# Important configurations for $N N$ processes in a Goldstone boson exchange model 

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#### Abstract

We study the short-range nucleon-nucleon interaction in a nonrelativistic chiral constituent quark model by diagonalizing a Hamiltonian containing linear confinement and a Goldstone boson exchange interaction between quarks. A finite six-quark basis obtained from single particle cluster model states was previously used. Here we show that the configurations which appear naturally through the use of molecular orbitals, instead of cluster model states, are much more efficient in lowering the six-quark energy. [S0556-2813(99)01403-X]


PACS number(s): 24.85.+p, 12.39.Fe, 13.75.Cs, 21.30. -x

## I. INTRODUCTION

Constituent quark models have been applied to the study of the nucleon-nucleon interaction. In a category of such models the Hamiltonian contains a kinetic term, a confinement term, and an effective one-gluon exchange (OGE) term. These models explain the short-range repulsion in the $N N$ systems as due to the color-magnetic part of the OGE interaction combined with quark interchanges between the $3 q$ clusters. Nevertheless, an effective meson-exchange potential, introduced through the coupling of mesons to $3 q$ cluster collectively, was required in order to reproduce the intermediate- and long-range attraction (for a review see, for example, Refs. [1-3]).

Another category is the hybrid models [4-6]. There, in addition to the OGE interaction, the quarks belonging to different $3 q$ clusters interact via pseudoscalar and scalar meson exchange. In these models the short-range repulsion in the $N N$ system is still attributed to the OGE interaction between the constituent quarks. The medium- and long-range attraction are due to meson exchange, as expected.

In a recent exploratory work [7], by using the BornOppenheimer approximation, we calculated an effective $N N$ interaction at zero separation distance, within the constituent quark model [8-10]. In this model the quarks interact via Goldstone boson exchange (GBE) instead of OGE of conventional models, and the hyperfine splitting in hadrons is obtained from the short-range part of the GBE interaction. An important merit of the GBE model is that it reproduces the correct order of positive and negative parity states in both nonstrange [9] and strange baryons [10] in contrast to any OGE model. In Ref. [7] we showed that the same short-range part of the GBE interaction, also induces a short-range repulsion in the $N N$ system. Moreover, the long- and middlerange attraction of the $N N$ potential will automatically appear due to the presence of a Yukawa potential tail in the qq interaction and due to $2 \pi$ (or sigma) exchanges.

In Ref. [7] the height of the repulsive core was about 800 MeV for the ${ }^{3} S_{1}$ channel and 1300 MeV for the ${ }^{1} S_{0}$ channel. Such a result has been obtained from diagonalizing the Hamiltonian of Ref. [9] in a six-quark cluster model basis

[^0]built from harmonic oscillator states containing up to two quanta of excitation. The six-quark states have orbital symmetries $[6]_{O}$ and $[42]_{O}$, so that they contain configurations of type $s^{6}, s^{4} p^{2}$, and $s^{5} 2 s$, with the center of mass motion removed. In the flavor-spin space only the symmetries [33], [51], and [411] were retained. As shown in Ref. [7] they produce the most important five basis states allowed by the Pauli principle. Due to the specific flavor-spin structure of the GBE interaction, we found that the state $\left|s^{4} p^{2}[42]_{o}[51]_{F S}\right\rangle$ was highly dominant at zero-separation between nucleons. The symmetry structure of this state implies the existence of a node in the nucleon-nucleon $S$-wave relative motion wave function at short distances. This nodal structure will induce an additional effective repulsion in dynamical calculations based, for example, on the resonating group method.

A central issue of the $N N$ problem is the construction of an adequate six-quark basis states. In principle the choice of basis is arbitrary if a sufficiently large basis is considered in the Hamiltonian diagonalization. But, as in practice one considers a finite set, its choice is very important. Reference [11] advocated the use of molecular-type single particle orbitals instead of cluster model-type states. These orbitals have the proper axially and reflectionally symmetries and can be constructed from appropriate combinations of two-center Gaussians. At zero separation the six-quark states obtained from such orbitals contain certain $p^{n} s^{6-n}$ components which are missing in the cluster model basis. In Ref. [12] it has been shown that for an OGE model used in the calculations of the $N N$ potential they lead to a substantial lowering of the lowest eigenstate, used in the calculation of the $N N$ potential. The molecular orbitals have also the advantage of forming an orthogonal and complete basis while the cluster model (twocenter) states are not orthogonal and are overcomplete.

Due to the predominance ( $93 \%$ ) of only one component, namely, $\left|s^{4} p^{2}[42]_{o}[51]_{F S}\right\rangle$, in the ground state wave function obtained in a cluster model basis [7] the GBE model is a more chalenging case to test the efficiency of a molecular orbital basis than the OGE model, where there is some mixture of states (see, e.g., Refs. [1,12]). Here we show that by using molecular orbitals the height of the repulsion reduces by about 22 and $25 \%$ in the ${ }^{3} S_{1}$ and ${ }^{1} S_{0}$ channels, respectively.

The paper is organized as follows. In Sec. II we briefly recall the procedure of constructing six-quark states from

TABLE I. Results of the diagonalization of the Hamiltonian (22)-(26) for $I S=(01)$. Column 1 : basis states, column 2: diagonal matrix elements $(\mathrm{GeV})$, column 3: eigenvalues $(\mathrm{GeV})$ in increasing order, column 4: lowest state amplitudes of components given in column 1. The results correspond to $\beta=0.437 \mathrm{fm}$. The diagonal matrix elements $H_{i i}$ and the eigenvalues are relative to $2 m_{N}=1939 \mathrm{MeV}$ (see text).

| State | $H_{i i}-2 m_{N}$ | Eigenvalues $-2 m_{N}$ | Lowest state amplitudes |
| :--- | :---: | :---: | :---: |
| $\left\|33[6]_{o}[33]_{F S}\right\rangle$ | 2.616 | 0.718 | -0.04571 |
| $\left\|33[42]_{o}[33]_{F S}\right\rangle$ | 3.778 | 1.667 | 0.02479 |
| $\left\|33[42]_{o}[51]_{F S}\right\rangle$ | 1.615 | 1.784 | -0.31762 |
| $\left\|33[42]_{o}[411]_{F S}\right\rangle$ | 2.797 | 2.309 | 0.04274 |
| $\left\|42^{+}[6]_{o}[33]_{F S}\right\rangle$ | 3.062 | 2.742 | -0.07988 |
| $\left\|42^{+}[42]_{o}[33]_{F S}\right\rangle$ | 2.433 | 2.784 | 0.12930 |
| $\left\|42^{+}[42]_{o}[51]_{F S}\right\rangle$ | 0.850 | 3.500 | -0.93336 |
| $\left\|42^{+}[42]_{o}[411]_{F S}\right\rangle$ | 3.665 | 3.752 | 0.00145 |
| $\left\|51^{+}[6]_{o}[33]_{F S}\right\rangle$ | 2.910 | 4.470 | -0.01789 |

molecular orbital single particle states. In Sec. III we describe the GBE Hamiltonian [9]. In Sec. IV we present our results for zero-separation $N N$ interaction derived in the Born-Oppenheimer approximation for the $I S=(10)$ and (01) sectors. The last section is devoted to summary and conclusions.

## II. SIX-QUARK STATES FROM MOLECULAR ORBITALS

Here we follow closely Ref. [11] where the use of molecular orbitals in the construction of six-quark states was originally proposed, instead of commonly used cluster model states. Let us denote by $Z$ the separation coordinate between the centers of the two clusters. At finite $Z$, in the simplest cluster model basis, each of the six quarks is decribed by an orbital wave function represented by a Gaussian centered either at $Z / 2$ or $-Z / 2$. These nonorthogonal states are denoted by $R$ (right) and $L$ (left), respectively,

$$
\begin{equation*}
R(\vec{r})=\Psi(\vec{r}-\vec{Z} / 2), \quad L(\vec{r})=\Psi(\vec{r}+\vec{Z} / 2) \tag{1}
\end{equation*}
$$

Alternatively, in a molecular basis we consider the two lowest states, $\sigma$ which is even and $\pi$ which is odd. These could be either the solutions of a static, axially, and reflectionally symmetric-independent particle model Hamiltonian (see, for example, Ref. [13]) or, as for the present purpose, can be constructed from $R$ and $L$ states.

First we introduce pseudoright and pseudoleft states $r$ and $l$ starting from the molecular orbitals $\sigma$ and $\pi$ as

$$
\left[\begin{array}{l}
r  \tag{2}\\
l
\end{array}\right]=2^{-1 / 2}(\sigma \pm \pi) \quad \text { for all } Z
$$

where

$$
\begin{equation*}
\langle r \mid r\rangle=\langle l \mid l\rangle=1, \quad\langle r \mid l\rangle=0 . \tag{3}
\end{equation*}
$$

On the other hand, starting from the cluster model states, one can construct good parity, orthonormal states for all $Z$ by setting

$$
\left[\begin{array}{l}
\sigma  \tag{4}\\
\pi
\end{array}\right]=[2(1 \pm\langle R \mid L\rangle)]^{-1 / 2}(R \pm L)
$$

which, introduced in Eq. (2), gives

$$
\left[\begin{array}{c}
r  \tag{5}\\
l
\end{array}\right]=\frac{1}{2}\left[\frac{R+L}{(1+\langle R \mid L\rangle)^{1 / 2}} \pm \frac{R-L}{(1-\langle R \mid L\rangle)^{1 / 2}}\right] .
$$

At $Z \rightarrow 0$ one has $\sigma \rightarrow s$ and $\pi \rightarrow p$ (with $m=0, \pm 1$ ), so that

$$
\left[\begin{array}{l}
r  \tag{6}\\
l
\end{array}\right]=2^{1 / 2}(s \pm p)
$$

and at $Z \rightarrow \infty$ one has $r \rightarrow R$ and $l \rightarrow L$.
From ( $r, l$ ) as well as from ( $\sigma, \pi$ ) orbitals one can construct six-quark states of required permutation symmetry. For the $S_{6}$ symmetries relevant for the $N N$ problem the transformations between six-quark states expressed in terms of $(r, l)$ and $(\sigma, \pi)$ states are given in Table I of Ref. [11]. This table shows that in the limit $Z \rightarrow 0$ six-quark states obtained from molecular orbitals contain configurations of type $s^{n} p^{6-n}$ with $n=0,1, \ldots, 6$. For example, the $[6]_{O}$ state contains $s^{6}, s^{6} p^{4}, s^{2} p^{4}$, and $p^{6}$ configurations and the [42] $]_{O}$ state associated to the $S$-channel contains $s^{4} p^{2}$ and $s^{2} p^{4}$ configurations. This is in contrast to the cluster model basis where $[6]_{O}$ contains only $s^{6}$ and $[42]_{O}$ only $s^{4} p^{2}$ configurations [14]. This suggests that the six-quark basis states constructed from molecular orbitals form a richer basis without introducing more single particle states. Here we examine its role in lowering the ground state energy of a six-quark system described by the Hamiltonian introduced in the next section.

Using Table I of Ref. [11] we find that the six-quark basis states needed for the ${ }^{3} S_{1}$ or ${ }^{1} S_{0}$ channels are

$$
\begin{align*}
\left|33[6]_{O}[33]_{F S}\right\rangle= & \left.\frac{1}{4} \right\rvert\,\left[\sqrt{5}\left(s^{6}-p^{6}\right)-\sqrt{3}\left(s^{4} p^{2}-s^{2} p^{4}\right)\right] \\
& \left.\times[6]_{O}[33]_{F S}\right\rangle  \tag{7}\\
\left|33[42]_{O}[33]_{F S}\right\rangle= & \sqrt{\frac{1}{2}}\left|\left[s^{4} p^{2}-s^{2} p^{4}\right][42]_{O}[33]_{F S}\right\rangle \tag{8}
\end{align*}
$$

$$
\begin{equation*}
\left|33[42]_{O}[51]_{F S}\right\rangle=\sqrt{\frac{1}{2}}\left|\left[s^{4} p^{2}-s^{2} p^{4}\right][42]_{O}[51]_{F S}\right\rangle, \tag{9}
\end{equation*}
$$

$$
\begin{align*}
\left|33[42]_{O}[411]_{F S}\right\rangle= & \sqrt{\frac{1}{2}}\left|\left[s^{4} p^{2}-s^{2} p^{4}\right][42]_{O}[411]_{F S}\right\rangle,  \tag{10}\\
\left|42^{+}[6]_{O}[33]_{F S}\right\rangle= & \left.\frac{1}{4} \sqrt{\frac{1}{2}} \right\rvert\,\left[\sqrt{15}\left(s^{6}+p^{6}\right)-\left(s^{4} p^{2}+s^{2} p^{4}\right)\right] \\
& \left.\times[6]_{O}[33]_{F S}\right\rangle,  \tag{11}\\
\left|42^{+}[42]_{O}[33]_{F S}\right\rangle= & \sqrt{\frac{1}{2}}\left|\left[s^{4} p^{2}+s^{2} p^{4}\right][42]_{O}[33]_{F S}\right\rangle,  \tag{12}\\
\left|42^{+}[42]_{O}[51]_{F S}\right\rangle= & \sqrt{\frac{1}{2}}\left|\left[s^{4} p^{2}+s^{2} p^{4}\right][42]_{O}[51]_{F S}\right\rangle,  \tag{13}\\
\left|42^{+}[42]_{O}[411]_{F S}\right\rangle= & \sqrt{\frac{1}{2}}\left|\left[s^{4} p^{2}+s^{2} p^{4}\right][42]_{O}[411]_{F S}\right\rangle,  \tag{14}\\
\left|51^{+}[6]_{O}[33]_{F S}\right\rangle= & \left.\frac{1}{4} \right\rvert\,\left[\sqrt{3}\left(s^{6}-p^{6}\right)+\sqrt{5}\left(s^{4} p^{2}-s^{2} p^{4}\right)\right] \\
& \left.\times[6]_{O}[33]_{F S}\right\rangle, \tag{15}
\end{align*}
$$

where the notation 33 and $\mathrm{mn}^{+}$in the left-hand side of each equality above means $r^{3} l^{3}$ and $r^{m} l^{n}+r^{n} l^{m}$ as in Ref. [11] (see also discussion below). Each wave function contains an orbital part $(O)$ and a flavor-spin part $(F S)$ which combined with the color singlet [222] $]_{C}$ state gives rise to a totally antisymmetric state. We restricted the flavor-spin states to $[33]_{F S},[51]_{F S}$, and $[411]_{F S}$ according to the discussion given in Sec. II of Ref. [7] where the most important states have been selected by using a schematic version of the Hamiltonian introduced in the next section.

In a cluster model, the most important basis states built from $s$ and $p$ harmonic oscillator states are

$$
\begin{gather*}
\left|s^{6}[6]_{o}[33]_{F S}\right\rangle,  \tag{16}\\
\left|s^{4} p^{2}[42]_{o}[33]_{F S}\right\rangle,  \tag{17}\\
\left|s^{4} p^{2}[42]_{o}[51]_{F S}\right\rangle,  \tag{18}\\
\left|s^{4} p^{2}[42]_{o}[411]_{F S}\right\rangle . \tag{19}
\end{gather*}
$$

These are the first four states given by Eq. (8) of Ref. [7]. The fifth one, containing the configuraiton $s^{5} 2 s$ is not considered here. Its role in lowering the ground state energy by a few MeV proved to be negligible. Besides being poorer in $s^{n} p^{6-n}$ configurations, as explained above, the number of basis states is smaller in the cluster model although we deal with the same $[f]_{O}$ and $[f]_{F S}$ symmetries and the same harmonic oscillator states $s$ and $p$ in both cases. This is due to the existence of three-quark clusters only in the cluster model states, while the molecular basis also allows configurations with five quarks to the left and one to the right, or vice versa, or four quarks to the left and two to the right or vice versa. At large separations these states act as "hidden
color'" states but at zero separation they bring a significant contribution, as we shall see below.

The matrix elements of the Hamiltonian (22) are calculated in the basis (7)-(15) by using the fractional parentage technique described in Refs. [14,15] and also applied in Ref. [7]. A program based on mathematica [16] has been created for this purpose. In this way every six-body matrix element reduces to a linear combination of two-body matrix elements of either symmetric or antisymmetric states for which Eqs. (3.3) of Ref. [8] can be used to integrate in the spin-flavor space. Then the linear combinations contain orbital two-body matrix elements of the type $\langle s s| V_{\gamma}|s s\rangle,\langle s s| V_{\gamma}|p p\rangle,\langle s p| V_{\gamma}|s p\rangle,\langle s p| V_{\gamma}|p s\rangle, \quad$ and $\langle p p| V_{\gamma}|p p\rangle_{L=0}$ where $\gamma=\pi, \quad \eta$, or $\eta^{\prime}$, see Eq. (25). Here we study the case $Z=0$ for which the following harmonic oscillator states are used:

$$
\begin{gather*}
|s\rangle=\pi^{-3 / 4} \beta^{-3 / 2} \exp \left(-r^{2} / 2 \beta^{2}\right)  \tag{20}\\
|p\rangle=8^{1 / 2} 3^{-1 / 2} \pi^{-1 / 4} \beta^{-5 / 2} r \exp \left(-r^{2} / 2 \beta^{2}\right) Y_{l m} \tag{21}
\end{gather*}
$$

In this basis the orbital two-body matrix elements of the linear confinement $V_{\text {conf }}=C r$ potential (23) are calculated analytically (see Appendix D of Ref. [7]).

## III. HAMILTONIAN

The GBE Hamiltonian considered below has the form [9]

$$
\begin{align*}
H= & \sum_{i} m_{i}+\sum_{i} \frac{\vec{p}_{i}^{2}}{2 m_{i}}-\frac{\left(\sum_{i} \vec{p}_{i}\right)^{2}}{2 \sum_{i} m_{i}}+\sum_{i<j} V_{\mathrm{conf}}\left(r_{i j}\right) \\
& +\sum_{i<j} V_{\chi}\left(r_{i j}\right) \tag{22}
\end{align*}
$$

with the linear confining interaction

$$
\begin{equation*}
V_{\mathrm{conf}}\left(r_{i j}\right)=-\frac{3}{8} \lambda_{i}^{c} \cdot \lambda_{j}^{c} C r_{i j} \tag{23}
\end{equation*}
$$

and the spin-spin component of the GBE interaction in its $\mathrm{SU}_{F}$ (3) form

$$
\begin{align*}
V_{\chi}\left(r_{i j}\right)= & \left\{\sum_{F=1}^{3} V_{\pi}\left(r_{i j}\right) \lambda_{i}^{F} \lambda_{j}^{F}+\sum_{F=4}^{7} V_{K}\left(r_{i j}\right) \lambda_{i}^{F} \lambda_{j}^{F}\right. \\
& \left.+V_{\eta}\left(r_{i j}\right) \lambda_{i}^{8} \lambda_{j}^{8}+V_{\eta^{\prime}}\left(r_{i j}\right) \lambda_{i}^{0} \lambda_{j}^{0}\right\} \vec{\sigma}_{i} \cdot \vec{\sigma}_{j}, \tag{24}
\end{align*}
$$

with $\lambda^{0}=\sqrt{2 / 3} \mathbf{1}$, where $\mathbf{1}$ is the $3 \times 3$ unit matrix. The interaction (24) contains $\gamma=\pi, K, \eta$, and $\eta^{\prime}$ meson-exchange terms and the form of $V_{\gamma}\left(r_{i j}\right)$ is given as the sum of two distinct contributions: a Yukawa-type potential containing the mass of the exchanged meson and a short-range contribution of opposite sign, the role of which is crucial in baryon spectroscopy. For a given meson $\gamma$, the exchange potential is

TABLE II. Same as Table I but for $I S=(10)$.

| State | $H_{i i}-2 m_{N}$ | Eigenvalues $-2 m_{N}$ | Lowest state amplitudes |
| :--- | :---: | :---: | :---: |
| $\left\|33[6]_{O}[33]_{F S}\right\rangle$ | 3.300 | 1.083 | -0.02976 |
| $\left\|33[42]_{o}[33]_{F S}\right\rangle$ | 4.367 | 2.252 | 0.01846 |
| $\left\|33[42]_{O}[51]_{F S}\right\rangle$ | 2.278 | 2.279 | -0.20460 |
| $\left\|33[42]_{o}[411]_{F S}\right\rangle$ | 3.191 | 2.945 | -0.04729 |
| $\left\|42^{+}[6]_{O}[33]_{F S}\right\rangle$ | 3.655 | 3.198 | -0.07215 |
| $\left\|42^{+}[42]_{O}[33]_{F S}\right\rangle$ | 2.796 | 3.317 | 0.13207 |
| $\left\|42^{+}[42]_{o}[51]_{F S}\right\rangle$ | 1.167 | 4.058 | -0.96531 |
| $\left\|42^{+}[42]_{o}[411]_{F S}\right\rangle$ | 4.405 | 4.459 | -0.00081 |
| $\left\|51^{+}[6]_{o}[33]_{F S}\right\rangle$ | 3.501 | 5.070 | -0.01416 |

$$
\begin{align*}
V_{\gamma}(r)= & \frac{g_{\gamma}^{2}}{4 \pi} \frac{1}{12 m_{i} m_{j}}\left\{\theta\left(r-r_{0}\right) \mu_{\gamma}^{2} \frac{e^{-\mu_{\gamma} r}}{r}\right. \\
& \left.-\frac{4}{\sqrt{\pi}} \alpha^{3} \exp \left[-\alpha^{2}\left(r-r_{0}\right)^{2}\right]\right\} . \tag{25}
\end{align*}
$$

For a system of $u$ and $d$ quarks only, as is the case here, the $K$ exchange does not contribute. In the calculations below we use the parameters of Refs. [9]. These are

$$
\begin{gather*}
\frac{g_{\pi q}^{2}}{4 \pi}=\frac{g_{\eta q}^{2}}{4 \pi}=0.67, \quad \frac{g_{\eta^{\prime} q}^{2}}{4 \pi}=1.206, \\
r_{0}=0.43 \mathrm{fm}, \alpha=2.91 \mathrm{fm}^{-1}, \\
C=0.474 \mathrm{fm}^{-2}, \quad m_{u, d}=340 \mathrm{MeV},  \tag{26}\\
\mu_{\pi}=139 \mathrm{MeV}, \quad \mu_{\eta}=547 \mathrm{MeV}, \quad \mu_{\eta^{\prime}}=958 \mathrm{MeV} .
\end{gather*}
$$

In principle it would be better to use a parametrization of the GBE interaction as given in Ref. [17] based on a semirelativistic Hamiltonian. However, in applying the quark cluster approach to two-baryon systems we are restricted to use a nonrelativistic kinematics and an $s^{3}$ wave function for the ground state baryon. With an $s^{3}$ variational solution the nonrelativistic Hamiltonian introduced above works generally well [18]. In particular, for the nucleon, the quantity $\langle N| H|N\rangle$ reaches its minimum at 969.6 MeV which is only about 30 MeV above the nucleon mass obtained in the dynamical three-body calculations of Ref. [9]. There the shifted Gaussian of Eq. (25) results from a pure phenomenological fit.

TABLE III. Parts of the energy expectation values $(\mathrm{GeV})$ of the dominant $6 q$ state in the cluster model and the molecular orbital basis for $I S=(01)$.

| Energy | Cluster model <br> $\left\|s^{4} p^{2}[42]_{O}[51]_{F S}\right\rangle$ | Molecular orbital <br> $\left\|42^{+}[42]_{O}[51]_{F S}\right\rangle$ |
| :--- | :---: | :---: |
| $K E$ | 2.840 | 3.139 |
| $V_{\text {conf }}$ | 0.385 | 0.364 |
| $V_{\chi}$ | -2.384 | -2.754 |
| $E$ | 0.841 | 0.749 |

## IV. RESULTS

We diagonalize the Hamiltonian (22) in the six-quark basis (7)-(15) and calculate the $N N$ interaction potential in the Born-Oppenheimer approximation

$$
\begin{equation*}
V_{N N}(Z)=\langle H\rangle_{Z}-\langle H\rangle_{\infty}, \tag{27}
\end{equation*}
$$

where $\langle H\rangle_{Z}$ is the lowest expectation value obtained from the diagonalization at a given $Z$ and $\langle H\rangle_{\infty}=2 m_{N}$ is the energy (mass) of two well separated nucleons. Here we study the case $Z=0$, relevant for short separation distances between the nucleons. In Tables I and II we present our results for $I S=(01)$ and (10), respectively, obtained from the diagonalization of $H$. From the diagonal matrix elements $H_{i i}$ as well as from the eigenvalues, the quantity $2 m_{N}$ $=1939 \mathrm{MeV}$ has been subtracted according to Eq. (27). Here $m_{N}$ is the nucleon mass calculated also variationally, with an $s^{3}$ configuration, as mentioned at the end of the previous section. This value is obtained for a harmonic oscillator parameter $\beta=0.437 \mathrm{fm}$ [19]. For sake of comparison with Ref. [7] we take same value of $\beta$ for the six-quark system as well.

In both $I S=(01)$ and (10) cases the effect of using molecular orbitals is rather remarkable in lowering the ground state energy as compared to the cluster model value obtained in the four-dimensional basis (16)-(19). Accordingly, the height of the repulsive core in the ${ }^{1} S_{3}$ channel is reduced from 915 MeV in the cluster model basis (see the Appendix) to 718 MeV in the molecular orbital basis. In the ${ }^{1} S_{0}$ channel the reduction is from 1453 to 1083 MeV . Thus the molecular orbital basis is much better, inasmuch as the same two single particle states $s$ and $p$ are used in both bases.

The previous study [7], performed in a cluster model basis indicated that the dominant configuration is associated to the symmetry $[42]_{O}[51]_{F S}$. It is the case here too and one can see from Tables I and II that the diagonal matrix element $H_{i i}$

TABLE IV. Same as Table III but for $I S=(10)$.

| Energy | Cluster model <br> $\left\|s^{4} p^{2}[42]_{O}[51]_{F S}\right\rangle$ | Molecular orbital <br> $\left\|42^{+}[42]_{o}[51]_{F S}\right\rangle$ |
| :--- | :---: | :---: |
| $K E$ | 2.840 | 3.139 |
| $V_{\text {conf }}$ | 0.385 | 0.364 |
| $V_{\chi}$ | -1.840 | -2.437 |
| $E$ | 1.385 | 1.066 |

TABLE V. Results of the diagonalization of the Hamiltonian (22)-(26) for $I S=(01)$. Column 1: basis states, column 2: diagonal matrix elements $(\mathrm{GeV})$, column 3: eigenvalues $(\mathrm{GeV})$ in increasing order for a $4 \times 4$ matrix, column 4 : components of the lowest state. The results correspond to $\beta=0.437 \mathrm{fm}$. The diagonal matrix elements and the eigenvalues are relative to $2 m_{N}=1939 \mathrm{MeV}$.

| State | Diag. elem $-2 m_{N}$ | Eigenvalues $-2 m_{N}$ | Lowest state amplitudes |
| :--- | :---: | :---: | :---: |
| $\left\|s^{6}[6]_{o}[33]_{F S}\right\rangle$ | 2.346 | 0.915 | -0.10686 |
| $\left\|s^{4} p^{2}[42]_{O}[33]_{F S}\right\rangle$ | 2.824 | 1.922 | 0.08922 |
| $\left\|s^{4} p^{2}[42]_{O}[51]_{F S}\right\rangle$ | 0.942 | 2.956 | -0.98854 |
| $\left\|s^{4} p^{2}[42]_{O}[411]_{F S}\right\rangle$ | 2.949 | 3.268 | 0.05843 |

of the state $\left|42^{+}[42]_{O}[51]_{F S}\right\rangle$ is far the lowest one, so that this state is much more favored than $\left|33[42]_{O}[51]_{F S}\right\rangle$. As explained above, such a state represents a configuration with two quarks on the left and four on the right around the symmetry center. At $Z \rightarrow \infty$ its energy becomes infinite, i.e., this state behaves as a hidden color state (see, e.g., Ref. [14]) and it decouples from the ground state. But at $Z=0$ it is the dominant component of the lowest state with a probability of $87 \%$ for $I S=(01)$ and $93 \%$ for $I S=(10)$. The next important state is $\left|33[42]_{O}[51]_{F S}\right\rangle$ with a probability of $10 \%$ for $I S=(01)$ and $4 \%$ for $I S=(10)$. The presence of this state will become more and more important with increasing $Z$. Asymptotically this state corresponds to a cluster model state with three quarks on the left and three on the right of the symmetry center.

To have a better understanding of the lowering of the six-quark energy we present in Tables III and IV the separate contribution of the kinetic energy $K E$, of the confinement $V_{\text {conf }}$ and of the GBE interaction $V_{\chi}$ to the dominant state in the cluster model $\left|s^{4} p^{2}[42]_{O}[51]_{F S}\right\rangle$ result and the dominant state in the molecular basis case, respectively. Table III corresponds to the ${ }^{3} S_{1}$ channel and Table IV to the ${ }^{1} S_{0}$ channel. We can see that $V_{\text {conf }}$ does not change much in passing from the cluster model to the molecular orbital basis. The kinetic energy $K E$ is higher in the molecular orbital basis which is natural because the $s^{2} p^{4}$ and $p^{6}$ configurations contribute with higher energies than $s^{6}$ and $s^{4} p^{2}$. Contrary, the contribution of the GBE interaction $V_{\chi}$ is lowered by several hundreds of MeV in both channels, so that $E=K E+V_{\text {conf }}+V_{\chi}$ is substantially lowered in the molecular orbital basis. This shows that the GBE interaction is more effective in the molecular orbital basis than in the cluster model basis. Note that $E$ differs from the value of the diagonal matrix elements of Tables I and II by the additional quantity $6 m-2 m_{N}$, where $m=m_{u}=m_{d}$.

The practically identical confinement energy in both bases shows that the amount of Van der Waals forces, as discussed in Ref. [7], remains the same. However, the soft attraction brought in by the Van der Waals forces does not play an
important role at short distances and it should be removed in further studies at intermediate distances.

For both $I S=(01)$ and (10) sectors we also searched for the minimum of $\langle H\rangle_{Z=0}$ as a function of the oscillator parameter $\beta$. For $I S=(01)$ the minimum of 572 MeV has been reached at $\beta=0.547 \mathrm{fm}$. For $I S=(10)$ the minimum of 715 MeV was obtained at $\beta=0.608 \mathrm{fm}$. These values are larger than the value of $\beta=0.437 \mathrm{fm}$ associated to the nucleon, which is quite natural because a six-quark system at equilibrium is a more extended object.

## V. SUMMARY AND CONCLUSIONS

We have calculated the $N N$ interaction potential at zero separation distance between nucleons by treating $N N$ as a six-quark system in a constituent quark model where the quarks interact via Goldstone boson (pseudoscalar meson) exchange. The orbital part of the six-quark states was constructed from molecular orbitals instead of the commonly used cluster model single particle states. The molecular orbitals posses the proper axially and reflectionally symmetries and are thus physically more adequate than the cluster model states. Due to their orthogonality property they are also technically more convenient. Here we constructed molecular orbitals from harmonic oscillator $s$ and $p$ states. Such molecular orbitals are a very good approximation [20] to the exact eigenstates of a "two-center" oscillator, frequently used in nuclear physics in the study of the nucleus-nucleus potential. The problem of calculating an $N N$ potential is similar in many ways.

We have shown that the upper bound of the ground state energy, and hence the height of the repulsive core in the $N N$ potential, is lowered by about 200 MeV in the ${ }^{3} S_{1}$ channel and by about 400 MeV in the ${ }^{1} S_{0}$ channel. Hence using molecular orbitals is more efficient than working with a cluster model basis. A repulsive core of several hundred MeV is still present in both channels. Due to the specific flavor-spin symmetry of the GBE interaction the molecular type component $\left|42^{+}[42]_{o}[51]_{F S}\right\rangle$ becomes dominant at short range

TABLE VI. Same as Table V but for $I S=(10)$.

| State | Diag. elem $-2 m_{N}$ | Eigenvalues $-2 m_{N}$ | Lowest state amplitudes |
| :--- | :---: | :---: | ---: |
| $\left\|s^{6}[6]_{O}[33]_{F S}\right\rangle$ | 2.990 | 1.453 | -0.10331 |
| $\left\|s^{4} p^{2}[42]_{O}[33]_{F S}\right\rangle$ | 3.326 | 2.436 | 0.09371 |
| $\left\|s^{4} p^{2}[42]_{O}[51]_{F S}\right\rangle$ | 1.486 | 3.557 | -0.98723 |
| $\left\|s^{4} p^{2}[42]_{O}[411]_{F S}\right\rangle$ | 3.543 | 3.899 | -0.07694 |

which implies that the $N N$ relative motion $S$-wave function has a node at short distance due to the presence of the configurations $s^{4} p^{2}$ and $s^{2} p^{4}$. The dominance of the $[51]_{F S}$ symmetry will reinforce the repulsion in dynamical calculations. In fact, it has been shown [1] that the phase shift calculated within the resonating group method with a pure $[51]_{F S}$ state shows a behavior typical for potentials with a repulsive core. In OGE models this effect is absent because none of the $[42]_{O}$ states is dominant (see, e.g., Ref. [12]). Note also that the configurations $s^{2} p^{4}$ or $p^{6}$ introduced through the molecular orbitals might have an influence on the momentum distribution of the $N N$ system as was discussed, for example, in Ref. [21] within the chromodielectric model.

The following step will be to calculate the $N N$ potential at $Z \neq 0$. The Yukawa potential tail in Eq. (25) will bring the
required long-range attraction. It would be interesting to find out the amount of middle-range attraction brought in by two correlated or uncorrelated pion exchanges.

## ACKNOWLEDGMENTS

We are very grateful to L. Wilets and L. Glozman for several useful comments.

## APPENDIX

Reference [7] presented results obtained from the diagonalization in a five-dimensional basis. For comparison, here we need to remove the fifth basis vector which does not have a corresponding one in the molecular basis. The results of the diagonalization in a four-dimensional basis are given in Tables V and VI for $I S=(01)$ and (10), respectively.
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