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THREE-BODY MOLECULAR DESCRIPTION OF ${}^9\text{Be}$ (I). Born-Oppenheimer approximation

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Received 18 July 1978

(Revised 30 March 1979)

Abstract: A three-cluster model composed of two α -particles and a neutron is used to describe the low-lying spectrum of ${}^9\text{Be}$. The resulting three-body problem is solved by the Born-Oppenheimer method for different two-body n - α and α - α potentials. Molecular energy curves are obtained that explain the binding mechanisms leading to both the ground state and first excited state of ${}^9\text{Be}$.

1. Introduction

In the past fifteen years there has been a considerable effort ¹⁾ to investigate the α -particle model in ${}^8\text{Be}$. Two-body α - α potentials have been used to reproduce the low energy spectrum of ${}^8\text{Be}$. The validity of the potential picture is supported by the rotational feature of the resonant levels for $J^\pi = 0^+, 2^+$ and 4^+ with a moment of inertia $M_\alpha R_\alpha^2$ corresponding to $R_\alpha \approx 4.5$ fm, and also by the large α -reduced width near the Wigner limit. Further evidence of $\alpha + \alpha$ cluster in ${}^8\text{Be}$ has been obtained through Hartree-Fock calculations where a symmetric localization of density results from the self-consistent wave function. Resonating group calculations have also been extremely successful in supplying some understanding on the nature of the α - α potential and the role of the Pauli principle on the molecular-like behavior of the α - α interaction. Although other channels such as ${}^6\text{Li} + d$ may be dynamically relevant to the understanding of the high energy excited states in ${}^8\text{Be}$ (20–30 MeV of excitation), the $\alpha + \alpha$ configuration seems to dominate the low energy level structure (up to 10 MeV of excitation).

The large binding energy of the α -particle suggests that identical arguments may be used to explain the low-lying levels of ${}^5\text{He}$ in terms of an effective $n - \alpha$ potential

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Resonating group calculations²⁾ also seem to support the $n+\alpha$ structure of the low-energy spectrum of ${}^5\text{He}$.

In the three-body sector where combinations of α -particles and nucleons may be considered, we find three configurations of interest. They are $\alpha+n+p$, $\alpha+\alpha+\alpha$ and $\alpha+n+\alpha$. The first two have been used in the past to explain with reasonable success the low energy levels of ${}^6\text{Li}$ [refs. ^{3,4)}] and ${}^{12}\text{C}$ [ref.⁵⁾], in particular those states that have a large α -decay width. In this work we attempt to study the configuration $\alpha+n+\alpha$ as a means to understand the low-lying states of ${}^9\text{Be}$. The energy of dissociation of ${}^9\text{Be}$ into $\alpha+n+\alpha$ is small (1.67 MeV) compared to the energy required to break up an α -particle (≈ 20 MeV). Since the low-energy levels of ${}^8\text{Be}$ and ${}^5\text{He}$ nuclei present a remarkable α -cluster structure, it is expected that the low-lying levels of ${}^9\text{Be}$ can be described as bound states or resonances of a three-body system composed of two α 's and a neutron n . From the pure three-body point of view, the $\alpha+n+\alpha$ system is also worthwhile considering. In the absence of a bound ${}^5\text{He}$ and ${}^8\text{Be}$ nuclei the ground state of $\alpha+n+\alpha$ results from a genuine three-body effect and in view of the resonant structure of both the $n-\alpha$ and $\alpha-\alpha$ interactions a rich structure of states may result in the three-body sector.

The variational method⁶⁾ and the Faddeev formalism⁷⁾ have been widely used in the past to obtain the bound states of the quantum mechanical nuclear three-body problem⁸⁾. On the contrary, in molecular physics, the large proton-electron mass ratio favors the use of molecular expansion methods⁹⁾ together with the Born-Oppenheimer approximation¹⁰⁾ to calculate the energy levels of three-body molecules such as $\text{H}_2^+(\text{p}+\text{e}^-+\text{p})$ and other more complicated molecular systems. Nevertheless, in a model three-body calculation involving two heavy particles and a lighter one, interacting through short range s-wave potentials, it has been shown recently¹¹⁾ that the Born-Oppenheimer (BO) method yields remarkably good results for the binding energies and wave functions even when the mass ratio m between the heavy and light particle is small ($m \geq 1$). Since the validity of the BO method for low mass ratios seems to be related to the short range nature of the two-body interaction between pairs¹¹⁾, we explore the analogy between the $\alpha+n+\alpha$ system and the H_2^+ molecule and make use of the BO method to obtain the bound states of the relevant three-body problem. Since an exact solution of the two-center problem may be obtained if the potentials are nonlocal but separable¹²⁾, we represent the $n-\alpha$ interaction by a separable potential that is both spin and angular momentum dependent and whose parameters are fitted to the low energy s_1 , p_1 and p_3 phase shift analyses. For the $\alpha-\alpha$ interaction both Ali-Bodmer¹³⁾ and Neudatchin *et al.*¹⁴⁾ local potentials are considered.

In sect. 2 we discuss the molecular approach and in sect. 3 the two-body $n-\alpha$ and $\alpha-\alpha$ interactions of our model are presented together with the resulting BO predictions for the low-lying levels of $\alpha+n+\alpha$. Some conclusions are given in sect. 4.

2. Molecular approach

In the Jacobian coordinates \mathbf{r} and \mathbf{R} of fig. 1 the three-body Schrödinger equation for the $\alpha + n + \alpha$ system is given by ($\hbar^2 = 1$; $m = m_n/m_n$; $2m_n = 1$)

$$\left[-\nabla_{\mathbf{R}}^2/\mu_{\alpha\alpha} - \nabla_{\mathbf{r}}^2/\mu + V_{n\alpha}(|\mathbf{r} + \frac{1}{2}\mathbf{R}|) + V_{n\alpha}(|\mathbf{r} - \frac{1}{2}\mathbf{R}|) + V_{\alpha\alpha}(\mathbf{R}) \right] \Psi(\mathbf{r}, \mathbf{R}) = E\Psi(\mathbf{r}, \mathbf{R}), \quad (1)$$

$$\mu_{\alpha\alpha} = \frac{1}{2}m, \quad \mu = 2m/(2m + 1),$$

where $\Psi(\mathbf{r}, \mathbf{R})$ is the exact wave function and E is the three-body binding energy.

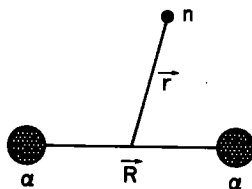


Fig. 1. The Jacobian coordinates of the three-body problem that are most convenient to molecular expansion methods.

The molecular approach⁹⁾ is based on the assumption that the wave function $\Psi(\mathbf{r}, \mathbf{R})$ can be approximately written as

$$\Psi(\mathbf{r}, \mathbf{R}) \approx \sum_i \psi_i(\mathbf{r}, \mathbf{R}) \Phi_i(\mathbf{R}), \quad (2)$$

where $\psi_i(\mathbf{r}, \mathbf{R})$ is an eigenfunction of the two-center problem

$$\left[-\nabla_{\mathbf{r}}^2/\mu + V_{n\alpha}(|\mathbf{r} + \frac{1}{2}\mathbf{R}|) + V_{n\alpha}(|\mathbf{r} - \frac{1}{2}\mathbf{R}|) \right] \psi_i(\mathbf{r}, \mathbf{R}) = \varepsilon_i(\mathbf{R}) \psi_i(\mathbf{r}, \mathbf{R}), \quad (3)$$

and $\varepsilon_i(\mathbf{R})$ is the corresponding negative energy eigenvalue that depends on the distance R between the α 's but not on the orientation in space of the \mathbf{R} vector. Substituting (2) in (1) and using the orthogonality properties of the $\psi_i(\mathbf{r}, \mathbf{R})$

$$\int d^3r \psi_i^*(\mathbf{r}, \mathbf{R}) \psi_j(\mathbf{r}, \mathbf{R}) = \delta_{ij}, \quad (4)$$

we obtain a set of coupled equations for the $\Phi_i(\mathbf{R})$

$$\left[-\nabla_{\mathbf{R}}^2/\mu_{\alpha\alpha} + V_{\alpha\alpha}(\mathbf{R}) + \varepsilon_i(\mathbf{R}) \right] \Phi_i(\mathbf{R}) = E\Phi_i(\mathbf{R}) - \sum_j A_{ij}(\mathbf{R}) \Phi_j(\mathbf{R}), \quad (5)$$

where the coupling coefficients are

$$A_{ij}(\mathbf{R}) = \frac{-1}{\mu_{\alpha\alpha}} \int d^3r \psi_i^*(\mathbf{r}, \mathbf{R}) \{ 2[\nabla_{\mathbf{R}} \psi_j(\mathbf{r}, \mathbf{R})] \cdot \nabla_{\mathbf{R}} + [\nabla_{\mathbf{R}}^2 \psi_j(\mathbf{r}, \mathbf{R})] \}. \quad (6)$$

In molecular physics the large proton-electron mass ratio is invoked as a justification for the BO approximation¹⁰⁾ which amounts to neglecting the coupling terms in eq. (5). Although in the present work the relevant mass ratio m is small ($m = 4$), we make use of the conclusions drawn in ref. ¹¹⁾ and neglect the coupling coefficients to obtain the negative energy spectrum of $\alpha + n + \alpha$. Thus

$$\Psi(r, R) \approx \psi_i(r, R)\Phi_i(R), \quad (7)$$

where

$$[-\nabla_R^2/\mu_{\alpha\alpha} + V_{\alpha\alpha}(R) + \varepsilon_i(R)]\Phi_i(R) = E\Phi_i(R). \quad (8)$$

The potential energy for the relative motion of the α 's is the sum of two terms. The first is the α - α potential that fits on-shell α - α scattering data and the second represents the effective interaction between the two α 's due to the presence of particle n .

Since the two-body n - α interaction of our model is nonlocal but separable, an exact solution of the two-center problem may be obtained¹²⁾. If the n - α potential is written in its most general form

$$V(q, q') = \sum_{l=0}^{l_{\max}} \sum_{j=l-\frac{1}{2}}^{l+\frac{1}{2}} \sum_{m=-j}^j \sum_n^{N_{lj}} g_{nlj}(q) \mathcal{Y}_{jl}^m(q) \lambda_{nlj} \mathcal{Y}_{nlj}^{m*}(q') \mathcal{Y}_{jl}^{m*}, \quad (9)$$

where

$$\mathcal{Y}_{jl}^m = (-i)^l \sum_{m's} \langle \frac{1}{2} l s m' | j m \rangle Y_l^{m'}(q') \chi_{\frac{1}{2}}^s, \quad (10)$$

and N_{jl} is the number of separable terms in each (jl) channel interaction, the two-center wave function $\psi(q, R)$ is given by

$$\psi_{M\Lambda i}(q, R) = \sum_{nljm} \frac{g_{nlj}(q) \mathcal{Y}_{jl}^m}{\varepsilon_{M\Lambda i}(R) - q^2/\mu} [\exp(-iq \cdot R/2) + \Lambda(-1)^l \exp(iq \cdot R/2)] \times \mathcal{D}_{mM}^j(\phi, \theta, 0) C_{nlj}^{M\Lambda i}(R). \quad (11)$$

The quantum number M is the projection of the neutron total angular momentum along the R -vector and Λ is the parity quantum number ($q \rightarrow -q, r \rightarrow -r$). The index " i " accounts for the possibility of different eigenvectors with the same M and Λ . \mathcal{D}_{mM}^j are the Wigner rotation matrices where ϕ and θ are the polar angles of the vector R . The energy eigenvalue $\varepsilon_{M\Lambda i}$ and the coefficients $C_{nlj}^{M\Lambda i}$ are obtained from the solution of a set of coupled homogeneous equations

$$\sum_{n'l'j'} \{ \lambda_{n'l'j'}^{-1} \delta_{nn'} \delta_{ll'} \delta_{jj'} - \mathcal{M}_{nlj, n'l'j'}^{M\Lambda}(\varepsilon_{M\Lambda}) \} C_{n'l'j'}^{M\Lambda} = 0, \quad (12)$$

with

$$\mathcal{M}_{nlj, n'l'j'}^{M\Lambda}(\varepsilon) = \int d^3q \frac{g_{nlj}(q) \mathcal{Y}_{jl}^M g_{n'l'j'}(q) \mathcal{Y}_{j'l'}^{M*}}{\varepsilon - (q^2/\mu)} [1 + \Lambda(-1)^l \exp(iq \cdot R)]. \quad (13)$$

For each value of R the energy eigenvalues ε_{MAi} are those values of ε for which the determinant of the homogeneous equation (12) vanishes, thus allowing for a solution C_{nij}^{MAi} . The number of coupled equations depends on M and does not exceed the total number of separable terms in the n - α interaction. If simple expressions are chosen for the form factors $g(q)$, the matrix elements $\mathcal{M}(\varepsilon)$ may be calculated analytically, otherwise a numerical integration can be easily performed.

3. Interactions and molecular results

3.1. TWO-BODY INTERACTIONS

As it has been previously pointed out the n - α interaction is represented by a separable potential that is both spin and angular momentum dependent and whose parameters are fitted to the low energy $s_{\frac{1}{2}}$, $p_{\frac{1}{2}}$ and $p_{\frac{3}{2}}$ n - α phase shifts. Unlike the p -wave phase shifts that are positive and present an unequivocal resonant structure¹⁵⁾, the s -wave phase shifts decrease monotonically from π or zero (depending on the absolute normalization) and seem to satisfy the relation $\delta_{\frac{1}{2}}^s(E_n = 0) - \delta_{\frac{1}{2}}^s(E_n = \infty) = \pi$. In the absence of a bound ${}^5\text{He}$ nuclei the modified Levinson's theorem¹⁶⁾ attributes the π discontinuity to the existence of a Pauli forbidden $s_{\frac{1}{2}}$ bound state in the $n + \alpha$ system. Since a two-body representation of the many-body n - α interaction has to simulate the presence of the forbidden state we follow the method proposed by Saito¹⁷⁾ and Kukulín, Neudatchin and Šmirnov¹⁸⁾. A one term s -wave separable potential $V_{n\alpha}^{0,\frac{1}{2}}$ is chosen that is strong enough to allow for an n - α bound state at 13.3 MeV[†] and that fits the s -wave phase shifts in the $E_n = 0$ –20 MeV range. Subsequently this bound state is subtracted by redefining the n - α interaction as

$$V_{n\alpha}^{0,\frac{1}{2}} = V_{n\alpha}^{0,\frac{1}{2}} + \Gamma |\phi_0\rangle \langle \phi_0|, \quad (14)$$

where $|\phi_0\rangle$ is the original bound state wave function and $\Gamma \rightarrow \infty$. Although $V_{n\alpha}^{0,\frac{1}{2}}$ allows for no negative energy bound state as required in the absence of a bound ${}^5\text{He}$ nuclei, the calculated phase shifts are identical to the ones resulting from $V_{n\alpha}^{0,\frac{1}{2}}$ and satisfy the condition $\delta_{\frac{1}{2}}^s(E_n + 0) - \delta_{\frac{1}{2}}^s(E_n = \infty) = \pi$ suggested by the phase shift analyses. Therefore the final $s_{\frac{1}{2}}$ n - α interaction to be used in the molecular calculation is a two-term separable potential where the second term is a projection operator on the bound state allowed by the first term. Since in most previous works^{3,4)} where the n - α interaction is represented by a separable potential, the forbidden state is simulated by an effective s -wave repulsion, we also consider another set of parameters for $V_{n\alpha}^{0,\frac{1}{2}}$ that make the n - α potential repulsive. This has the advantage that there

[†] The Wood-Saxon potential that fits $n\alpha$ scattering data allows for a $1s$ bound state at 13.3 MeV [ref. 19)].

are no $n-\alpha$ bound states to be subtracted but the resulting phase shifts do not satisfy the π discontinuity. For the p -wave interaction a simple one-term separable potential is adopted that is sufficiently attractive to reproduce the resonant structure of the $p_{\frac{1}{2}}$ and $p_{\frac{3}{2}}$ phase shift analyses in the 0–20 MeV energy region. Among the several possible form factors that have been used in the past ^{3,4} for $V_{n\alpha}^{lj}$ we choose

$$g_{lj}(q) = q^l / (q^2 + \beta_{lj}^2)^{l+1}, \quad (15)$$

that leads to two-body solutions that have the correct threshold and asymptotic behavior. The parameters of the $V_{n\alpha}^{lj}$ interaction in each (lj) channel are shown in table 1.

TABLE I
Parameters of the two-body $n-\alpha$ interaction

	$s_{1/2}$ (attractive)	$s_{1/2}$ (repulsive)	$p_{1/2}$	$p_{3/2}$
β	1.494 fm^{-1}	0.7 fm^{-1}	1.177 fm^{-1}	1.449 fm^{-1}
$2\mu'\lambda$	-9.283 fm^{-3}	3.770 fm^{-3}	-13.873 fm^{-5}	-60.708 fm^{-5}

The $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ (repulsive) parameters are from ref. ¹⁸) and μ' is the $n-\alpha$ reduced mass, $\mu' = m/(m+1)$.

The $\alpha-\alpha$ interaction is represented by a phenomenological local potential whose parameters are fitted to the s -, d -, and g -wave $\alpha-\alpha$ phase shifts. Both Ali-Bodmer ¹³) and Neudatchin *et al.* ¹⁴) potentials have been adopted in the molecular calculation. Since the Neudatchin *et al.* potential is strong enough to allow for $1s$, $2s$ and $1d$ bound states of $\alpha+\alpha$, the relevant states to $\alpha+n+\alpha$ emerging from eq. (8) are $3s$, $2d$ and $1g$.

3.2. MOLECULAR RESULTS

With the two-body $n-\alpha$ interaction described above we solve first eq. (12) to obtain the eigenvalues $\varepsilon_{MA}(R)$ of the two-center problem. The results of this calculation are shown in fig. 2 for $V_{n\alpha}^{0,\frac{1}{2}}$ attractive and in fig. 3 for $V_{n\alpha}^{0,\frac{1}{2}}$ repulsive. Since the $p_{\frac{1}{2}}$ $n-\alpha$ potential is solely responsible for $\varepsilon_{\frac{3}{2}A}(R)$, the $\frac{3}{2}A$ molecular curves are identical in both figures (since $\varepsilon_{\frac{3}{2}+}(R) \leq \varepsilon_{\frac{3}{2}-}(R = \infty)$ for all R the $\frac{3}{2}+$ curve has been omitted for clarity). Unlike the $\frac{3}{2}-$ solution that exists for all R , the $\frac{3}{2}+$ emerges around $R = 7.4$ fm and joins the $\frac{3}{2}-$ at $R = \infty$. Although there is no $p_{\frac{1}{2}}$ bound state in the $n+\alpha$ system, the $\frac{3}{2}-$ curve converges to a very small value of the energy at $R = \infty$ ($\varepsilon_{\frac{3}{2}A}(\infty) = 0.48$ MeV). This is an inherent feature of the molecular treatment that results from using in eq. (3) the reduced mass μ of the "united atom" ($R = 0$) for all values of R including the "separated atom" limit ($R \rightarrow \infty$) (see ref. ¹¹). The asymptotic behavior has little or no effect in a bound state calculation but may be crucial in the scattering region where it leads to an incorrect scattering threshold ²⁰). In fig. 2 the dashed

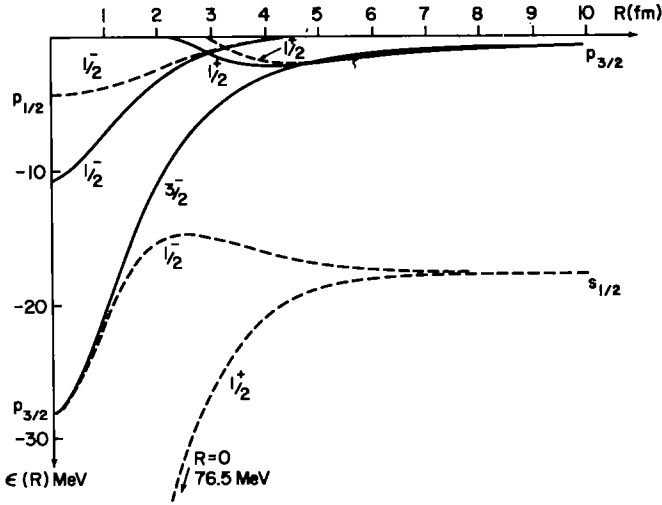


Fig. 2. The two-center binding energy $\varepsilon(R)$ versus R for an attractive $s_{1/2}$ n - α interaction and different values of M and Λ . The dashed lines correspond to $\Gamma = 0$ while the solid lines to $\Gamma = \infty$.

lines correspond to $\Gamma = 0$ in eq. (14) ($s_{1/2}$ n - α bound state not subtracted) and the solid lines to $\Gamma = \infty$. For $R > 7.4$ fm the lowest $\frac{1}{2}^-$ curves in both figures behave like $\varepsilon_{\frac{1}{2},\Lambda}(R)$ and for that reason have not been drawn in that region. Although all $\varepsilon_{\frac{1}{2},\Lambda}(R)$ eigenvalues depend on the way the $s_{1/2}$ Pauli forbidden $n + \alpha$ state is treated by the two-body n - α interaction the $\frac{1}{2}^-$ eigenvalues are the most affected. The striking feature in fig. 2 is that in the limit $R \rightarrow 0$ the lowest $\frac{1}{2}^-$ and $\frac{3}{2}^-$ eigenvalues (solid curves) stay undegenerate while the corresponding states in fig. 3 approach each other to

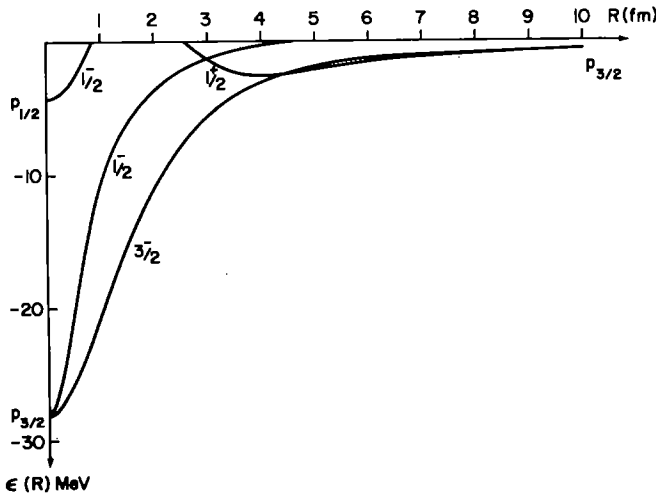


Fig. 3. The two-center binding energy $\varepsilon(R)$ versus R for a repulsive $s_{1/2}$ n - α interaction and different values of M and Λ .

form the $p_{\frac{3}{2}}$ bound state of the "united atom." This indicates that the spherical symmetry is not restored in the limit $R \rightarrow 0$ whenever the Pauli excluded $s_{\frac{1}{2}} n + \alpha$ state is simulated by an attractive $n - \alpha$ interaction with the bound state subtracted[†]. It is interesting to note that in the two-center Hartree-Fock calculation of Okabe, Abe and Tanaka²¹⁾ where the Pauli principle is fully accounted for (they use nine-particle Slater determinants) the lowest $\frac{3}{2}^-$ and $\frac{1}{2}^-$ energy curves are also non-degenerate in the limit $R \rightarrow 0$. Although in their work the dynamics is treated in a completely different way the energy curves they obtain have essentially the same meaning as ours. Therefore it may be appropriate to conclude that in the interaction between composite particles the subtraction method of Kukulin *et al.*¹⁸⁾ provides a better representation of Pauli forbidden states than a simple effective repulsion. The remaining molecular curves to be discussed are the second $\frac{1}{2}^-$ energy eigenvalue curve and the lowest positive parity $\varepsilon_{\frac{3}{2}^+}(R)$. While in fig. 3 there is a second $\frac{1}{2}^-$ energy curve for $0 \leq R < 0.8$ fm that coincides at $R = 0$ with the $p_{\frac{3}{2}}$ bound state of the "united atom", the corresponding state in fig. 2 only exists for $\Gamma = 0$. Once the $s_{\frac{1}{2}}$ $n - \alpha$ bound state is subtracted ($\Gamma = \infty$) the second $\frac{1}{2}^-$ curve disappears from the negative energy region. On the contrary the $\frac{1}{2}^+$ molecular curve is little affected by the nature of the $n - \alpha$ interaction. It emerges at $R \approx 2.5$ fm and for $R > 4.5$ fm is the lowest eigenvalue solution of the two-center problem. Since there is no $s_{\frac{1}{2}}$ bound state of $n + \alpha$ (except for $\Gamma = 0$) the $\frac{1}{2}^+$ curve cannot subside all the way until $R = 0$. Its existence is mainly due to the p-wave $n - \alpha$ interaction that is allowed to contribute with increasing weight for larger values of R . It is again worthwhile noting that the relative position of the $\frac{1}{2}^+$ and $\frac{3}{2}^-$ curves is consistent with the results of the Hartree-Fock calculation of Okabe *et al.*²¹⁾ where for $R > 5$ fm the $\frac{1}{2}^+$ is the lowest energy solution.

As it has been previously pointed out the next step of the BO method involves the solution of eq. (8) to obtain the three-body binding energy. The potential energy for the relative motion of the α 's is the sum of the $\alpha - \alpha$ two-body interaction with the lowest $\varepsilon_{MA}(R)$ of a given parity. In fig. 4 we show the effective

$$v_{\alpha\alpha}^{MA}(R) = V_{\alpha\alpha}(R) + \varepsilon_{MA}(R), \quad (16)$$

for the case of Ali-Bodmer $\alpha - \alpha$ potential. The dotted line is the Ali-Bodmer potential alone and the full lines correspond to adding the $\frac{3}{2}^-$ and $\frac{1}{2}^+$ energy curves of fig. 2 to $V_{\alpha\alpha}$. While $\varepsilon_{\frac{3}{2}^-}(R)$ essentially deepens the $\alpha - \alpha$ effective potential the main effect of $\varepsilon_{\frac{1}{2}^+}(R)$ is to increase its range. As shown in table 2 both the $v_{\alpha\alpha}^{\frac{1}{2}^-}$ and $v_{\alpha\alpha}^{\frac{1}{2}^+}$ allow for an $L = 0$ eigenstate of (8) in contrast to no bound states when the Ali-Bodmer potential is used alone, $v_{\alpha\alpha}^{\frac{1}{2}^-}$ also allows for an $L = 2$ three-body bound state that is less bound than the $L = 0$ eigenvalue resulting from $v_{\alpha\alpha}^{\frac{1}{2}^+}$. The same calculation was

[†] At $R = 0$ the s-wave components of the $n - \alpha$ interaction have no effect on the $\frac{1}{2}^-$ eigenvalues (see eq. (11)). Therefore $\varepsilon_{1/2^-}(R = 0) = \varepsilon_{3/2^-}(R = 0)$ and the spherical symmetry is locally recovered. For $R \neq 0$ but infinitesimally close to zero the limit $\Gamma \rightarrow \infty$ takes over and creates a spherical asymmetry that leads to a non-infinitesimal difference between eigenvalues corresponding to different M -values.

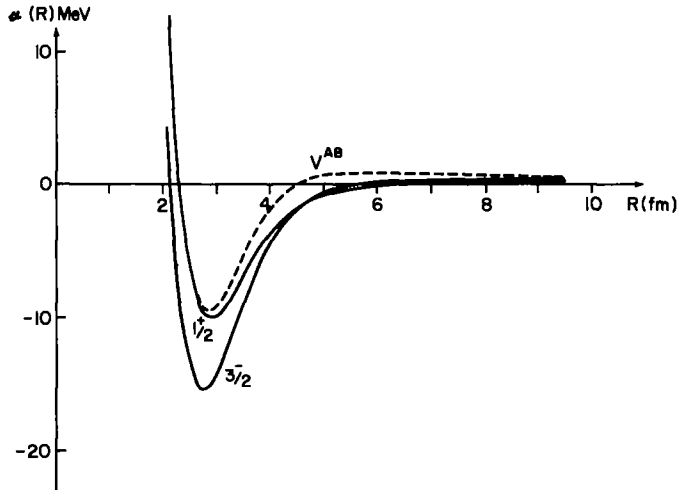


Fig. 4. The potential energy $v(R)$ for the relative motion of the α 's versus R . V^{AB} is Ali-Bodmer α - α potential alone.

done with Neudatchin *et al.* Wood-Saxon potential ¹⁴) which by itself allows for two $L = 0$ and one $L = 2$ bound states. Since these states are meant to simulate Pauli forbidden states in the $\alpha + \alpha$ system it is not *a priori* clear whether the forbidden states in $\alpha + n + \alpha$ should be eigenstates of

$$\nabla_R^2/\mu_{\alpha\alpha} + V_{\alpha\alpha}(R) + \varepsilon_{MA}(R), \quad (17)$$

or

$$\nabla_R^2/\mu_{\alpha\alpha} + V_{\alpha\alpha}(R). \quad (18)$$

In the first case the calculation is simple and the bound states of $\alpha + n + \alpha$ are the 3s and 2d eigenvalues of the operator (17) that are shown in table 2 for two different $\varepsilon_{MA}(R)$. If the forbidden states of $\alpha + n + \alpha$ are eigenvalues of (18) then we have to proceed as in eq. (14) and redefine the α - α potential in (8) as

$$V_{\alpha\alpha} = V_{\alpha\alpha} + \Gamma_1 |1s\rangle\langle 1s| + \Gamma_2 |2s\rangle\langle 2s| + \Gamma_3 |1d\rangle\langle 1d|. \quad (19)$$

TABLE 2
Born-Oppenheimer spectrum of $\alpha + n + \alpha$

	Ali-Bodmer		Kukulin, <i>et al.</i>	
	fig. 2	fig. 3	fig. 2	fig. 3
$\frac{1}{2}^- \quad l = 2$	-1.05	-1.05	-2.67	-2.67
$\frac{1}{2}^+ \quad l = 0$	-1.70	-1.65	-1.59	-1.56
$\frac{3}{2}^- \quad l = 0$	-3.85	-3.85	-6.10	-6.10

The bound state of $\alpha + n + \alpha$ are the low-energy eigenvalues of the resulting inhomogeneous differential equation and the corresponding eigenstates are orthogonal to the eigenstates of (18). Compared to the values shown in table 2 this method lowers the binding energy of the ground state by 0.7 MeV and leaves all the other states unchanged. Although the three-body energy levels of $\alpha + n + \alpha$ we obtain are lower than the known experimental values, the ones obtained with the Ali-Bodmer potential have the correct relative position. The first excited state is the $\frac{1}{2}^+$, $L = 0$ state which is 1.95 MeV above the ground state. Since the resulting BO wave functions are not eigenfunctions of the total three-body angular momentum J we abstain from making a direct comparison with experiment. In a subsequent publication we will present the results of a full molecular calculation where some of the coupling coefficients will be retained (see eqs. (5)–(8)) and the three-body wave function is constructed to be a pure state of the total J .

4. Discussion

In the previous sections we have used the BO method to obtain the low-lying levels of ${}^9\text{Be}$ as a three-body molecular system composed of two α -particles and a neutron n . The molecular approach provides a very simple and transparent explanation of the level structure of ${}^9\text{Be}$. The presence of the neutron n is crucial to the existence of a bound ${}^9\text{Be}$ nuclei. It creates an effective potential between the α 's that when added to the two-body α - α interaction generates sufficient attraction to allow for three-body bound states. In the model the $p_{\frac{1}{2}}$ n - α interaction is solely responsible for the ground state energy (its absolute value depends also on the two-body α - α potential that has been chosen) and the corresponding wave function has no nodes (see eq. (11)). The low-lying positive parity state is essentially due to a long range force between the α -particles that is mediated by the neutron. This long range force is particularly sensitive to the strength of the p -wave n - α interaction. In view of the simplicity of the BO method it is our hope that the molecular approach may be useful in studying threebody cluster structure in heavier nuclei such as ${}^{25}\text{Mg}$ (${}^{12}\text{C} + n + {}^{12}\text{C}$), ${}^{29}\text{Si}$ (${}^{12}\text{C} + n + {}^{16}\text{O}$) and others that can be dissociated in two closed shell nuclei and a nucleon. Another interesting subject of research is to study the best way to simulate Pauli forbidden states in the two-body interaction between composite particles. The BO method was able to show that some components of the effective α - α interaction resulting from the presence of particle n are extremely sensitive to the nature of the s -wave n - α interaction. Nevertheless because the difference was on the $\frac{1}{2}^-$ molecular energy curve we cannot make a definite statement as how this change will affect the three-body observables. This will be studied in a subsequent publication where a coupled channel calculation based on both $\frac{3}{2}^-$ and $\frac{1}{2}^-$ two-center eigenfunctions will be performed.

Two of the authors (A.C.F. and J.R.) are grateful to the National Science Founda-

tion (USA) and the Institute of Cultural Relations (Hungary) for the exchange grant which made this collaboration possible. They also would like to thank the Central Research Institute for Physics (Budapest) and the University of Maryland (College Park) for their hospitality. One of us (A.C.F.) wishes to thank M. K. Banerjee and W. F. Hornyak for useful discussions and the Computer Science Center of the University of Maryland for its generous collaboration.

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