Decoding the double heavy tetraquark state $T_{cc}^+$

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We analyse the deuteron-like $T_{cc}^+$ state observed by the LHCb Collaboration from the perspective of the quark clustering. The $T_{cc}^+$ state implies the possible existence of other compact doubly heavy tetraquark states.

Recently, the LHCb Collaboration reported the doubly charmed state $T_{cc}^+$ with $J^P = 0^+$ in the $D^0 \bar{D}^0 \pi^+$ invariant mass spectrum [1]. Its extremely small binding energy and width can match very well with the prediction of the $DD^*$ molecular state [2, 3]. The deuteron-like molecule configuration is manifest from its characteristic size. The discovery of the $T_{cc}^+$ is a great breakthrough in hadron physics after the state $\Xi_{cc}^+$, which provides an excellent platform to investigate the low energy strong interactions.

Inspired by the $T_{cc}^+$, we employed the quark model to systematically investigate the double heavy tetraquark states with the molecule configuration [4]. We extracted the binding energy of the $T_{cc}^+$ to be 0.34 MeV, which agrees with LHCb’s measurement very well. The $T_{cc}^+$ is a loosely bound deuteron-like state with a huge size around 4.32 fm. The long-range $\pi$ and intermediate-range $\sigma$ exchange interactions and coupled channel effect play a pivotal role. In the molecule configuration $[bq\bar{q}]_1 [b\bar{q}]_1$, the $T_{bb}$ state with $0^+$ is sensitive to different dynamical effects and may have three different physical pictures: the compact state, deuteron-like state, or hydrogen molecule-like state. Their binding energies are less than 50 MeV and qualitatively consistent with the latest lattice QCD predictions [5].

Prior to the $T_{cc}^+$, many theoretical explorations have focused on the stability of the doubly heavy tetraquark states since the pioneering work [6]. The $T_{bb}$ state with $0^+$ was widely accepted as the most promising stable doubly heavy tetraquark state with a binding energy around $-200$ MeV relative to the $BB^*$ threshold [7]. However, the energy of the $T_{cc}^+$ with $0^+$ hovers over the $DD^*$ threshold in the range of 300 MeV. Its stability is highly model dependent.

In the nonrelativistic quark models, the diquark configuration $[QQ][\bar{q}\bar{q}]$ ($Q = c$ and $b$, $q = u$ and $d$) is apt to yield a deep compact bound state while the molecule configuration $[Qq][\bar{Q}\bar{q}]$ is prone to produce a shallow bound state. One can consult the latest review on the doubly heavy tetraquark states [8, 9]. In this work, we attempt to decode the underlying mechanism of these two obviously different physical pictures from the perspective of the quark clustering.

Gell-Mann first proposed the possibility of the diquark in his pioneering work in 1964 [10]. It seems that there exists some phenomenological evidence of the relevance of the diquarks in hadron physics [11, 12]. We want to emphasize that the diquark is not a point-like fundamental object as the quark. Throughout this work, we use the diquark to denote the possible quark clustering and correlations. In fact, the diquark is a spatially extended object with various color-flavor-spin-space configurations. The substructure of the diquarks may affect the structure of the multiquark states.

We define the color quantum number $c = 0$ and $c = 1$ for the diquark in the color 3 and 6 representation respectively. For the heavy diquark $[QQ]$, its spin $s$, isospin $i$, orbit angular excitation $l$, and color $c$ should satisfy the constraint $s + i + l + c = odd$ due to the Pauli principle. The $S$-wave diquark $[QQ]_3$ must be spin triplet. Its Coulomb interaction is strongly attractive because the large mass of the heavy quarks decreases the kinetic energy and allows them to approach each other. The heavier the heavy quark, the stronger the Coulomb interaction. Its color-magnetic interaction is weakly repulsive because it is suppressed by the heavy quark mass. Thus, the $S$-wave diquark $[QQ]_3$ is favored.

The $S$-wave diquark $[QQ]_6$ must be spin singlet. Both the color-magnetic interaction and Coulomb interaction are repulsive so that this type of the heavy diquark is disfavored. However, the diquark-antidiquark configuration $[QQ]\bar{QQ}_{[6]}$ is predominant in the fully-heavy tetraquark ground states due to the strong Coulomb attraction and confinement potential between the two color sextet subclusters [14]. For the excited diquarks $[QQ]_{[3]}$ and $[QQ]_{[6]}$, their color-magnetic interaction is weak. The Coulomb interaction decreases because they are spatially more extended. The orbital excitation tends to increase the kinetic energy. Thus, the excited diquarks are heavier than the $S$-wave diquark.

For the light diquark $[qq]$, the situation is opposite to that of the heavy diquark $[QQ]$ because of the obvious mass difference. The color-magnetic interaction tends to prevail over the Coulomb interaction in the diquark $[qq]$. Its spin $s$, isospin $i$, orbit angular excitation $l$, and color $c$ obey the constraint $s + i + l + c = even$. The $S$-wave diquark $[qq]$ has four possible spin-isospin-color combinations. The spin singlet, isospin singlet and color triplet diquark is often called the good diquark, which is simultaneously favored by the Coulomb interaction, color-magnetic interaction as well as the one-pion-exchange interaction. Other combinations are sometimes called bad
diquarks. A good diquark $[qq]_3$ and a good anti-diquark $\bar{q}q[3]$ generally do not form a stable tetraquark state because of the low mass threshold of two light pseudoscalar mesons.

A good diquark $[Q\bar{Q}]_3$ and a good antidiquark $[\bar{q}q]\bar{3}$ are an optimal combination to produce a possible stable tetraquark state with $0^+$. The Coulomb interaction in the diquark $[QQ]_3$ alone can ensure that the doubly heavy tetraquark lies below the threshold of two $Q\bar{q}$ mesons if the mass ratio of $M_{Q\bar{Q}}$ and $m_q$ exceeds a critical value. In the limit of the very large $M_{Q\bar{Q}}$, the diquark $[QQ]_3$ shrinks into a tiny and compact core because of the strong Coulomb interaction while the light quarks move around the $QQ$-core. The doubly heavy tetraquark states look like a helium-like QCD-atom. Moreover, the color-magnetic interaction and pseudoscalar meson exchange force are also very strong if one takes chiral symmetry into account in the good antiquark $\bar{q}q\bar{3}$. To some extent, the good antidiquark $[\bar{q}q]\bar{3}$ plays the similar role of the electron pair in the hydrogen molecule, where the two electrons are in spin singlet and form a $\sigma$-bond. Furthermore, the above two binding mechanisms are independent and do not occur in the threshold of two $Q\bar{q}$ mesons, which is beneficial to produce the compact tetraquark states with $0^+$.

The doubly heavy tetraquark states have two completely equivalent color configurations $13$: \{12 $\otimes$ 134, 8_{12} $\otimes$ 8_{34}\} for $[Q_1\bar{q}_2][Q_3\bar{q}_4]$ and \{3_{13} $\otimes$ 3_{24}, 6_{13} $\otimes$ 6_{24}\} for $[Q_1Q_3][\bar{q}q\bar{4}]$, where the subscript represents the quark index. For the tetraquark states with $0^+$, their spin configurations are also equivalent $12$: \{12 $\otimes$ 134, 112 $\otimes$ 0_{34}, 0_{12} $\otimes$ 134\} and \{113 $\otimes$ 124, 113 $\otimes$ 0_{24}, 0_{13} $\otimes$ 124\}. For the orbital space, one can define the relative coordinates $r_{ij}$ and $r_{i,j,k,l}$ as

$$r_{ij} = r_i - r_j, \quad r_{i,j,k} = \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2} - \frac{m_3 r_3 + m_4 r_4}{m_3 + m_4},$$

where $\{r_{12}, r_{34}, r_{12,34}\}$ and $\{r_{13}, r_{24}, r_{13,24}\}$ are the Jacobi coordinates of the molecule configuration and the diquark configuration, respectively. They can reciprocally transform into each other through a unitary matrix depending on the quark masses.

To obtain the diquark-antidiquark components in the molecular ground state $[Q_1\bar{q}_2][Q_3\bar{q}_4]$, one can express the orbit wave function $\phi(r_{12}, r_{34}, r_{12,34})$ in terms of the explicit diquark configuration, namely $\phi(r_{12}, r_{34}, r_{12,34}) = \phi'(r_{13}, r_{24}, r_{13,24})$. We adopt the Gaussian function as the orbit trial wave function. The coordinate-related parts can be expressed as

$$e^{-\nu r_{12} - \nu r_{34} - \nu r_{12,34} - \nu r_{24}} e^{-a r_{13} - b r_{13,24} - c r_{13,24}} \chi e^{-d r_{24} - e r_{24} - f r_{24} - g r_{24} - h r_{13,24}},$$

in which the coefficients $a$-$f$ depend on the variational parameters $\nu$ and the elements of the transformation matrix from $\{r_{12}, r_{34}, r_{12,34}\}$ to $\{r_{13}, r_{24}, r_{13,24}\}$. With the cumbersome angular momentum algebra $13$, one can show that the wave function $\phi'(r_{13}, r_{24}, r_{13,24})$ includes all possible relative orbital angular momenta $l_{13}, l_{24}$ and $l_{13,24}$ associated with the relative motions $r_{13}, r_{24},$ and $r_{13,24}$, respectively, which should satisfy $l_{13} + l_{24} + l_{13,24} = 0$ or 2 and $l_{13} + l_{24} + l_{13,24} = \text{even}$ due to the parity conservation. The details of the wave function can be found in the supplemental materials at the bottom of this paper. After accomplishing the above procedures, the diquark $[Q_1Q_3]$ and the antidiquark $[\bar{q}q\bar{4}]$ are either symmetric or antisymmetric. Then, one can apply the Pauli principle to two pairs of identical quarks, and naturally arrive at the diquark-antidiquark structure.

In fact, the above procedures are just making a rough partial wave analysis on the eigenvector of the ground molecular state $[Q_1\bar{q}_2][Q_3\bar{q}_4]$ according to the Pauli principle, which deserves further investigation. Higher partial wave components are less important from the nucleon-nucleon scattering.

In general, a multiquark state should be a mixture of all possible color components, including the color singlets and hidden color configurations. Taking the $T_{cc}$ state with $0^+$ as an example, it contains two color singlets $D^*D$ and $D^*D^*$ and two hidden color octets $D_{q5}D_8$ and $D_{q5}D_8$. However, the deuteron-like configuration of the $T_{cc}$ indicates that the hidden color components do not play critical role because the color confinement interaction is suppressed in the distance larger than 1 fm when we adopt the screened confinement potential $4$. The states with various components and the percentage of each are listed in Table I. One can find that the colorless components in the $T_{cc}$ state occupy 81% while the percentage of the hidden color components is 19%. The distance between the two subclusters is 2.62 fm, which clearly supports the deuteron-like configuration. In addition, we also give numerical results when the state contains the color singlet components $DD^*$ and $D^*D^*$ only. The difference between the two cases is very small, which also holds for the state $T_{cc}^-$. These numerical results indeed justify the consideration of all possible colorless components only in the deuteron-like configuration $4$. On the other hand, the hidden color component is an inevitable new degree of freedom of the multi-quark states which is absent in ordinary hadrons. The physical effects of the hidden color components especially in the deeply bound multiquark states are interesting and deserve further investigation.

The ground state $[Q_1Q_3][\bar{q}q\bar{4}]$ with $0^+$ only contains two channels, see the cases (1) and (2) in Table II, which are the generally adopted diquark-antidiquark configurations. After coupling the two channels, the two states $[c_1c_3][\bar{q}q\bar{4}]$ and $[b_1b_3][\bar{q}q\bar{4}]$ with $0^+$ can generate deep compact bound states with the binding energy of about $-60$ MeV and $-205$ MeV, respectively. The binding energy mainly come from the contributions of the strong Coulomb interaction, color-magnetic interaction and meson exchange interaction. The optima spin-isospin-color-orbit combination (i.e., the case (1)) is dominant with a probability almost reaching 100%, so that the coupled channel effect is insignificant in the cases (1) and (2). In
TABLE I: Components, ratio, and binding energy $E_b$.

| State | Component | $E_b$ (MeV) | Ratio (%) |
|-------|-----------|-------------|-----------|
| $T_{cc}^+$ | $D^+D^*/D^*/D^*$ | $-1.2 \pm 0.2$ | $74.2 : 6.8$ |
| | $D^+D_s/D^+_s/D^+_s$ | $0.2 : 18.8$ |
| $T_{cc}^{++}$ | $D^+D^*/D^*/D^*$ | $-0.9 \pm 0.2$ | $98.8 : 1.2$ |
| $T_{bb}$ | $B^+B^*/B^*/B^*$ | $-48.9 \pm 0.2$ | $49.0 : 40.0$ |
| | $B^+_sB^+_s/B^+_sB^+_s$ | $7.0 : 4.0$ |
| $T_{bb}^{--}$ | $B^+B^*/B^*/B^*$ | $-43.8 \pm 0.2$ | $62.4 : 37.6$ |

TABLE II: Probability of various combinations of $[Q_1Q_2]$ and $[\bar{q}_2\bar{q}_4]$ in the state $[Q_1Q_2][\bar{q}_2\bar{q}_4]$ and their energy in unit of MeV. Orbit stands for the angular momenta $l_{13}$, $l_{24}$ and $l_{13,24}$.

| Case | Color | Spin | Orbit | $|c_1c_3||\bar{q}_2\bar{q}_4|$ | $|b_1b_3||\bar{q}_2\bar{q}_4|$ |
|------|-------|------|-------|----------------|----------------|
| (1)  | $3 \otimes 3$ | $1 \oplus 0$ | $000$ | $3820, 98.7\%$ | $10355, 99.8\%$ |
| (2)  | $6 \otimes 6$ | $0 \oplus 1$ | $000$ | $4112, 1.3\%$ | $10679, 0.2\%$ |
| (3)  | $3 \otimes 3$ | $0 \oplus 1$ | $110$ | $4439, 1.5\%$ | $10973, 0.3\%$ |
| (4)  | $6 \otimes 6$ | $1 \oplus 0$ | $110$ | $4285, 98.5\%$ | $10841, 99.7\%$ |
| (5)  | $3 \otimes 3$ | $1 \oplus 0$ | $011$ | $4440, 8\%$ | $10987, 8\%$ |
| (6)  | $6 \otimes 6$ | $1 \oplus 0$ | $101$ | $4311, 9\%$ | $10873, 8\%$ |

TABLE III: Probability of various combinations of $[Q_1Q_2]$ and $[\bar{q}_2\bar{q}_4]$ in the state $[Q_1Q_2][\bar{q}_2\bar{q}_4]$ with $01^+$.  

| Case | Color | Spin | Orbit | $T_{cc}^+$ | $T_{cc}^{++}$ | $T_{bb}$ | $T_{bb}^{--}$ |
|------|-------|------|-------|---------|---------|--------|---------|
| (a)  | $3 \otimes 3$ | $1 \oplus 0$ | $000$ | $13.6\%$ | $8.4\%$ | $13.4\%$ | $11.0\%$ |
| (b)  | $6 \otimes 6$ | $0 \oplus 1$ | $000$ | $17.8\%$ | $16.9\%$ | $22.8\%$ | $22.0\%$ |
| (c)  | $3 \otimes 3$ | $0 \oplus 1$ | $000$ | $13.6\%$ | $8.4\%$ | $13.4\%$ | $11.0\%$ |
| (d)  | $6 \otimes 6$ | $1 \oplus 0$ | $000$ | $17.8\%$ | $16.9\%$ | $22.8\%$ | $22.0\%$ |
| (e)  | $3 \otimes 3$ | $1 \oplus 0$ | $000$ | $12.4\%$ | $16.5\%$ | $10.5\%$ | $11.3\%$ |
| (f)  | $6 \otimes 6$ | $1 \oplus 0$ | $000$ | $24.8\%$ | $33.0\%$ | $17.5\%$ | $22.7\%$ |

addition, we present four lowest excited states with $01^+$, which are much higher than the ground states. The cases (3) and (4) have the same orbital excitation mode, where the coupled channel effect is also very weak and the color configuration $6 \otimes 6$ is dominant. The cases (5) and (6) can not couple with each other due to their different excitation modes and the absence of noncentral forces in the model [4]. Furthermore, we find that the coupled channel effect is always very weak between the same orbital excitation modes after checking some higher excited states.

In order to illustrate the underlying mechanism of these two different physical pictures clearly, we decompose the ground state $[Q_1Q_2][\bar{q}_2\bar{q}_4]$ with $01^+$ as the superposition of a large number of the $[Q_1Q_2][\bar{q}_2\bar{q}_4]$ states with various angular excitations of $l_{13}$, $l_{24}$ and $l_{13,24}$. According to the spin-color-isospin symmetry, six types of the $[Q_1Q_3]$ and $[\bar{q}_2\bar{q}_4]$ combinations can satisfy the Pauli principle and the parity conservation, see Table III. $e$ and $o$ represent even and odd, respectively. For example, the $eoe$ represents $(000, 020, 220, 222, 224)$, etc., which are orthogonal bases and do not mix with each other because of the lack of noncentral force in the model [3]. With the probability of each component in the states in Table I and their color-spin wave functions, we can approximately exhibit the percentage of each type of the $[Q_1Q_3]$ and $[\bar{q}_2\bar{q}_4]$ combination in the states if we ignore the very weak coupled channel effect among the modes with the same orbital excitations, which are presented in Table III.

In principle, we can also expand the $[Q_1Q_3][\bar{q}_2\bar{q}_4]$ state in terms of the molecular $[Q_1\bar{q}_2][Q_3\bar{q}_4]$ bases. On the contrary, the Pauli principle does not act on the molecules $[Q_1\bar{q}_2]$ and $[Q_3\bar{q}_4]$ so that their orbitally excited modes $l_{12}$ and $l_{134}$ can not be determined precisely as the identical $[Q_1Q_3]$ and $[\bar{q}_2\bar{q}_4]$ in Table III. There are many different combinations of the orbitally excited mode (parity) for each isospin-spin-color combination if one attempts to expand the $[Q_1Q_3][\bar{q}_2\bar{q}_4]$ state in terms of the molecular $[Q_1\bar{q}_2][Q_3\bar{q}_4]$ bases. In another word, one can make such expansions only according to isospin-spin-color combinations, which leads to the fact that it is difficult to extract some accurate and transparent information on the molecular $[Q_1\bar{q}_2][Q_3\bar{q}_4]$ configuration from the diquark state $[Q_1Q_3][\bar{q}_2\bar{q}_4]$.

In addition, we calculate the errors of the percentage, mass and binding energy of the double heavy tetraquark states in the two configurations, which are introduced by the uncertainty of the adjustable model parameters in the Minuit program. The errors of the percentage of each configuration in three Tables are less than 0.1%. The mass errors in Table II are around 10 MeV. Those of the excited states (i.e., the cases (3)-(6)) are 8-9 MeV while those of the ground states (i.e., the cases (1) and (2)) are 12-13 MeV. The definition of binding energy, $E_b = E_4 - E_{m_{123}}$, can greatly reduce the influence of the uncertainty of the energy of the double heavy tetraquark state $E_4$ and its corresponding twomeson threshold $E_{m_{123}}$ on the binding energy. Therefore, the $E_b$ errors are very small, about 0.2 MeV, in Table I.

The optima isospin-color-spin-orbit combination only exists in the case (a) in Table III. The percentage of the optima combination in the $T_{cc}^+$ ($T_{bb}^{--}$) is in fact less than 13.6\% (13.4\%) because the case (a) contains the contributions from the other orbitally excited components. Compared with the $T_{cc}^{++}$ ($T_{bb}^{--}$), the $T_{cc}^+$ ($T_{bb}^{--}$) has a larger percentage of the favorable optima combination and a larger binding energy. In strong contrast, the probability of the optima combination is almost 100\% in the state $|c_1c_3||\bar{q}_2\bar{q}_4|$ (|$b_1b_3||\bar{q}_2\bar{q}_4$), which provides a strong attraction to generate a deep bound state. The optima combination should therefore be responsible for the formation of the shallow bound states from the prospective of diquarks.
The corresponding SU(2) groups of the isospin, $V$-spin and $U$-spin are three subgroups of the flavor SU(3) group. Therefore, the isospin, $V$-spin, and $U$-spin antisymmetric states, such as $T_{cc}$ with $01^+$ and $T_{bb}$ with $\frac{1}{2}1^+$, should share the same symmetry in their wave functions so that their behaviors should be analogous. For the state $T_{bb}$ with $\frac{1}{2}1^+$, the molecule configuration can form a stable state with a binding energy of about $-10$ MeV, which implies the existence of the deep bound diquark configuration $[b_1 b_3][\bar{u}_2 \bar{s}_4]$. Its binding energy is about $-50$ MeV in the present calculation. However, the state $T_{cc}$ with $\frac{1}{2}1^+$ can not produce a stable state in either molecule or diquark configuration. The optima isospin $(V$-spin$)$-color-spin-orbit combination is just a necessary condition to produce a stable double heavy tetraquark state. As a result, it is easy to understand why there do not exist the stable doubly heavy tetraquark states which contain the isospin, $U$-spin or $V$-spin symmetric light antidiquarks in various theoretical frameworks.

The compact structure of the ground state $[c_1 c_3][\bar{q}_2 \bar{q}_4]$ arises from the strong attractive interaction within the $[c_1 c_3]$ and $[\bar{q}_2 \bar{q}_4]$ diquarks and the strong color force between the $[c_1 c_3]$ and $[\bar{q}_2 \bar{q}_4]$. In contrast, in the state $[c_1 \bar{q}_2][c_3 q_4]$, the majority of the bad diquarks with various orbitally excited modes are spatially extended while the $c_1$ and $q_2$ ($c_3$ and $q_4$) are tightly bound into a meson by the strong color force, which leads to the loosely bound molecular state.

In principle, if all possible orbital excitations are considered properly, either the diquark or molecule bases are complete and orthogonal so that one can apply either set of these bases to make the model calculations. One can decompose the complete bases into two subsets: one is for the ground states and the other for the excited states. Note that the corresponding subsets in the diquark and molecule bases are not equivalent. The wave function of the ground state does not mix with those of the orbitally excited states if the model Hamiltonian does not contain the noncentral forces such as the spin-orbital and $S$-$D$ wave mixing interactions as in Ref. [4]. The ground state bases with the diquark or molecule configurations alone are enough to describe its corresponding physical state in the model without the noncentral interactions. On the other hand, the diquark and molecule configurations have different orbitally excited modes. The construction of the trial wave function in the model space depends on the orbitally excited modes in the realistic calculations, which may result in the difference between two configurations.

The existence of the deuteron-like $T_{cc}$ state implies the advent of other compact double heavy tetraquark states. The doubly charmed baryon $\Xi_{cc}^{++}$ indicates the possible existence of the similar doubly charmed hadron with the light quark replaced by a strongly correlated light antidiquark. These interesting states may also be searched for in the relativistic heavy-ion collisions at ultrarelativistic energies [10, 17].

**Conflict of interest**

The authors declare that they have no conflict of interest.

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**Supplemental materials**

Completely equivalent color configurations \{1_{12} \otimes 1_{34}, 8_{12} \otimes 8_{34}\} and \{3_{13} \otimes 3_{24}, 6_{13} \otimes 6_{24}\},

\[
\begin{pmatrix}
1_{12} \otimes 1_{34} \\
8_{12} \otimes 8_{34}
\end{pmatrix} = \begin{pmatrix}
\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}
\end{pmatrix}
\begin{pmatrix}
3_{13} \otimes 3_{24} \\
6_{13} \otimes 6_{24}
\end{pmatrix}.
\]

Completely equivalent spin configurations \{1_{12} \oplus 1_{34}, 1_{12} \oplus 0_{34}, 0_{12} \oplus 1_{34}\} and \{1_{13} \oplus 1_{24}, 1_{13} \oplus 0_{24}, 0_{13} \oplus 1_{24}\},

\[
\begin{pmatrix}
1_{12} \oplus 1_{34} \\
1_{12} \oplus 0_{34} \\
0_{12} \oplus 1_{34}
\end{pmatrix} = \begin{pmatrix}
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{pmatrix}
\begin{pmatrix}
1_{13} \oplus 1_{24} \\
1_{13} \oplus 0_{24} \\
0_{13} \oplus 1_{24}
\end{pmatrix}.
\]

A unitary transformation matrix

\[
\begin{pmatrix}
\mathbf{r}_{12} \\
\mathbf{r}_{34} \\
\mathbf{r}_{12,34}
\end{pmatrix} = \begin{pmatrix}
\frac{m_3}{m_1+m_3} & \frac{-m_2}{m_1+m_2} & 1 \\
\frac{m_3}{m_1+m_3} & \frac{m_2}{m_1+m_2} & 1 \\
\frac{m_3}{m_1+m_3} & \frac{m_2}{m_1+m_2} & 1
\end{pmatrix}
\begin{pmatrix}
\mathbf{r}_{13} \\
\mathbf{r}_{24} \\
\mathbf{r}_{13,24}
\end{pmatrix}.
\]

Gaussian wave function

\[
\psi_{lm}^G(\mathbf{x}) = \sum_{n=1}^{n_{max}} c_n N_{nl} x^l e^{-\nu_n x^2} Y_{lm}(\mathbf{x}),
\]

\[
\phi(\mathbf{r}_{12}, \mathbf{r}_{34}, \mathbf{r}_{12,34}) = \psi_{00}^G(\mathbf{r}_{12}) \psi_{00}^G(\mathbf{r}_{34}) \psi_{00}^G(\mathbf{r}_{12,34}).
\]

Wave function expansion

\[
e^{-dr_{13} r_{24} - cr_{13} r_{13,24} - fr_{24} r_{13,24}} = \frac{1}{4\sqrt{\pi}} \sum_{l_{13}=0}^\infty \sum_{l_{24}=0}^\infty \sum_{l_{13,24}=0}^\infty \left[ |Y_{l_{13}}(r_{13}) Y_{l_{24}}(r_{24})|^2 i_{l_{13}} l_{13,24} \frac{I_{l_{13}} l_{24} - l_{13,24}}{I_{l_{13}} l_{24}} \left| \psi_{00}^G(\mathbf{r}_{12}) \psi_{00}^G(\mathbf{r}_{34}) \psi_{00}^G(\mathbf{r}_{12,34}) \right| \right]
\]

\[
\times \left( \frac{z_{r_{13} r_{24}}}{2dr_{13} r_{24}} I_{l_{1}+\frac{1}{2}}(dr_{13} r_{24}) \right) \left( \frac{z_{r_{13} r_{13,24}}}{2cr_{13} r_{13,24}} I_{l_{2}+\frac{1}{2}}(cr_{13} r_{13,24}) \right) \left( \frac{z_{r_{24} r_{13,24}}}{2fr_{24} r_{13,24}} I_{l_{3}+\frac{1}{2}}(fr_{24} r_{13,24}) \right),
\]

where \(I_\alpha(x)\) are the modified Bessel functions.