th/84th percentile to the medians give the lower/upper systematic uncertainties. To combine the systematic errors with the statistical errors the jackknife errors of the medians are added in quadrature. This results in

$$\alpha_5 = 0.35_{-0.04}^{+0.05}, \quad (4.2a)$$

$$d_5 = 0.42_{-0.08}^{+0.08} \text{ fm}. \quad (4.2b)$$

The fit function (1.3) with these parameters can be seen in Figure 4.1.

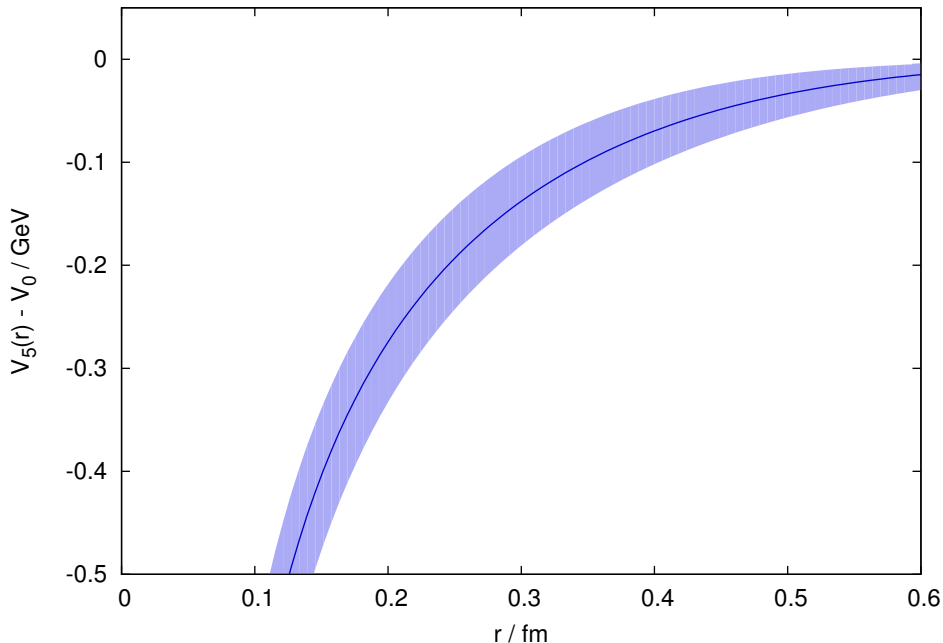


Figure 4.1: Parametrization of the $\bar{b}\bar{b}$ potential V_5 in the isosinglet channel. Fit function (1.3) with the parameters (4.2).

4.2 Energy of the four quark system

The energy of the system is given by the eigenvalue of equation (3.31). A bound state is found if $E < m_B + m_B^*$ and the binding energy in this case is $E_{\text{bind}} = m_B + m_B^* - E$.

To be able to compute the energy we first have to discuss the values of the fit parameters for V_j , which could not be determined in the previous section. The short range behavior of the potentials is expected to be dominated by the interaction of the \bar{b} quarks. In the attractive case (V_5) they are expected to form a color triplet and in the repulsive case (V_j) a color sextet. For both these multiplets one can compute the associated potentials in leading order perturbation theory, which leads to:

$$V^{\text{trip}}(r) = -\frac{2\alpha_s}{3}r \quad (4.3)$$

$$V^{\text{sext}}(r) = \frac{\alpha_s}{3}r, \quad (4.4)$$

where α_s denotes the coupling constant. This suggests the estimate $\alpha_j = \alpha_5/2$ and $d_j = d_5$.

Since this is a rough estimate only we will use the following strategy to gauge the influence of α_j and d_j on the energy: denoting the central values for α_5 and d_5 from (4.2) by $\alpha_{5,c}$ and $d_{5,c}$ we make the following choices for α_j and d_j , which are consistent with the lattice data:

$$\alpha_j \in \{0, \alpha_{5,c}/4, \alpha_{5,c}/2\} \quad \text{and} \quad (4.5a)$$

$$d_j \in \{d_{5,c}/4, d_{5,c}/2, d_{5,c}\}. \quad (4.5b)$$

For each of these choices the energy for all fits from section 4.1 is computed, constructing a distribution for the energy this way. The resulting distributions can then be compared for the different values of α_j and d_j .

For $\alpha_j = 0$ the repulsive potential vanishes, this should lead to the largest binding energy. Even in this case, however, one runs into the problem that some fits lead to no binding at all.

Specifically, this happens for the fits with $t_{\min} = 8a$ and $t_{\max} = 9a$. These fit have the common feature that d_5 is relatively small, which results in a shorter range of the potential. To get a better understanding of the situation, see Figure 4.2, where effective masses $m_{\text{eff}}(t, r) = \frac{1}{a} \log \left(\frac{C(t, r)}{C(t+a, r)} \right)$ are shown which are used to extract the potential V_5 .

As one can see, the statistical errors are significantly higher for $t_{\min} = 8$ and $t_{\max} = 9$ compared to the case where $t_{\min} = 5$ and $t_{\max} = 8$. Also the difference between $m_{\text{eff}}(t_{\min}, r)$ and $m_{\text{eff}}(t_{\max}, r)$ is much larger in the former case, for a sensible extraction of the potential, however, $V(r)$ should be read off from a plateau of m_{eff} . On the other hand, one can argue that these differences (especially when $m_{\text{eff}}(t_{\max}, r)$ is smaller) indicate, that the plateau for $t_{\min} = 5a$ and $t_{\max} = 8a$ is contaminated with excited states. This however should mainly influence V_0 , which is discarded anyway.

We therefore pursue the strategy that has been explained above without using the fits with $t_{\min} = 8a$ and $t_{\max} = 9a$, keeping, however, in mind that the reasoning to exclude them is heuristic only. For $\alpha_j = \alpha_{5,c}/2$ and $d_j = d_5$ the resulting binding energy is

$$E_{\text{bind}} = 59_{-42}^{+39} \text{ MeV} \quad (4.6)$$

and in all other cases from (4.5)

$$E_{\text{bind}} = 60_{-41}^{+39} \text{ MeV}. \quad (4.7)$$

This shows that α_j and d_j only have little influence on the binding energy (about 1 – 2 MeV) and that the confidence level for this $ud\bar{b}\bar{b}$ tetraquark state is around 1.5σ (with the caveat that we had to exclude some fits).

A plot of the wave function χ and the associated radial probability density $|\chi_1|^2 + |\chi_2|^2$ for a specific choice for the parameters of V_5 and V_j can be seen in Figure 4.3.

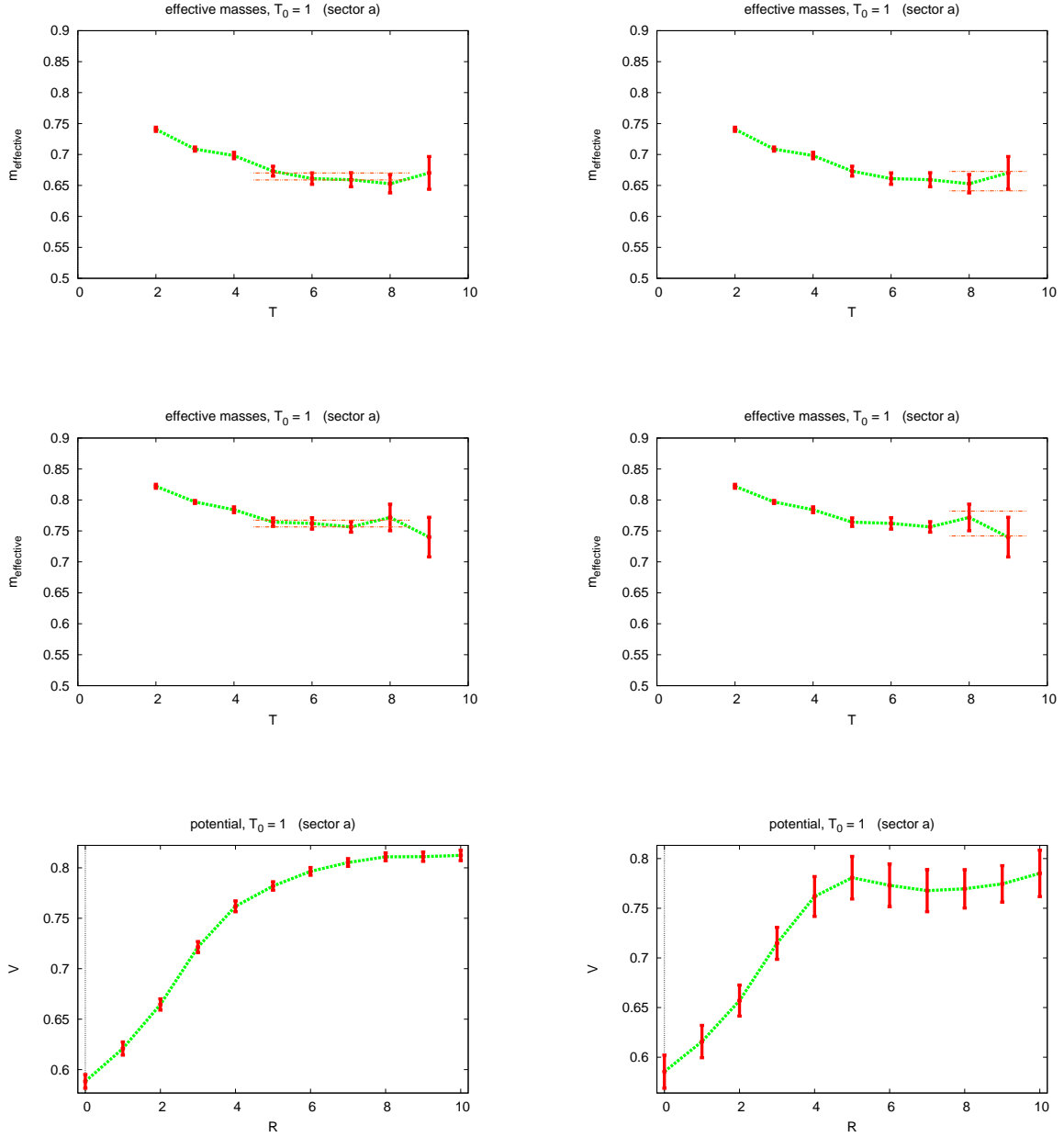


Figure 4.2: Effective masses and the resulting potential V_5 . In the first line the spatial separation of the \bar{b} quarks is $r = 2a$, in the second line $r = 4a$. On the left side $t_{\min} = 5a$ and $t_{\max} = 8a$, on the right side $t_{\min} = 8a$ and $t_{\max} = 9a$.

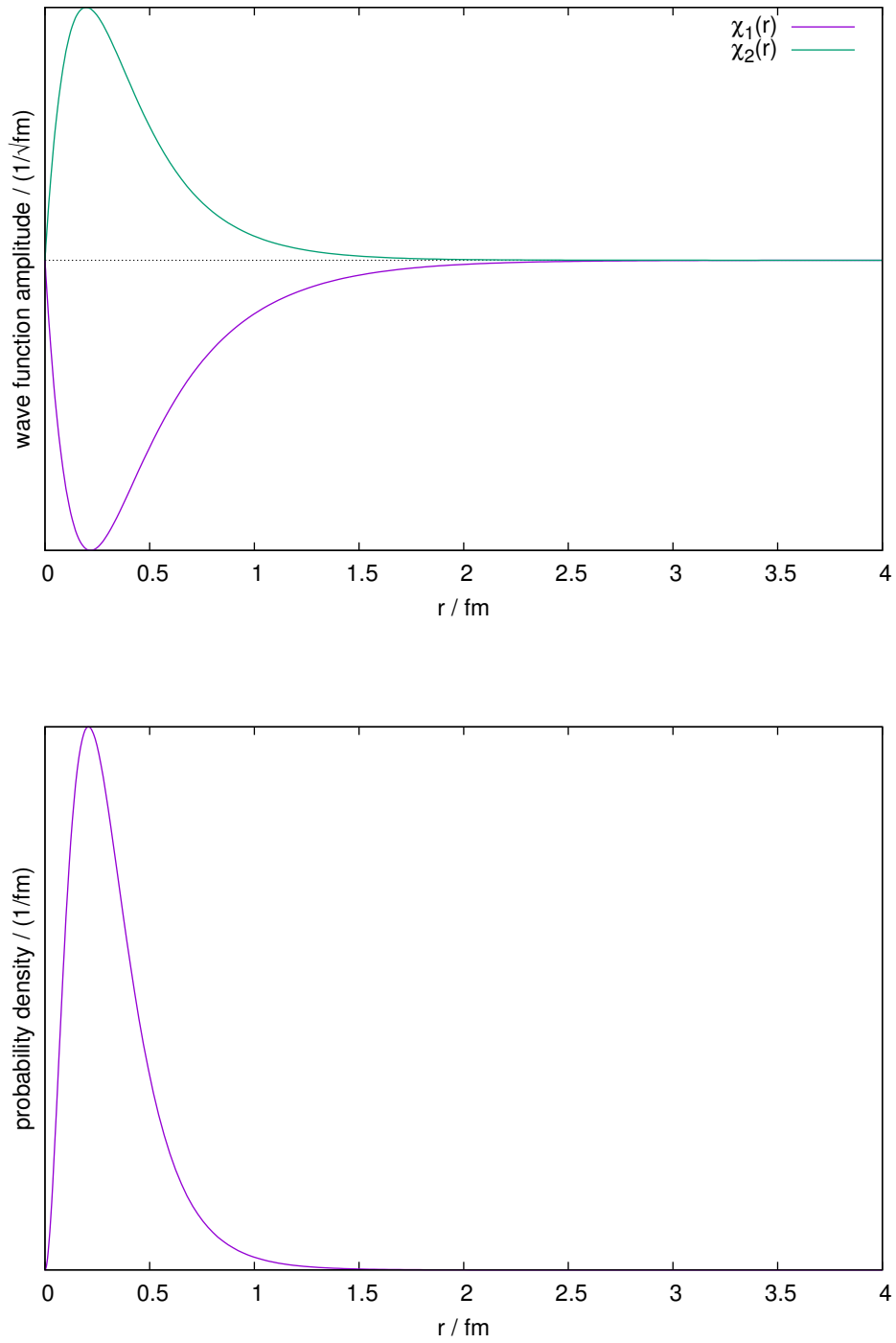


Figure 4.3: Wave function χ and probability density to find the \bar{b} quarks at separation r . For the potentials V_5 and V_j the values (cf. equation (4.2)) $\alpha_5 = 0.35$, $d_5 = 0.42$ fm, $\alpha_j = \alpha_5/2$ and $d_j = d_5$ were chosen. The resulting binding energy is 51 Mev.

4.3 Further sources of systematic errors

As indicated in [12] and [11] there are additional sources of systematic errors:

- The light u/d quarks are unphysically heavy in the lattice computations, corresponding to a pion mass of $m_\pi \approx 340$ MeV. Lighter masses for these quarks should enhance the binding since they lead to $B^{(*)}$ mesons with larger radii and therefore reduce screening.
- The lattice results are not precise enough to resolve light meson exchange resulting in long range interactions. Furthermore these interactions are suppressed due to the unphysically heavy u/d quarks. Resolving this should also lead to larger binding energy.
- Finite volume effects are expected to be suppressed exponentially. This suppression can be estimated by $\exp(-m_\pi L)$, where L is the periodic spatial volume of the lattice. In practice, even for simple quantities where statistical errors are much smaller than for our calculations, $m_\pi \gtrsim 3 \dots 4$ is usually sufficient for the finite volume effects to be negligible compared to the statistical errors. Since $m_\pi L = 3.3$ in our case, finite volume effects are expected not to influence the result significantly. Furthermore, Figure 4.3 indicates that the spatial extension of the lattice $L \approx 1.9$ fm is large enough to resolve a tetraquark state.
- The mass difference between B and B^* which is due to spin interactions between the heavy and light quark has been taken into account. The spin interactions between the \bar{b} quarks however have still been neglected. Since they are of the order $1/m_b^2$ in quark models they presumably have little influence on the result.

Chapter 5

Conclusion and Outlook

Comparing our results to the binding energies obtained in [11] shows that the inclusion of heavy spin effects weakens the binding energy. Nevertheless we still have found indications for a tetraquark state with $I(J^P) = 0(1^+)$.

In the near future we are planning to extrapolate to physical u/d quark masses. Preliminary results confirm the expectation from section 4.3 that this should enhance binding. Furthermore, it would be interesting to not only study bound states but also resonances. Finally, once these investigations are finished for the $qq\bar{b}\bar{b}$ systems they can be extended to $q\bar{q}b\bar{b}$ systems, which are more interesting from an experimental standpoint, especially in light of the observations by the BELLE collaboration [2].

Appendix A

Gamma matrices

We use the conventions of [26], the Euclidean gamma matrices γ_μ , $\mu = 1, 2, 3, 4$ obey

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}\mathbf{1}. \quad (\text{A.1})$$

If we define γ_5 to be

$$\gamma_5 = \prod_{\mu=1}^4 \gamma_\mu, \quad (\text{A.2})$$

then equation (A.1) is extended to the cases where μ or ν are equal to five.

Throughout this thesis the chiral representation is employed. In this representation the Euclidean gamma matrices have the following explicit form

$$\gamma_{1,2,3} = \begin{pmatrix} 0 & -i\sigma_{1,2,3} \\ i\sigma_{1,2,3} & 0 \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} 0 & \mathbf{1}_{2 \times 2} \\ \mathbf{1}_{2 \times 2} & 0 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} \mathbf{1}_{2 \times 2} & 0 \\ 0 & \mathbf{1}_{2 \times 2} \end{pmatrix}, \quad (\text{A.3})$$

and fulfill in addition to equation (A.1)

$$\gamma_\mu = \gamma_\mu^\dagger = \gamma_\mu^{-1}. \quad (\text{A.4})$$

The defining equations for the charge conjugation Matrix \mathcal{C} are

$$\mathcal{C}\gamma_\mu\mathcal{C}^{-1} = -\gamma_\mu^T, \quad \mu = 1, 2, 3, 4, \quad (\text{A.5})$$

which implies that in the chiral representation \mathcal{C} is given (up to a phase factor) by

$$\mathcal{C} = i\gamma_2\gamma_4. \quad (\text{A.6})$$

Bibliography

- [1] K. A. Olive et al. “Review of Particle Physics”. In: *Chin. Phys.* C38 (2014), p. 090001. DOI: 10.1088/1674-1137/38/9/090001.
- [2] A. Bondar et al. “Observation of two charged bottomonium-like resonances in $Y(5S)$ decays”. In: *Phys. Rev. Lett.* 108 (2012), p. 122001. DOI: 10.1103/PhysRevLett.108.122001. arXiv: 1110.2251 [hep-ex].
- [3] Z. Q. Liu et al. “Study of $e^+e^- \rightarrow \pi^+\pi^- J/\psi$ and Observation of a Charged Charmoniumlike State at Belle”. In: *Phys. Rev. Lett.* 110 (2013), p. 252002. DOI: 10.1103/PhysRevLett.110.252002. arXiv: 1304.0121 [hep-ex].
- [4] K. Chilikin et al. “Observation of a new charged charmoniumlike state in $\bar{B}^0 \rightarrow J/\psi K^- \pi^+$ decays”. In: *Phys. Rev.* D90.11 (2014), p. 112009. DOI: 10.1103/PhysRevD.90.112009. arXiv: 1408.6457 [hep-ex].
- [5] T. Xiao et al. “Observation of the Charged Hadron $Z_c^\pm(3900)$ and Evidence for the Neutral $Z_c^0(3900)$ in $e^+e^- \rightarrow \pi\pi J/\psi$ at $\sqrt{s} = 4170$ MeV”. In: *Phys. Lett.* B727 (2013), pp. 366–370. DOI: 10.1016/j.physletb.2013.10.041. arXiv: 1304.3036 [hep-ex].
- [6] M. Ablikim et al. “Observation of a Charged Charmoniumlike Structure in $e^+e^- \rightarrow \pi^+\pi^- J/\psi$ at $\sqrt{s} = 4.26$ GeV”. In: *Phys. Rev. Lett.* 110 (2013), p. 252001. DOI: 10.1103/PhysRevLett.110.252001. arXiv: 1303.5949 [hep-ex].
- [7] M. Ablikim et al. “Observation of a charged charmoniumlike structure in $e^+e^- \rightarrow (D^* \bar{D}^*)^\pm \pi^\mp$ at $\sqrt{s} = 4.26$ GeV”. In: *Phys. Rev. Lett.* 112.13 (2014), p. 132001. DOI: 10.1103/PhysRevLett.112.132001. arXiv: 1308.2760 [hep-ex].
- [8] M. Ablikim et al. “Observation of a Charged Charmoniumlike Structure $Z_c(4020)$ and Search for the $Z_c(3900)$ in $e^+e^- \rightarrow \pi^+\pi^- h_c$ ”. In: *Phys. Rev. Lett.* 111.24 (2013), p. 242001. DOI: 10.1103/PhysRevLett.111.242001. arXiv: 1309.1896 [hep-ex].
- [9] M. Ablikim et al. “Observation of a charged $(D\bar{D}^*)^\pm$ mass peak in $e^+e^- \rightarrow \pi D\bar{D}^*$ at $\sqrt{s} = 4.26$ GeV”. In: *Phys. Rev. Lett.* 112.2 (2014), p. 022001. DOI: 10.1103/PhysRevLett.112.022001. arXiv: 1310.1163 [hep-ex].
- [10] M. Ablikim et al. “Observation of $e^+e^- \rightarrow \pi^0\pi^0 h_c$ and a Neutral Charmoniumlike Structure $Z_c(4020)^0$ ”. In: *Phys. Rev. Lett.* 113.21 (2014), p. 212002. DOI: 10.1103/PhysRevLett.113.212002. arXiv: 1409.6577 [hep-ex].
- [11] Pedro Bicudo et al. “Evidence for the existence of $ud\bar{b}\bar{b}$ and the non-existence of $ss\bar{b}\bar{b}$ and $cc\bar{b}\bar{b}$ tetraquarks from lattice QCD”. In: *Phys. Rev.* D92.1 (2015), p. 014507. DOI: 10.1103/PhysRevD.92.014507. arXiv: 1505.00613 [hep-lat].

- [12] Pedro Bicudo and Marc Wagner. “Lattice QCD signal for a bottom-bottom tetraquark”. In: *Phys. Rev. D* 87.11 (2013), p. 114511. DOI: 10.1103/PhysRevD.87.114511. arXiv: 1209.6274 [hep-ph].
- [13] M. Born and R. Oppenheimer. “Zur Quantentheorie der Molekeln”. In: *Annalen der Physik* 389.20 (1927), pp. 457–484. ISSN: 1521-3889. DOI: 10.1002/andp.19273892002. URL: <http://dx.doi.org/10.1002/andp.19273892002>.
- [14] Marc Wagner. “Forces between static-light mesons”. In: *PoS LATTICE2010* (2010), p. 162. arXiv: 1008.1538 [hep-lat].
- [15] Marc Wagner. “Static-static-light-light tetraquarks in lattice QCD”. In: *Acta Phys. Polon. Supp.* 4 (2011), pp. 747–752. DOI: 10.5506/APhysPolBSupp.4.747. arXiv: 1103.5147 [hep-lat].
- [16] Yoshiaki Koma and Miho Koma. “Spin-dependent potentials from lattice QCD”. In: *Nucl. Phys. B* 769 (2007), pp. 79–107. DOI: 10.1016/j.nuclphysb.2007.01.033. arXiv: hep-lat/0609078 [hep-lat].
- [17] Yoshiaki Koma, Miho Koma, and Hartmut Wittig. “Nonperturbative determination of the QCD potential at $O(1/m)$ ”. In: *Phys. Rev. Lett.* 97 (2006), p. 122003. DOI: 10.1103/PhysRevLett.97.122003. arXiv: hep-lat/0607009 [hep-lat].
- [18] Annabelle Uenver. “Lattice study of possibly existing tetraquarks”. MA thesis. Goethe university Frankfurt, 2014.
- [19] Maxima. *Maxima, a Computer Algebra System. Version 5.30.0*. 2014. URL: <http://maxima.sourceforge.net/>.
- [20] Stephen Godfrey and Nathan Isgur. “Mesons in a relativized quark model with chromodynamics”. In: *Phys. Rev. D* 32 (1 July 1985), pp. 189–231. DOI: 10.1103/PhysRevD.32.189. URL: <http://link.aps.org/doi/10.1103/PhysRevD.32.189>.
- [21] Dimitrij A. Varšalovič, Anatolij N. Moskalev, and Valerij K. Chersonskij. *Quantum theory of angular momentum : irreducible tensors, spherical harmonics, vector coupling coefficients, 3nj symbols*. Singapore [u.a.]: World Scientific Publ., 1988. ISBN: 9971509962.
- [22] Ramamurti Shankar. *Principles of quantum mechanics*. New York, NY: Plenum, 1980. URL: <https://cds.cern.ch/record/102017>.
- [23] Norbert Straumann. *Quantenmechanik. Ein Grundkurs über nichtrelativistische Quantentheorie*. 2nd ed. Springer-Verlag Berlin Heidelberg, 2013. 450 pp. ISBN: 978-3-642-32174-0. DOI: 10.1007/978-3-642-32175-7.
- [24] Brian Gough. *GNU Scientific Library Reference Manual - Third Edition*. 3rd. Network Theory Ltd., 2009. ISBN: 0954612078, 9780954612078.
- [25] Krzysztof Cichy et al. “Overlap valence quarks on a twisted mass sea: a case study for mixed action Lattice QCD”. In: *Nucl. Phys. B* 869 (2013), pp. 131–163. DOI: 10.1016/j.nuclphysb.2012.12.011. arXiv: 1211.1605 [hep-lat].
- [26] Christof Gattringer and Christian B. Lang. “Quantum chromodynamics on the lattice”. In: *Lect. Notes Phys.* 788 (2010), pp. 1–343. DOI: 10.1007/978-3-642-01850-3.

Acknowledgement

I want to thank Prof. Marc Wagner for his great supervision. His constant willingness to discuss problems and possible solutions was of great help. Furthermore I want to thank him for providing me the opportunity to visit the conference Excited QCD 2015, which was a great experience.

Next, I want to thank Prof. Pedro Bicudo for useful discussions during his stays in Frankfurt, especially for introducing me to the method to numerically solve the coupled channel equation as it is explained in section 3.4.

Finally, I thank Antje Peters for providing me with the fit results that have been used in chapter 4.