# Important configurations in six-quark $\boldsymbol{N}-\boldsymbol{N}$ states 

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#### Abstract

We present an analysis of six-quark basis states constructed from molecular-type single-particle orbitals. In the present work, we employ a nonrelativistic constituent quark model with one-gluon exchange approximated by a spin-spin interaction. The orbitals are constructed from appropriate combinations of two-center Gaussians. The calculations are performed in the limit of zero separation, and is deemed relevant to short distances. We study the contributions of configurations which are natural in the molecular basis but had been neglected previously in cluster model calculations. We find a dramatic lowering of the energy due to these configurations.


## I. INTRODUCTION

A description of the nucleon-nucleon interaction is one of the fundamental challenges of quantum chromodynamic (QCD) models in the low energy (confinement) regime. Of the various models which have been discussed in the literature, here we address those containing explicit quark structure. These include both constituent quark nonrelativistic potential models, and current quark relativistic bag or soliton models. A common problem which all quark models face is the representation of the quark wave functions for various nucleon-nucleon "separations."

In a previous paper, ${ }^{1}$ we discussed the important advantages of molecular orbitals. We presented a classification scheme and the explicit construction of sixquark basis states which are relevant to $N-N$ scattering and bound states.

Molecular orbitals are natural to mean field or general independent particle model (IPM) approximations. Among the various quantum numbers characterizing an IPM state, we call special attention to parity, since single-particle parity is conserved during a collision within the mean-field approximation.

The nonrelativistic cluster model has been used extensively to calculate the $N-N$ interaction. In that model, single-particle wave functions are the nonorthogonal "right" and "left" orbitals

$$
R_{n}(\mathbf{r})=\psi_{n}(\mathbf{r}-\mathbf{Z} / 2)
$$

and

$$
L_{n}(\mathbf{r})=\psi_{n}(\mathbf{r}+\mathbf{Z} / 2),
$$

where $Z$ is the intercluster distance and $\psi_{n}$ is frequently taken to be the ground state ( $n=0$ ) oscillator function of width independent of $\boldsymbol{Z}$. As discussed in Ref. 1, orthogonal molecular-type wave functions can be constructed as simple linear combinations of the cluster functions $R_{n}$ and $L_{n}$. There we considered explicitly the case $n=0$. For that case (suppressing $n$ ), the two molecular orbitals
of even and odd parity are

$$
\left[\begin{array}{l}
\sigma(\mathbf{r})  \tag{1.1}\\
\pi(\mathbf{r})
\end{array}\right) \equiv[2(1 \pm\langle R \mid L\rangle)]^{-1 / 2}[R(\mathbf{r}) \pm L(\mathbf{r})]
$$

For the scattering problem, it is convenient to construct orthogonal pseudo-right and pseudo-left orbitals, $r_{n}(\mathbf{r})$ and $l_{n}(\mathbf{r})$, which for large separations approach $R_{n}(\mathbf{r})$ and $L_{n}(\mathbf{r})$ :

$$
\left(\begin{array}{l}
r(\mathbf{r}) \\
l(\mathbf{r})
\end{array}\right] \equiv 2^{-1.2}[\sigma(\mathbf{r}) \pm \pi(\mathbf{r})]
$$

The use of orthogonal functions greatly simplifies the mathematics of generating states of the proper space-spin-isospin-color symmetries.

Of course, both the cluster model states and the molecular states form a complete basis set. However, there are configurations which appear naturally in the molecular basis but which hitherto have been ignored in cluster model calculations. These configurations were listed explicitly in Ref. 1.

In order to evaluate the importance of the neglected configurations, we consider here the case of zero separation (the united cluster) because it is especially simple and because it offers an extreme case of configuration mixing. Our conclusions will be relevant for short separations. In this study, we diagonalize a commonly used nonrelativistic Hamiltonian in six-quark basis states. We use only configurations which are generated by the lowest cluster model functions, namely $0 s$ states. Therefore, in the following we suppress the subscript $n$. At $Z=0$, the corresponding molecular basis has two functions, $s$ and $p$ ( $m=0$ ), and the corresponding pseudo-right and -left functions read

$$
\left[\begin{array}{l}
r(\mathbf{r}) \\
l(\mathbf{r})
\end{array}\right]=2^{-1 / 2}[s(\mathbf{r}) \pm p(\mathbf{r})] .
$$

From the $s$ and $p$ orbitals, various six-quark configurations can be constructed; they are of the type $s^{n} p^{6-n}$ or $r^{n} l^{6-n}$, with $n=0,1,2, \ldots, 6$. In Table I of

Ref. 1 we gave the transformation between the ( $r, l$ ) and $(\sigma, \pi)$ representations. Note that for $Z=0, \sigma \rightarrow s$ and $\pi \rightarrow p$.

In the cluster model, the nonorthogonal $R$ and $L$ functions have been used only to construct configurations of the type $R^{3} L^{3}$, which are then properly symmetrized and normalized. Care must be taken in the spherical limit because $R$ and $L$ become identical, and spatially antisymmetric pairs vanish. A proper limiting procedure is obtained by letting $Z \rightarrow 0$ in the functions and in the overall normalization (see Ref. 2).

Harvey has selected those configurations which approach, asymptotically, the physical $N N$ and $\Delta \Delta$ states and a particular hidden color state $C C$. As a function of $Z$, these states will here still be denoted by $N N, \Delta \Delta$, and $C C$. If we reexpand these three configurations in terms of molecular parity eigenstates, we find that the admixture of various single-particle parities varies with $Z$. As $\boldsymbol{Z} \rightarrow \infty$, they all contain equal probabilities of even and odd parity functions, but at $Z=0$ they contain only $s^{6}$ and $s^{4} p^{2}$ components for $T=0, S=1$ or $T=1, S=0$, and $s^{5} p$ and $s^{3} p^{3}$ for $T=0, S=0$. The explicit spherical structure is given below.

This paper is offered as an aid to the practitioners of cluster model and mean-field calculations in order to simplify their work, to provide group theoretical coefficients for constructing basis states, and to identify important basis configurations so as to reduce computation time.

## II. THE SIX-QUARK BASIS STATES

The six-quark basis states constructed in Ref. 1 are totally antisymmetric. The group theoretic classification scheme is an extension of that done by Harvey. ${ }^{2}$ Thus we build a totally antisymmetric state of six quarks according to

$$
\begin{equation*}
\Psi_{6}=\left(\left\{\psi_{6}[f] C_{6}\left[f^{\prime}\right]\right\}_{\left[f^{\prime \prime}\right]} \Gamma_{6}\left(\left[f^{\prime \prime}\right] T S\right)\right)_{\left[1^{6}\right]} \tag{2.1}
\end{equation*}
$$

i.e., we first couple an orbital function $\psi_{6}$ of partition [ $f$ ] to an $\mathrm{SU}_{c}(3)$ singlet color function $C_{6}$ of partition $\left[f^{\prime}\right]$ to give a state belonging to the [ $\tilde{f}^{\prime \prime}$ ] representation of the permutation group $S_{6}$. This is combined with the spinisospin state $\Gamma_{6}$ of dual symmetry $\left[f^{\prime \prime}\right]$ to form a totally antisymmetric state.

In order to calculate matrix elements of a model Hamiltonian (see Sec. III), it is necessary to resolve the functions $\psi_{6}, C_{6}$, and $\Gamma_{6}$ as linear combinations of products $\psi_{4} \phi_{2}, C_{4} c_{2}$, and $\Gamma_{4} \gamma_{2}$, i.e., into states of four and two quarks so as to reduce the calculation of six-body matrix elements to two-body matrix elements. The required linear combinations are obtained with the help of coefficients of fractional parentage (cfp).

For the orbital space, Harvey ${ }^{2}$ has provided the coefficients for states $\psi_{6}[f]$ having configurations of the type $r^{3} l^{3}$, i.e., three quarks which are asymptotically in a left ( $l$ ) cluster and three in a right ( $r$ ) cluster. The coefficients we need are the same as for his $a^{3} b^{3}$ ( $\equiv S_{+}^{3} S_{-}^{3}$ ) configurations. Our classification scheme, ${ }^{1}$ based on molecular orbitals, introduces extra configurations $r^{4} l^{2}$ and $r^{2} l^{4}$ (four and two quarks in each cluster), and $r^{5} l$ and $l^{5} r$ (five and one per cluster). Here we ignore the configurations $r^{6}$ and $l^{6}$; they are spurious
in the limit of infinite separation and they do not couple to $N N$ and $\Delta \Delta$ states at zero separation. Using the same phase conventions as Harvey, we have calculated the corresponding cfp. They are presented in Tables I and II. Cases not shown are trivial: Either 1 or 0 .

As pointed out by Harvey, the color cfp are not required in practice because they disappear into the normalization property. In spin-isospin space, we consider within our classification scheme all the $\operatorname{SU}(4)$ representations of Harvey's Table I. With the exception of the \{411\} representation one can find the corresponding cfp in either Ref. 2 or 3. As demonstrated in Sec. III, the \{411\}, together with many others (those without an asterisk in Harvey's Table I), can be neglected and it is therefore unnecessary to calculate such cfp.

Another necessary ingredient of the six-quark state is the so-called $\bar{K}$ matrix. The $\bar{K}$ matrix is a linear combination of terms which are products of specific factors of Clebsch-Gordan coefficients of the symmetric group $S_{6}$ and $S_{5}$. They appear from the coupling of the orbital to the color space. For details, see Appendix B of Ref. 2. Harvey has calculated the elements of the $\bar{K}$ matrices of the "asterisked" $\mathrm{SU}(4)$ representations. They contain dibaryon states. The others are asymptotically unphysical and play the role of "hidden color" states. One purpose of the present work is to study quantitatively their contribution at $Z=0$. In Table III we present the $\bar{K}$ matrix elements for all representations without an asterisk. We follow the notation of Ref. 2.

## III. THE QUARK-QUARK INTERACTION

To examine the utility of molecular orbitals over cluster states, here we consider a nonrelativistic constituent quark model. In such models, a description of one-gluon exchange is given by the usual magnetic hyperfine interaction. ${ }^{4}$ For simplicity in the present study, we restrict ourselves to the spin-spin term. In baryon spectroscopy, ${ }^{5,6}$ this is the major contribution to the spectrum. Thus we consider the Hamiltonian ( $\hbar=c=1$ )

$$
\begin{align*}
H= & \sum_{i}\left[m_{i}+\frac{p_{i}^{2}}{2 m_{i}}\right)-\frac{1}{2 M} P^{2} \\
& +\sum_{i<j} \hat{\lambda}_{i} \cdot \hat{\lambda}_{j}\left[v_{c}\left(r_{i j}\right)+\sigma_{i} \cdot \sigma_{j} v_{\sigma}\left(r_{i j}\right)\right] \tag{3.1}
\end{align*}
$$

where $M=\sum_{i} m_{i}, \mathbf{P}=\sum_{i} \mathbf{p}_{i}$, and the $\hat{\lambda}$ are the set $\lambda^{\alpha}$ ( $\alpha=1, \ldots, 8$ ), the generators of the $\mathrm{SU}(3)$ color group. For $v_{c}$ as a function of the interquark spacing $r$ we use the parametrized form of Ref. 7,

$$
\begin{equation*}
v_{c}=A e^{-r^{2} / \alpha^{2}}+B r^{2}+C \tag{3.2}
\end{equation*}
$$

and $v_{\sigma}$ is simply the contact term

$$
\begin{equation*}
v_{\sigma}=D \delta(\mathbf{r}) \tag{3.3}
\end{equation*}
$$

The parameters $A, B, C, D$, and $\alpha$, together with the harmonic oscillator size parameter $\beta$, have been fit in Ref. 7 to the baryon spectrum. Among the sets offered there, we have selected

$$
\begin{align*}
& A=0, \quad B=-621 \mathrm{MeV} \mathrm{fm}^{-2} \\
& C=776 \mathrm{MeV}, \quad D=-109.5 \mathrm{MeV} \mathrm{fm}^{3}  \tag{3.4}\\
& \alpha=0.2737 \mathrm{fm}, \quad B=0.456 \mathrm{fm}
\end{align*}
$$

TABLE I. Orbital two-body fractional parentage coefficients for the symmetry states [ $f$ ] containing the configurations $r^{4} l^{2}$ or $r^{2} l^{4}$.

| [4]:[2] |  |  |  |  | [4]:[11] |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $r^{4} l^{2}$ | $r^{4}: l^{2}$ |  | $r^{2} l^{2}: r^{2}$ | $r^{3} l: r l$ | $r^{3} l: r l$ |
| [6] | $\sqrt{\frac{1}{15}}$ |  | $\sqrt{\frac{6}{15}}$ | $\sqrt{\frac{8}{15}}$ | 0 |
| [51] | $\sqrt{\frac{1}{3}}$ |  | $-\sqrt{\frac{1}{2}}$ | $\sqrt{\frac{1}{6}}$ | -1 |
| [42] | $\sqrt{\frac{6}{10}}$ |  | $\sqrt{\frac{1}{10}}$ | $-\sqrt{\frac{3}{10}}$ | 0 |
|  |  | [31]:[2] |  |  | [31]:[11] |
| $r^{4} l^{2}$ | $r^{4}: l^{2}$ |  | $r^{2} l^{2}: r^{2}$ | $r^{3} l: r l$ | $r^{3} l: r l$ |
| [51] | 0 |  | $-\sqrt{\frac{1}{2}}$ | $\sqrt{\frac{1}{2}}$ | 0 |
| [42] | 0 |  | $\sqrt{\frac{1}{2}}$ | $\sqrt{\frac{1}{2}}$ | -1 |
|  |  | [4]:[2] |  |  | [4]:[11] |
| $r^{2} l^{4}$ | $l^{4}: r^{2}$ |  | $r^{2} l^{2}: l^{2}$ | $r l^{3}: r l$ | $r l^{3}: r l$ |
| [6] | $\sqrt{\frac{1}{15}}$ |  | $\sqrt{\frac{6}{15}}$ | $\sqrt{\frac{8}{15}}$ | 0 |
| [51] | $\sqrt{\frac{1}{3}}$ |  | $-\sqrt{\frac{1}{2}}$ | $\sqrt{\frac{1}{6}}$ | +1 |
| [42] | $\sqrt{\frac{6}{10}}$ |  | $\sqrt{\frac{1}{10}}$ | $-\sqrt{\frac{3}{10}}$ | 0 |
|  |  | [31]:[2] |  |  | [31]:[11] |
| $r^{2} l^{4}$ | $l^{4}: r^{2}$ |  | $r^{2} l^{2}: l^{2}$ | $r l^{3}: r l$ | $r l^{3}: r l$ |
| [51] | 0 |  | $\sqrt{\frac{1}{2}}$ | $\sqrt{\frac{1}{2}}$ | 0 |
| [42] | 0 |  | $-\sqrt{\frac{1}{2}}$ | $\sqrt{\frac{1}{2}}$ | +1 |

The kinetic term is treated nonrelativistically, with quark mass $m=362 \mathrm{MeV}$. The results given in the next section are relative to two-nucleon masses, which each is $M_{N}=940 \mathrm{MeV}$.

Each six-quark basis state considered in the calculation has been expanded in terms of products of antisymmetric states of four and two particles by using the technique described in Ref. 2 and the tables available therein and in this paper in Sec. I. In this way, any six-body matrix ele-

TABLE II. Same as Table I but for the configurations $r^{5} l$ or $r l^{5}$.

|  | $[4]:[2]$ |  | $[4]:[11]$ |
| :--- | :--- | :---: | :---: |
| $r^{5} l$ | $r^{4}: r l$ | $r^{3} l: r^{2}$ | $r^{4}: r l$ |
| $[6]$ | $\sqrt{\frac{1}{3}}$ | $\sqrt{\frac{2}{3}}$ | 0 |
| $[51]$ | $\sqrt{\frac{2}{3}}$ | $-\sqrt{\frac{1}{3}}$ | -1 |
|  |  |  | $[4]:[11]$ |
|  | $[4]:[2]$ |  | $l^{4}: r l$ |
| $r l^{5}$ | $l^{4}: r l$ | $r l^{3}: l^{2}$ |  |
|  | $\sqrt{\frac{1}{3}}$ | $\sqrt{\frac{2}{3}}$ | 0 |
| $[6]$ | $\sqrt{\frac{2}{3}}$ | $-\sqrt{\frac{1}{3}}$ | +1 |
| $[51]$ |  |  |  |

ment becomes a linear combination of two-body matrix elements. In Table IV we give all necessary two-body matrix elements obtained for $v_{c}$ [see (Eq. 3.2)] and $v_{\sigma}$ [see Eq. (3.3)] with the parametrization (3.4).

In Table II of Ref. 1 we listed all available six-quark states obtained from our truncated molecular orbital space and all $S U(4)$ isospin-spin representations which lead to totally antisymmetric states. In this way we obtained a space spanned by 16 vectors for the $T=0, S=1$ or $T=1, S=0$ sectors, by seven vectors for the $T=0, S=0$ sector, and by 25 vectors for the $T=1, S=1$ sector. The present study tries to answer the question as to which of these vectors are the most important and if a reduction of the basis of each sector can be made without altering the results.

## IV. RESULTS

We have performed numerical calculations for the sectors $T=0, S=1$ and $T=0, S=0$. The output of the matrix diagonalization is given in Tables V and VI, respectively. In the first column of each table we list the basis states in the notation of Ref. 1. The $N N$ and $\Delta \Delta$ states, together with the $C C$ state, have been defined by Har$v^{2,8}$ for the cluster basis. In the $Z \rightarrow 0$ limit, they have a different orbital space content in the cluster and in the molecular bases. In the cluster basis they are

$$
\begin{align*}
& N N(\text { cluster })=\frac{1}{3}\left(\left(s^{6}[6]\{33\}\right)+2\left(s^{4} p^{2}[42]\{33\}\right)-2\left(s^{4} p^{2}[42]\{51\}\right)\right), \\
& \Delta \Delta(\text { cluster })=\frac{1}{\sqrt{45}}\left(2\left(s^{6}[6]\{33\}\right)+4\left(s^{4} p^{2}[42]\{33\}\right)+5\left(s^{4} p^{2}[42]\{51\}\right)\right),  \tag{4.1}\\
& C C(\text { cluster })=\frac{1}{\sqrt{5}}\left(2\left(s^{6}[6]\{33\}\right)-\left(s^{4} p^{2}[42]\{33\}\right)\right)
\end{align*}
$$

for $(T=0, S=1)$ or ( $T=1, S=0)$, and

$$
\begin{align*}
& N N(\text { cluster })=\frac{1}{\sqrt{45}}\left(\sqrt{5}\left(s^{5} p[51]\{42\}\right)+2\left(s^{3} p^{3}[33]\{42\}\right)+6\left(s^{3} p^{3}[33]\{6\}\right)\right), \\
& \Delta \Delta(\text { cluster })=\frac{1}{\sqrt{45}}\left(\sqrt{20}\left(s^{5} p[51]\{42\}\right)+4\left(s^{3} p^{3}[33]\{42\}\right)-3\left(s^{3} p^{3}[33]\{6\}\right)\right),  \tag{4.2}\\
& C C(\text { cluster })=\frac{1}{3}\left(+2\left(s^{5} p[51]\{42\}\right)-\sqrt{5}\left(s^{3} p^{3}[33]\{42\}\right)\right)
\end{align*}
$$

TABLE III. The matrices $\bar{K}\left(f[p q] f^{\prime}\left[p^{\prime} q^{\prime}\right] \mid f^{\prime \prime}\left[p^{\prime \prime} q^{\prime \prime}\right]\right)$. For each distinct matrix, the first line indicates $[f]\left[f^{\prime}\right]$ and the line below it gives $p q p^{\prime} q^{\prime}$ with an overbar for a symmetric and a tilde for an asymmetric pair. The rows are labeled by $\left[f^{\prime \prime}\right] p^{\prime \prime} q^{\prime \prime}$. For details, see Ref. 2.

| $f^{\prime \prime}$ | [51] [222] |  |  | [51] [222] |
| :---: | :---: | :---: | :---: | :---: |
|  |  | $\overline{11} \overline{33} \quad \overline{12} \overline{33} \quad \overline{12} \quad 23$ |  | $\begin{array}{lllllll}11 & 23 & \overline{12} & \widetilde{23} & \overline{12} & \overline{33}\end{array}$ |
| [321] | $\overline{12}$ | $\left(-\sqrt{\frac{1}{5}}\right.$ | 12 | $\left(\left.\begin{array}{lll}\sqrt{\frac{3}{5}} & -\sqrt{\frac{2}{5}} 0\end{array} \right\rvert\,\right.$ |
|  | $\overline{13}$ | 0 | 13 | $-\sqrt{\frac{3}{5}}$ |
|  | $\overline{23}$ | $\left(\begin{array}{lll}1 & 0 & 0\end{array}\right]$ | 23 | $\begin{array}{lll}-1 & 0 & 0\end{array}$ |
| [321] | $\overline{12}$ | [42] [222] |  | [42] [222] |
|  |  | $\begin{array}{llllllllllll}11 & \overline{33} & \overline{12} & \overline{33} & \overline{22} & \overline{33} & \overline{12} & \widetilde{23}\end{array}$ |  | $\begin{array}{llllllll}11 & \widetilde{23} & \overline{12} & \widetilde{23} & \overline{22} & \widetilde{23} & \overline{12} & \overline{33}\end{array}$ |
|  |  | $\left\|\begin{array}{cccc}0 & -\sqrt{\frac{1}{3}} & 0 & -\sqrt{\frac{2}{3}} \\ \sqrt{\frac{8}{15}} & 0 & -\sqrt{\frac{5}{15}} & \sqrt{\frac{2}{15}} \\ 0 & -\sqrt{\frac{3}{5}} & 0 & -\sqrt{\frac{2}{5}}\end{array}\right\|$ | 12 | $\left\|-\sqrt{\frac{8}{27}}-\sqrt{\frac{3}{27}} \sqrt{\frac{10}{27}} \sqrt{\frac{6}{27}}\right\|$ |
|  | $\overline{13}$ |  | 13 | $\left\lvert\, \begin{array}{llll}0 & -1 & 0 & 0\end{array}\right.$ |
|  | $\overline{23}$ |  | 23 | $-\sqrt{\frac{8}{15}}-\sqrt{\frac{1}{15}}$ |
| [42] | $\frac{\overline{11}}{\overline{22}} \overline{12}$ | [42] [222] | 12 | $\left(\begin{array}{ccccc}\overline{11} & \frac{23}{2} & \overline{12} & \widetilde{23} & \overline{22} \\ \text { 23 } & \widetilde{12} & \overline{33} \\ \left(\sqrt{\frac{3}{10}}\right. & \sqrt{\frac{6}{10}} & 0 & \left.\sqrt{\frac{1}{10}}\right)\end{array}\right)$ |
|  |  | $\begin{array}{lllllllllllll}11 & \overline{33} & \overline{12} & \overline{33} & \overline{22} & \overline{33} & \overline{12} & \widetilde{23}\end{array}$ |  |  |
|  |  | $\left(\begin{array}{lllll}\sqrt{\frac{1}{20}} & 0 & \sqrt{\frac{10}{20}} & \sqrt{\frac{9}{20}}\end{array}\right.$ |  |  |
|  |  | $\left(\begin{array}{llll}1 & 0 & 1 & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{3}\end{array}\right.$ |  |  |
|  |  | $\left\lvert\, \begin{array}{llll}0 & -\sqrt{\frac{2}{5}} & 0 & \sqrt{\frac{3}{5}}\end{array}\right.$ |  |  |
| [3111] | $\frac{\overline{11}}{14}$ | [42] [222] | 14 | [42] [222] |
|  |  | $\overline{11} \overline{33} \quad \overline{12} \overline{33} \quad \overline{22} \overline{33} \quad \overline{12} \overline{23}$ |  | $\begin{array}{lllllllllll}\overline{11} & \overline{23} & \overline{12} & \overline{23} & \overline{22} & \overline{23} & \overline{12} & \overline{33}\end{array}$ |
|  |  | $\left(\begin{array}{cccc}-\sqrt{\frac{1}{3}} & 0 & 0 & +\sqrt{\frac{2}{3}}\end{array}\right.$ |  | $\left(+\sqrt{\frac{25}{54}}-\sqrt{\frac{6}{54}} \sqrt{\frac{20}{54}}-\sqrt{\frac{3}{54}}\right)$ |
|  |  | $\left(\begin{array}{llll}0 & \sqrt{\frac{2}{3}} & 0 & -\sqrt{\frac{1}{3}}\end{array}\right]$ | $\widetilde{34}$ | $\left(\begin{array}{llll}\sqrt{\frac{1}{6}} & \sqrt{\frac{2}{6}} & 0 & \sqrt{\frac{3}{6}}\end{array}\right.$ |
| [33] | $\overline{22}$ | [33] [222] | $\overline{12}$ | [33] [222] |
|  |  | $\overline{22} \overline{33} \quad \overline{12} \sqrt{23}$ |  | $\begin{array}{lll} 22 & 23 & 12 \\ \left(\sqrt{\frac{3}{4}}\right. & \left.\sqrt{\frac{1}{4}}\right) \end{array}$ |
|  |  | $22\left(-\sqrt{\frac{1}{2}} \sqrt{\frac{1}{2}}\right)$ |  |  |
| [411] | [33] [222] |  | $\widetilde{13}$ | [33] [222] |
|  | $\overline{11}$ | $\overline{22} \overline{33} \quad \overline{12} \sqrt{23}$ |  | $\overline{22} \sqrt{23} \quad \sqrt{12} \overline{33}$ |
|  |  | $\sqrt{\frac{1}{2}}-\sqrt{\frac{1}{2}}$ |  | 10 |
|  |  | $\begin{array}{ll}\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}}\end{array}$ | 23 | $0 \quad-1$ |

for $(T=0, S=0)$. In the molecular basis the same states have a richer structure. From Refs. 1, 2, and 8 we obtain

$$
\begin{align*}
& N N(\text { molec })=\frac{1}{3}\left(\frac{\sqrt{5}}{4}\left(\left(s^{6}[6]\{33\}\right)-\left(p^{6}[6]\{33\}\right)\right)-\frac{\sqrt{3}}{4}\left(\left(s^{4} p^{2}[6]\{33\}\right)-\left(s^{2} p^{4}[6]\{33\}\right)\right)\right. \\
&\left.+\sqrt{2}\left(\left(s^{4} p^{2}[42]\{33\}\right)-\left(s^{2} p^{4}[42]\{33\}\right)\right)-\sqrt{2}\left(\left(s^{4} p^{2}[42]\{51\}\right)-\left(s^{2} p^{4}[42]\{51\}\right)\right)\right] \\
& \begin{aligned}
\Delta \Delta(\text { molec })=\frac{1}{\sqrt{45}} & {\left[\frac{\sqrt{5}}{2}\left(\left(s^{6}[6]\{33\}\right)-\left(p^{6}[6]\{33\}\right)\right)-\frac{\sqrt{3}}{2}\left(\left(s^{4} p^{2}[6]\{33\}\right)-\left(s^{2} p^{4}[6]\{33)\right)\right.\right.} \\
& \left.+2 \sqrt{2}\left(\left(s^{4} p^{2}[42]\{33\}\right)-\left(s^{2} p^{4}[42]\{33\}\right)\right)+\frac{5}{\sqrt{2}}\left(\left(s^{4} p^{2}[42]\{51\}\right)-\left(s^{2} p^{4}[42]\{51\}\right)\right)\right] \\
C C(\text { molec })=\frac{1}{\sqrt{5}} & {\left[\frac{\sqrt{5}}{2}\left(\left(s^{6}[6]\{33\}\right)-\left(p^{6}[6]\{33\}\right)\right)-\frac{\sqrt{3}}{2}\left(\left(s^{4} p^{2}[6]\{33\}\right)-\left(s^{2} p^{4}[6]\{33\}\right)\right)\right.}
\end{aligned}  \tag{4.3}\\
&\left.\quad-\frac{1}{\sqrt{2}}\left(\left(s^{4} p^{2}[42]\{33\}\right)-\left(s^{2} p^{4}[42]\{33\}\right)\right)\right]
\end{align*}
$$

for $T=0, S=1$ (or $T=1, S=0$ ), and

$$
\begin{align*}
& \begin{aligned}
& N N(\text { molec })=\frac{1}{\sqrt{45}}\left(\frac{\sqrt{30}}{4}\left(\left(s^{5} p[51]\{42\}\right)-\left(s p^{5}[51]\{42\}\right)\right)-\frac{\sqrt{5}}{2}\left(s^{3} p^{3}[51]\{42\}\right)\right. \\
&\left.+2\left(s^{3} p^{3}[33]\{42\}\right)+6\left(s^{3} p^{3}[33]\{6\}\right)\right) \\
& \Delta \Delta(\text { molec })=\frac{1}{\sqrt{45}} {\left[\frac{\sqrt{30}}{2}\left(\left(s^{5} p[51]\{42\}\right)-\left(s p^{5}[51]\{42\}\right)\right)-\sqrt{5}\left(s^{3} p^{3}[51]\{42\}\right)\right.} \\
&\left.+4\left(s^{3} p^{3}[33]\{42\}\right)-3\left(s^{3} p^{3}[33]\{6\}\right)\right), \\
& C C(\text { molec })=\frac{1}{3}\left[\frac{\sqrt{6}}{2}\left(\left(s^{5} p[51]\{42\}\right)-\left(s p^{5}[51]\{42\}\right)\right)-\left(s^{3} p^{3}[51]\{42\}\right)-\sqrt{5}\left(s^{3} p^{3}[33]\{42\}\right)\right)
\end{aligned}
\end{align*}
$$

for $(T=0, S=0)$, i.e., for each $s^{n} p^{n-3}(n \neq 3)$, a complementary configuration appears in the molecular basis. For other six-quark states the limiting configurations can be read directly from Table I of Ref. 1 by making the replacement $\sigma \rightarrow s, \pi \rightarrow p$.

Due to the complex structure of the states, we found it more convenient to work out analytically the six-quark matrix elements in the ( $r, l$ ) single-particle basis (Ref. 1, Table I, second column) and return to the ( $s, p$ ) states at the level of two-body matrix elements only.

In the second and fourth columns of Tables V and VI we give the expectation values of the Hamiltonian (3.1) for each six-quark state in the cluster $(R, L)$ basis and in the molecular ( $r, l$ ) basis, respectively. The third column is the result of diagonalization of a $3 \times 3$ matrix in the

TABLE IV. Two-body matrix elements for the confinement potential, Eq. (3.2), and the spin-spin interaction of Eq. (3.3) with the parameters of Eq. (3.4).

|  | $v_{c}$ | $v_{\sigma}$ |
| :--- | :---: | :---: |
| $\langle s s\| v\|s s\rangle$ | 388.62 | -73.32 |
| $\langle p p\| v\|p p\rangle$ | 130.36 | -54.99 |
| $\langle s s\| v\|p p\rangle$ | 129.13 | -36.66 |
| $\langle s p\| v\|s p\rangle$ | 259.49 | -36.66 |

( $R, L$ ) basis. This is what the cluster model calculations of Ref. 9 would give at zero separation. The fifth column and beyond are the results of diagonalization of matrices of various sizes in the molecular ( $r, l$ ) basis.

For both sectors, the $3 \times 3(r, l)$ matrix gives higher energies than the ( $R, L$ ) basis. However, the enlargement of the space by the addition of the asymptotically unphysical $42^{ \pm}, 51^{ \pm}$configurations has a dramatic effect in lowering the ground state energies in both sectors. The last column in these tables gives the amplitudes of the corresponding basis states in the ground state wave function.

Let us first look at the effect of the nonasterisked isospin-spin states neglected by Harvey. In the examples considered here, these are the three $\{321\}$ states of the $T=0, S=1$ sector and the $\{222\}$ state of the $T=0, S=0$ sector. One sees that they contribute only 2 MeV and 1 MeV , respectively, to the lowering of the ground state. The other nonasterisked configurations have a similar effect. The reason is that they couple to other states only through the spin-spin interaction (and the tensor interaction if included), and this contribution is much smaller than that of the confining potential. Therefore all nonasterisked configurations can be safely neglected.

In both the $(0,1)$ and $(0,0)$ sectors there are three basis states which appear to dominate the lowest eigenstate. In

TABLE V. Results of the diagonalization of the Hamiltonian (3.1) in various six-quark bases, built from cluster model $R, L$ or molecular $r, l$ orbitals, for the $T=0, S=1$ sector. Column one: the basis state; column two: diagonal matrix elements in the cluster model; column three: eigenvalues $(3 \times 3)$ for the cluster model; column four: diagonal matrix elements for the molecular orbital basis, columns five-ten: eigenvalues for matrices of various sizes; column eleven: the components of the lowest state associated with the largest matrix.

| Channel | $R, L$ (cluster) |  | $r, l$ (molecular) |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $1 \times 1$ | $3 \times 3$ | $1 \times 1$ | $3 \times 3$ | $4 \times 4$ | $5 \times 5$ | $6 \times 6$ | $7 \times 7$ | $10 \times 10$ | Lowest state components |
| $N N$ | 903 | 592 | 961 | 952 | 423 | 415 | 413 | 311 | 309 | 0.84784 |
| $\Delta \Delta$ | 1372 | 1163 | 1687 | 1594 | 1590 | 1440 | 1308 | 1292 | 1285 | 0.03965 |
| $C C$ | 1083 | 1603 | 1840 | 1942 | 1939 | 1869 | 1495 | 1494 | 1490 | 0.05947 |
| $\left(42^{+}[6]\{33\}\right)$ |  |  | 2099 |  | 2635 | 2344 | 2158 | 1578 | 1573 | 0.43544 |
| $\left(42^{+}[42]\{33\}\right)$ |  |  | 2223 |  |  | 2742 | 2344 | 2159 | 1655 | 0.09132 |
| $\left(42^{+}[42]\{51\}\right)$ |  |  | 1658 |  |  |  | 2750 | 2344 | 2107 | $-0.03052$ |
| $\left(51^{+}[6]\{33\}\right)$ |  |  | 1613 |  |  |  |  | 2903 | 2162 | 0.27613 |
| $(42+[51]\{321\})$ |  |  | 1879 |  |  |  |  |  | 2345 | $-0.01055$ |
| $(42+[42]\{321\})$ |  |  | 2136 |  |  |  |  |  | 2722 | $-0.01678$ |
| (33[42] 321$\}$ ) |  |  | 2485 |  |  |  |  |  | 2933 | -0.023 19 |

the $(0,1)$ sector, these are the first, fourth, and seventh in the list, and together carry a total probability of $98.5 \%$. In the $(0,0)$ sector the states are the first, fourth, and fifth, carrying a total probability of $99.9 \%$. As discussed further in the following, the $\Delta \Delta$ and $C C$ basis states apparently are not important. To verify this, we have diagonalized the corresponding $3 \times 3$ Hamiltonian matrices in each of these sectors.
For the $(0,1)$ sector we obtain a lowest eigenvalue of 329 MeV compared with 309 MeV for the $10 \times 10$ matrix, and 592 MeV for the ( $R, L$ ) cluster $3 \times 3$ matrix.

For the ( 0,0 ) sector, we obtain 215 MeV , only 2 MeV higher than using the $6 \times 6$ matrix, in contrast with 914 MeV for the ( $R, L$ ) cluster $3 \times 3$ matrix.

These results show that the molecular $N N$ basis state is the main component in the lowest eigenstate, and that molecular $\Delta \Delta$ and $C C$ components are not important. It also shows that among the configurations $r^{n} l^{6-n}$, with $n$ different from 3, the totally symmetric state ${ }^{6}$ is far more important than the mixed symmetry states [42] for $T=0, S=1$. Its role can be explained through its large coupling to the $N N$ state, dominated by the confining potential. Table IV shows, in fact, that the two-body matrix elements are a few times larger for the confining potential than for the spin-spin interaction. It turns out systemati-
cally that whenever the symmetry of the wave functions allows only a spin-spin coupling, this is an order of magnitude smaller than the other matrix elements and has little effect in the diagonalization, as shown above for nonasterisked configurations. The three states which we have identified in each sector are sufficient to obtain results dramatically lower than the three component ( $R, L$ ) results.

We can understand more about the first three vectors in both models with the help of the details given below. An alternative way would have been to work directly with the symmetry states instead of performing the transformations (4.1)-(4.4). In Tables VII and VIII we give the matrix elements of $H$, Eq. (3.1), for the symmetry states for the $T=0, S=1$ and $T=0, S=0$ sectors, respectively, in both the cluster and molecular models. Let us consider the $T=0, S=1$ sector. From Eq. (4.1) we see that within the cluster model the $s^{4} p^{2}$ limiting configuration appears with probability $0.89,0.91$, and 0.2 in the $N N, \Delta \Delta$, and $C C$ states, respectively. One might expect that the $C C$ state would be below the nearly degenerate $N N$ and $\Delta \Delta$ states because it carries less diagonal excitation energy due to the smaller probability of two quarks in the $p$ state. But from Table VII one can see that the coupling between symmetry states has an im-

TABLE VI. Same as Table V, but for the $T=0, S=0$ sector and at most a $6 \times 6$ matrix in the molecular basis.

| Channel | $R, L$ (cluster) |  | $r, l$ (molecular) |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $1 \times 1$ | $3 \times 3$ | $1 \times 1$ | $3 \times 3$ | $4 \times 4$ | $5 \times 5$ | $6 \times 6$ | Lowest state Components |
| $N N$ | 1046 | 914 | 1070 | 1068 | 253 | 214 | 213 | 0.73981 |
| $\Delta \Delta$ | 1446 | 1251 | 1644 | 1606 | 1604 | 1155 | 1154 | 0.00936 |
| CC | 1800 | 2128 | 2226 | 2266 | 2266 | 1605 | 1594 | 0.02428 |
| (42-[51]\{42\}) |  |  | 1592 |  | 2408 | 2282 | 2045 | 0.64484 |
| ( $51^{-}[51]\{42\}$ ) |  |  | 1456 |  |  | 2731 | 2285 | 0.19061 |
| (33[33]\{222\}) |  |  | 2038 |  |  |  | 2735 | 0.02979 |

TABLE VII. The matrix of $H$ in the symmetry basis $|i\rangle(i=1,3)$ used to define the $N N, \Delta \Delta$, and $C C$ states in the $T=0, S=1$ sector. In the cluster model, $|1\rangle=\left(s^{6}[6]\{33\}\right) ;|2\rangle=\left(s^{4} p^{2}[42]\{33\}\right)$; $|3\rangle=\left(s^{4} p^{2}[42]\{51\}\right)$. In the molecular orbital basis, $|1\rangle=\frac{1}{4}\left(\sqrt{5}\left(\left(s^{6}[6]\{33\}\right)-\left(p^{6}[6]\{33\}\right)\right)\right.$ $\left.-\sqrt{3}\left(\left(s^{4} p^{2}[6]\{33\}\right)-\left(s^{2} p^{4}[6]\{33\}\right)\right)\right) ; \quad|2\rangle=1 / \sqrt{2}\left(\left(s^{4} p^{2}[42]\{33\}\right)-\left(s^{2} p^{4}[42]\{33\}\right)\right) ; \quad|3\rangle$ $=1 / \sqrt{2}\left(\left(s^{4} p^{2}[42]\{51\}\right)-\left(s^{2} p^{4}[42]\{51\}\right)\right)$.

|  | $R, L$ (cluster) |  |  | $r, l$ (molecular) |  |  |
| :--- | ---: | :---: | :---: | :---: | :---: | :---: |
| State | 1 | 2 | 3 | 1 | 2 | 3 |
| 1 | 726.3 | -265.6 | 103.1 | 1590.1 | -331.1 | 105.9 |
| 2 | -265.6 | 1447.0 | 206.4 | -331.1 | 1514.4 | 347.6 |
| 3 | 103.1 | 206.4 | 1185.2 | 105.9 | 347.6 | 1383.4 |

portant role in changing this picture. We find that it lowers the $N N$ state from 1270 MeV to 903 MeV and it lifts the $\Delta \Delta$ state from 1254 MeV to 1372 MeV and the CC state from 917 MeV to 1185 MeV . We stress that the coupling is not always pure magnetic. In the abovementioned case the [6]\{33\} and [42]\{33\} states have a nonzero spin-independent coupling (confinement) due to their identical isospin-spin structure. This contribution represents $92 \%$ of the entire coupling of the two states. The $N N, \Delta \Delta$, and $C C$ approach each other sufficiently to couple among themselves and produce the results of the third column of Table V .

For molecular orbitals the situation is more complicated due to the excitation of two, four, and six quarks into $p$ states. It turns out that the symmetry states [6] 333$\}$ and $[42]\{33\}$ appear nearly degenerate and slightly higher than the [42] $\{51\}$ state (see Table VII). This indicates that a part of the excitation of the $p^{6}$ configuration appearing in [6] $\{33\}$ is compensated by the spin-spin interaction. The coupling between the symmetry states pulls down the $N N$ state separating it from the $\Delta \Delta$ state by about 700 MeV . The rernaining coupling becomes so weak that the $N N, \Delta \Delta$, and $C C$ states practically do not mix any more, as seen from Table $V$.

A similar discussion can be carried out for the $T=0, S=0$ sector with the help of Eqs. (4.2) and (4.4) and Table VIII. The conclusion is that the Harvey transformations (4.1)-(4.4) produce an important subdiagonalization.

By extrapolation one can also draw conclusions about the $T=1, S=0$ sector. This differs from the $T=0, S=1$ sector through the effect of the spin-spin interaction only. As the coupling is dominated by the confinement potential, one would expect that the most important states for
the $T=1, S=0$ sector should be the same as for the $T=0, S=1$ sector.

For the $T=1, S=1$ sector, one can certainly neglect all the nonasterisked isospin-spin states as for the other cases. This sector contains $N N, \Delta \Delta$, and $N \Delta$ as physical states. The $N N$ state probably has non-negligible coupling to unphysical states of the type (51-[51]\{42\}) and (41-[51]\{42\}). As these have a multiplicity of two each, there will be in all five important basis vectors contributing to the lowest state after the Harvey transformation. ${ }^{2,8}$

The calculations discussed above were done for a value of $\beta$ which minimizes the ground state energy of a threequark system. Such a value does not minimize the energy of a six-quark system. We therefore studied the effect of the six-quark energies due to variation of $\beta$. The result is displayed in Figs. 1 and 2 for the ( $T=0, S=1$ ) and ( $T=0, S=0$ ) sectors, respectively. The new minimum is reached within $10 \%$ of the three-quark value in all cases, and the qualitative discussion above holds.

A quantity of interest is the $p$-state occupation. For the ten state molecular basis, we find, for the ground state, the probabilities in the $(0,1)$ sector

$$
\begin{aligned}
& P\left(s^{6}\right)=0.3746, \quad P\left(s^{4} p^{2}\right)=0.3801 \\
& P\left(s^{2} p^{4}\right)=0.2459, \quad P\left(p^{6}\right)=0.0002
\end{aligned}
$$

for a total $p$-quark probability of $29 \%$; the number of $p$ quarks is six times this number. In the three state cluster basis, the corresponding number is only $6.5 \%$.

In the $(0,0)$ sector, we find

$$
P\left(s^{5} p\right)=0.1286, \quad P\left(s^{3} p^{3}\right)=0.5663, \quad P\left(s p^{5}\right)=0.3062
$$

for a p-quark probability of $56 \%$ compared with the

TABLE VIII. Same as Table VII, but for the $T=0, S=0$ sector. In the cluster model, $|1\rangle=-\left(s^{5} p[51]\{42\}\right), \quad|2\rangle=-\left(s^{3} p^{3}[33]\{42\}\right) ;|3\rangle=-\left(s^{3} p^{3}[33]\{6\}\right)$. In the molecular basis, $|1\rangle=-\sqrt{6} / 4\left(\left(s^{5} p[51]\{42\}\right)-\left(s p^{5}[51]\{42\}\right)+\frac{1}{2}\left(s^{3} p^{3}[51]\{42\}\right) ; \quad|2\rangle=-\left(s^{3} p^{3}[33]\{42\}\right) ; \quad|3\rangle\right.$ $=-\left(s^{3} p^{3}[33]\{6\}\right)$.

|  | $R, L$ (cluster) |  |  | $r, l$ (molecular) |  |  |  |
| :---: | ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| State | 1 | 2 | 3 | 1 | 2 | 3 |  |
| 1 | 1033.8 | -204.5 | -107.1 | 1681.6 | -343.5 | -142.1 |  |
| 2 | -204.5 | 2047.3 | -215.1 | -343.5 | 2047.3 | -215.1 |  |
| 3 | -107.1 | -215.1 | 1211.4 | -142.1 | -215.1 | 1211.4 |  |



FIG. 1. The lowest state energy as a function of the oscillator size parameter $\beta$ for the $T=0, S=1$ sector. The arrow indicates the three-quark minimum.
three-state cluster basis result of $27 \%$. The $p$-quark probabilities are significantly higher than what is obtained in the more restrictive cluster calculations.

The quark mean-square radius is proportional to $\frac{3}{2}$ times the $s$-quark probability plus $\frac{5}{2}$ times the $p$-quark probability, and is also proportional to $\beta^{2}$. This leads to an increase in the rms radius, relative to three-quark bags, of $14 \%$ for the $(0,1)$ sector and $22 \%$ for the $(0,0)$ sector.

More generally, one requires the expectation value of the Hamiltonian as a function of $Z$, and here we have calculated only the $Z=0$ point relative to $Z=\infty$. As


FIG. 2. Same as Fig. 1, but for the $T=0, S=0$ sector.
should be well known, even this does not solve the scattering or bound state problem, because one must calculate the dynamics of the process (see, for example, Harvey, LeTourneux, and Lorazo, Ref. 9).

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