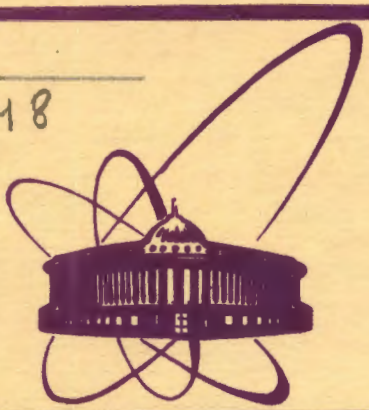

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E4 - 12394

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THREE-BODY MOLECULAR DESCRIPTION OF ^{9}Be.

II. Adiabatic One-Level Approximation with Correct Angular Momentum

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Submitted to "Nuclear Physics"

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E4 - 12394

Молекулярная модель для описания ядра ^{9}Be.
II. Адиабатическое одноуровневое приближение

В кластерной $\alpha+\alpha+n$ модели ядра ^{9}Be получено уравнение Шредингера для волновой функции с правильной четностью и угловым моментом. С помощью этого уравнения рассчитаны спектр и волновые функции низколежащих состояний. Проведено сравнение с экспериментом.

Работа выполнена в Лаборатории теоретической физики, ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1979

Revai J., Matveenko A.V.

E4 - 12394

Three-Body Molecular Description of ^{9}Be.
II. Adiabatic One-Level Approximation with Correct Angular Momentum

The low lying spectrum of the ^{9}Be nucleus is calculated in an $\alpha+\alpha+n$ three-body model. The molecular approach to this three-body problem based on the exact evalution of the two-center wave functions for separable $n-\alpha$ potentials is considered in detail. The numerical results are obtained in a generalized Born-Oppenheimer approximation which preserves total angular momentum and parity.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1979

1. INTRODUCTION

It is commonly believed (see, e.g., ref. [1]) that the low-lying states of the ^{9}Be nucleus can be well described in terms of an $\alpha+\alpha+n$ model. Most recently this idea has found its realization in the framework of microscopical variational calculations [2-4] (generator coordinate method, resonating group method); the antisymmetrized trial wave functions depend on all nucleon coordinates, eight of them form two α-clusters, and the relative motion of these two clusters and the remaining neutron is suitably parametrized. This means that the dynamics is completely attributed to the three-cluster relative motion, and the presence of the eight individual particles of the two α-s manifests itself only through the Pauli principle.

Therefore, if the effect of the overall antisymmetrization could be appropriately incorporated into the intercluster interaction [5-7], the solution of the dynamical three-body equations for the $\alpha+\alpha+n$ system could yield a deeper understanding of the low-lying states of ^{9}Be. Unfortunately - to our knowledge - the only Faddeev calculation of this system was done in 1970 by R.Grubman and T.Whitten [8]. This work was aimed at reproducing only the ground state binding energy (E^{B}_{calc} =1.22 MeV) since the method used for treating the Coulomb force was valid only for negative total energies. There was also no discussion of the effects of the Pauli principle.

Thus, the complete dynamical treatment of the $\alpha+\alpha+n$ system does not exist yet. In our opinion the three-body molecular approach is a step towards this goal; an attempt, which, in spite of its calculational simplicity, offers some physical and easily visualizable insight into the structure of this nucleus.

In a previous paper [9] the Born-Oppenheimer Approximation (BOA) was considered for the ^{9}Be; it has been shown, that even this simplest form of the molecular treatment of this three-body system can provide a qualitative

description of the low-lying states of ^{9}Be. In this picture, the presence of the neutron produces an effective potential between the two α-particles which, when added to the original $\alpha-\alpha$ - interaction, is strong enough to account for the weak three-body binding in the ground state of ^{9}Be. The long-range character of the positive-parity part of the effective force indicates the presence of low-lying positive-parity states in the ^{9}Be spectrum.

The main difficulty of the BOA which does not allow making quantitative statements on its ground is the non-conservation of total angular momentum in the BOA. In the present paper we demonstrate how the conservation of the total spin and parity can be explicitly incorporated into the molecular approach and derive the "minimal extension" of the BOA having the correct quantum numbers.

In section II we give a short review of the molecular approach to the three-body problem; section III contains the derivation of the basic system of coupled equations of the molecular treatment; in section IV we introduce the adiabatic one-level approximation and in section V we present the results of its application to ^{9}Be; in section VI we draw some conclusions.

II. REVIEW OF THE MOLECULAR APPROACH

The description of the $\alpha+\alpha+n$ three-body system can be conveniently performed using the Jacobian coordinate and momentum variables

$$\vec{\mathcal{R}} = \frac{1}{2m_\alpha + m_n}(m_\alpha \vec{r}_{\alpha_1} + m_\alpha \vec{r}_{\alpha_2} + m_n \vec{r}_n); \quad \vec{\mathcal{P}} = \vec{p}_{\alpha_1} + \vec{p}_{\alpha_2} + \vec{p}_n$$

$$\vec{R} = \vec{r}_{\alpha_1} - \vec{r}_{\alpha_2}; \quad \vec{P} = \tfrac{1}{2}(\vec{p}_{\alpha_1} - \vec{p}_{\alpha_2}),$$

$$\vec{r} = \vec{r}_n - \frac{1}{2}(\vec{r}_{\alpha_1} + \vec{r}_{\alpha_2}); \quad \vec{p} = \frac{1}{2m_\alpha + m_n}(2m_\alpha \vec{p}_n - m_n(\vec{p}_{\alpha_1} + \vec{p}_{\alpha_2})). \tag{1}$$

After separating the center of mass variables $(\vec{\mathcal{R}}, \vec{\mathcal{P}})$ the Hamiltonian can be written as

$$\mathcal{H} = \frac{1}{2\mu}\hat{P}^2 + \frac{1}{2m}\hat{p}^2 + \hat{v}_{n\alpha}(\vec{r} - \frac{1}{2}\vec{R}) + \hat{v}_{n\alpha}(\vec{r} + \frac{1}{2}\vec{R}) + \hat{v}_{\alpha\alpha}(R) \tag{2}$$

with the reduced masses

$$\mu = \frac{1}{2}m_\alpha, \quad m = \frac{2m_\alpha m_n}{2m_\alpha + m_n}. \tag{3}$$

The basic idea of the molecular approach to the solution of the three-body problem

$$(\mathcal{H} - E)\Psi(\vec{r}, \vec{R}) = 0 \tag{4}$$

is to expand the three-body wave function $\Psi(\vec{r}, \vec{R})$ in terms of the eigenfunctions $\Phi_i(\vec{r};\vec{R})$ of the two-center Hamiltonian $\hat{h}_{t.c.}$:

$$\hat{h}_{t.c.} = \frac{1}{2m}\hat{p}^2 + \hat{v}_{n\alpha}(\vec{r} - \frac{1}{2}\vec{R}) + \hat{v}_{n\alpha}(\vec{r} + \frac{1}{2}\vec{R}),$$

$$\hat{h}_{t.c.}\Phi_i(\vec{r};\vec{R}) = \epsilon_i(R)\Phi_i(\vec{r};\vec{R}). \tag{5}$$

The expansion

$$\Psi(\vec{r}, \vec{R}) = \sum_j \Phi_j(\vec{r};\vec{R})u_j(\vec{R}) \tag{6}$$

combined with the projection of the Schrödinger equation (4)

$$\int \Phi_i^*(\vec{r};\vec{R})(\mathcal{H} - E)\Psi(\vec{r};\vec{R})\,d\vec{r} = 0$$ *

leads to the following set of coupled equations for the expansion coefficients $u_i(\vec{R})$:

$$(-\frac{1}{2\mu}\Delta_{\vec{R}} + \hat{v}_{\alpha\alpha}(R) + \epsilon_i(R) - E)u_i(R) =$$

$$= \frac{1}{2\mu}\sum_j \{\int \Phi_i^*(\vec{r};\vec{R})\Delta_{\vec{R}}\Phi_j(\vec{r};\vec{R})\,d\vec{r} +$$

$$+ 2\int \Phi_i^*(\vec{r};\vec{R})\vec{\nabla}_{\vec{R}}\Phi_j(\vec{r};\vec{R})\,d\vec{r}\,\vec{\nabla}_{\vec{R}}\}u_j(\vec{R}). \tag{7}$$

*Here and in the following, if not necessary, the spin variable of the neutron is not explicitly indicated; summation over the spin coordinate is understood whenever integration over the coordinate or momentum variable of the neutron occurs.

The practical application of the molecular approach depends on the solvability of the two-center problem (5). In the present work we use separable n–α interactions for which the two-center problem can be solved exactly. Since we shall need them later, let use recall briefly the main properties of these two-center functions. The separable n–α potential can be written as

$$\hat{v}_{n\alpha} = \sum_{\ell=0}^{\ell_{max}} \sum_{j=\ell-1/2}^{\ell+1/2} \sum_{m=-j}^{j} \sum_{n=1}^{N_{\ell j}} |n\ell jm\rangle \lambda_{n\ell_j} \langle n\ell jm| , \qquad (8)$$

where the ket-vectors are defined through the form factors $g_{n\ell_j}(p)$ as

$$\langle \vec{p}, s | n\ell jm \rangle = g_{n\ell_j}(p) i^{-\ell} \mathcal{Y}^{\ell}_{jm}(\Omega_p, s),$$
$$\mathcal{Y}^{\ell}_{jm}(\Omega_p, s) = \sum_{\mu\sigma} (\ell\mu\, 1/2\,\sigma | jm) Y_{\ell\mu}(\Omega_p) \chi_{1/2\,\sigma}(s). \qquad (9)$$

In eq. (8) ℓ_{max} defines the number of partial waves in which the potential acts, N_{ℓ_j} fixes the number of separable terms in each wave. The solution of the two-center problem for two potentials of the form (8) is obtained as [10]

$$|\Phi_{M\Lambda_i}\rangle = \hat{G}_0(\epsilon_{M\Lambda_i}) \sum_{n\ell jm} (e^{-\frac{i}{2}\vec{R}\vec{p}} + \Lambda(-1)^{\ell} e^{\frac{i}{2}\vec{R}\vec{p}}) |n\ell jm\rangle D^{j}_{mM}(\Phi,\theta,0) C^{n\ell_j}_{M\Lambda_i}(R), \qquad (10)$$

where $\hat{G}_0(z)$ is the free Green operator of eq. (5): $\hat{G}_0(z) = (z - \frac{1}{2m}\hat{p}^2)^{-1}$. D^{j}_{mM} is the Wigner rotation matrix*, Φ and θ being the polar angles of $\vec{R}$. The meaning of the quantum numbers is the following: M is the projection of the neutron angular momentum along the direction of $\vec{R}$; Λ is associated with a symmetry following from the identity of the two α-particles, in the coordinate system (1) it coincides with the parity against the inversion $\hat{\pi} \to (\vec{p} \to -\vec{p},\ \vec{r} \to -\vec{r})$; i denotes the missing labels, which might be necessary to specify a state. The energy eigenvalue $\epsilon_{M\Lambda_i}(R)$ and the coefficients $C^{n\ell_j}_{M\Lambda_i}(R)$ are obtained from the set of homogeneous algebraic equations

* Throughout the paper we use the convention

$$D^{j}_{mm'}(\alpha,\beta,\gamma) = \langle jm | e^{-i\alpha\hat{J}_z} e^{-i\beta\hat{J}_y} e^{-i\gamma\hat{J}_z} | jm' \rangle .$$

$$\sum_{\beta'} \{ \lambda^{-1}_{\beta} \delta_{\beta\beta'} - \langle \beta M | G_0(\epsilon)(1 + \Lambda(-1)^{\ell} e^{iR\hat{p}_z}) | \beta' M \rangle \} C^{\beta'}_{M\Lambda}(R) = 0 \qquad (11)$$

with the notation $\beta = \{n\ell j\}$. For a given value of R the energy eigenvalues $\epsilon_{M\Lambda_i}(R)$ are those values of ϵ for which the determinant of eq. (11) vanishes, allowing a solution $C^{\beta}_{M\Lambda_i}(R)$; the missing equation for determining the coefficients is the normalization condition

$$\langle \Phi_{M'\Lambda'i'} | \Phi_{M\Lambda i} \rangle = \delta_{MM'} \delta_{\Lambda\Lambda'} \delta_{ii'} . \qquad (12)$$

The simplest realization of the molecular approach is the BOA, in which only one term in expansion (6) is retained, and the r.h.s. of eq. (7) is neglected. The application of the BOA for the ^{9}Be case was considered in detail in [9], here we want to point out only one specific features of the BOA: it does not conserve the total angular momentum. Indeed, in the BOA we have a spherically symmetric Schrödinger equation in variable $\vec{R}$, and thus the total wave function will have the form $\Phi_i(\vec{r};\vec{R}) u_L(R) Y_{LM}(\theta,\Phi)$ which is obviously not an eigenfunction of the total angular momentum.

In principle, it would be possible to follow the familiar angular momentum projection procedure to construct good angular momentum states from the "deformed" BOA solution Ψ_{BOA}:

$$\Psi^{JM}_{BOA} = \hat{P}^{JM} \Psi_{BOA},$$
$$E^{J}_{BOA} = \langle \Psi^{JM}_{BOA} | \hat{H} | \Psi^{JM}_{BOA} \rangle : \langle \Psi^{JM}_{BOA} | \Psi^{JM}_{BOA} \rangle ,$$

$\hat{P}^{JM}$ being a suitable projection operator. There are two possible objections to this procedure:

a) the resulting wave functions and energy values are no longer solutions of, may be, approximate but still dynamical equations; we would have a mixture of a dynamical and a variational calculation;

b) for the two-centre functions (10) the practical realization of the projection is more difficult than the correct treatment of the angular momentum from the very beginning.

III. DERIVATION OF THE COUPLED SYSTEM IN R

Let us rewrite (10) in momentum representation:

$$\Phi_{M\Lambda i}(\vec{p};\vec{R}) = \sum_{\beta m} (e^{-\frac{i}{2}\vec{R}\vec{p}} + \Lambda(-1)^{\ell} e^{\frac{i}{2}\vec{R}\vec{p}}) i^{-\ell} \mathcal{Y}^{\ell}_{jm}(\Omega_p s) D^{j}_{mM}(\Phi,\theta,0) \phi^{\beta}_{M\Lambda i}(p,R), \tag{13}$$

where the notation

$$\phi^{\beta}_{M\Lambda i}(p,R) = C^{\beta}_{M\Lambda i}(R) g_{\beta}(p)(\epsilon_{M\Lambda i}(R) - \frac{1}{2m}p^2)^{-1} \tag{14}$$

was introduced. Our task is the evaluation of the r.h.s. of eq. (7):

$$X = \frac{1}{2\mu}\sum_{M'i'}\{\int \Phi^{*}_{M\Lambda i}(\vec{p};\vec{R})\Delta_{\vec{R}}\Phi_{M'\Lambda i'}(\vec{p};\vec{R})d\vec{p} + 2\int \Phi^{*}_{M\Lambda i}(\vec{p};\vec{R})\vec{\nabla}_{\vec{R}}\Phi_{M'\Lambda i'}(\vec{p};\vec{R})d\vec{p}\,\vec{\nabla}_{\vec{R}}\}u_{M'\Lambda i'}(R). \tag{15}$$

In writing (15), besides the explicit indication of the quantum numbers of the two-center functions, we have taken into account that $\hat{p}^2$ commutes with $\hat{\pi}_r$, and thus no coupling in Λ occurs. Before calculating X we note that at this point our approach differs from the one used in molecular physics: since our two-center functions (13) are explicitly given for arbitrary direction of $\vec{R}$, there is no need to introduce a "body-fixed" frame (with z axis along $\vec{R}$) and thus in our formalism no Coriolis interaction occurs.

The calculation of X is straightforward but tedious; the main steps are:

- the evaluation of the effect of the operators $\Delta_{\vec{R}}$ and $\vec{\nabla}_{\vec{R}}$ upon the functions (13);
- spin-angular integration using elementary angular-momentum algebra;
- summations over the magnetic quantum numbers using the orthogonality properties and Clebsch-Gordan expansion of the rotaion matrices.

The result is as follows:

$$X = \frac{1}{2\mu}\sum_{i'}\{[D^{M\Lambda}_{ii'}(R) + N^{M\Lambda}_{ii'}(R)\frac{1}{R^2}(2M^2 - \frac{M^2}{\sin^2\theta} - 2M\frac{\cos\theta}{\sin^2\theta}i\frac{\partial}{\partial\Phi}) +$$

$$+ B^{M\Lambda}_{ii'}(R)\partial_o]u_{M\Lambda i'}(\vec{R}) + Q^{M\Lambda+}_{ii'}(R)(\partial_+ + (M+1)\frac{\cos\theta}{\sin\theta})u_{M+1\Lambda i'}(\vec{R}) + \tag{16}$$

$$+ Q^{M\Lambda-}_{ii'}(R)(\partial_- + (M-1)\frac{\cos\theta}{\sin\theta})u_{M-1\Lambda i'}(\vec{R})\}$$

with the notation chain:

$$D^{M\Lambda}_{ii'}(R) = \sum_{\beta\beta' L} A^{L}_{\beta\beta'}\langle j'ML0|jM\rangle \langle \beta iM|\hat{d}(p,R)|\beta' i'M\rangle_p , \tag{17}$$

$$N^{M\Lambda}_{ii'}(R) = \sum_{\beta\beta' L} A^{L}_{\beta\beta'}\langle j'ML0|jM\rangle \langle \beta iM|f(p,R)|\beta' i'M\rangle_p , \tag{18}$$

$$B^{M\Lambda}_{ii'}(R) = \sum_{\beta\beta' L} A^{L}_{\beta\beta'}\langle j'ML0|jM\rangle \langle \beta iM|\hat{b}(p,R)|\beta' i'M\rangle_p , \tag{19}$$

$$Q^{M\Lambda\pm}_{ii'}(R) = \frac{1}{R^2}\sum_{\beta\beta' L} A^{L}_{\beta\beta'}\{\langle j'ML0|jM\rangle\sqrt{(j'\mp M)(j'\pm M+1)}\langle \beta iM|f(p,R)|\beta' i'M\pm1\rangle_p - \tag{20}$$

$$- \frac{1}{2}\langle j'M\pm1\, L\mp1|jM\rangle\sqrt{L(L+1)}\langle \beta iM|g(p,R)|\beta' i'M\pm1\rangle_p\},$$

$$A^{L}_{\beta\beta'} = 2\cdot i^{\ell'+\ell+L}(2L+1)(-1)^{j'+\frac{1}{2}}\sqrt{(2\ell'+1)(2j'+1)}\langle \ell'0L0|\ell0\rangle \begin{Bmatrix} \ell' & \frac{1}{2} & j' \\ j & L & \ell \end{Bmatrix} \tag{21}$$

The matrix elements $\langle \beta iM|\hat{O}(p,R)|\beta' i'M'\rangle_p$ denote the integral over p:

$$\langle \beta iM|\hat{O}(p,R)|\beta' i'M'\rangle_p = \int_0^{\infty} p^2 dp\, \phi^{\beta}_{M\Lambda i}(p,R)\hat{O}(p,R)\phi^{\beta'}_{M'\Lambda i'}(p,R) \tag{22}$$

while the operators and functions occuring in these matrix elements in eqs. (17)-(20) are defined as

$$\hat{d}(p,R) = f(p,R)(-\frac{1}{4}p^2 + \frac{1}{R^2}\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R} - \frac{1}{R^2}j'(j'+1)) - h(p,R)\frac{\partial}{\partial R} +$$

$$+ \frac{1}{2R^2}g(p,R)(j(j+1) - j'(j'+1) - L(L+1)), \tag{23}$$

$$\hat{b}(p,R) = 2f(p,R)\frac{\partial}{\partial R} - h(p,R), \qquad (24)$$

$$f(p,R) = \delta_{L0} + \Lambda(-1)^{\ell'} j_L(pR);\ g(p,R) = \frac{1}{3}\delta_{L1} pR - \Lambda(-1)^{\ell'} j_L(pR),$$

$$h(p,R) = \frac{1}{3}\delta_{L1} p - \Lambda(-1)^{\ell'}\frac{\partial}{\partial R} j_L(pR). \qquad (25)$$

The set of differential operators $\partial_0, \partial_\pm$ is defined as

$$\partial_0 = \frac{\partial}{\partial R};\ \partial_\pm = \mp\frac{\partial}{\partial\theta} - \frac{i}{\sin\theta}\frac{\partial}{\partial\Phi}. \qquad (26)$$

It is seen immediately from eq. (16) that coupling occurs only between functions $u_{M\Lambda i}$ and $u_{M'\Lambda i'}$ for which $\Delta M = M' - M = 0, \pm 1$. The next thing to be noted is that the normalization condition (12) written out in detail coincides with (18), so we have

$$N^{M\Lambda}_{ii'}(R) = \delta_{ii'}. \qquad (27)$$

This fact enables us to rewrite eq. (7) in the form:

$$\left[-\frac{1}{2\mu R^2}\left(\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\Phi^2} - 2iM\frac{\cos\theta}{\sin^2\theta}\frac{\partial}{\partial\Phi} - \frac{M^2}{\sin^2\theta} + 2M^2\right) + v_{aa}(R) + \epsilon_{M\Lambda i}(R) - E\right]u_{M\Lambda i}(\vec{R}) =$$

$$= \frac{1}{2\mu}\sum_{i'}\{(D^{M\Lambda}_{ii'}(R) + B^{M\Lambda}_{ii'}(R)\frac{\partial}{\partial R})u_{M\Lambda i'}(\vec{R}) + Q^{M\Lambda+}_{ii'}(R)(\partial_+ + (M+1)\frac{\cos\theta}{\sin\theta})u_{M+1\,\Lambda i'}(\vec{R}) +$$

$$+ Q^{M\Lambda-}_{ii'}(R)(\partial_- + (M-1)\frac{\cos\theta}{\sin\theta})u_{M-1\,\Lambda i'}(\vec{R})\}. \qquad (28)$$

The system (28) allows an exact separation of angular dependence of the functions $u_{M\Lambda i}(\vec{R})$ in the form:

$$u_{M\Lambda i}(\vec{R}) = u^J_{M\Lambda i}(R) D^J_{-M_J-M}(\Phi,\theta,0). \qquad (29)$$

Substituting (29) into eq. (28) and taking into account that

$$(\partial_\pm + (M\pm1)\frac{\cos\theta}{\sin\theta})D^J_{-M_J-(M\pm1)}(\Phi,\theta,0) = -\sqrt{(J\mp M)(J\pm M+1)}D^J_{-M_J-M}(\Phi,\theta,0) \qquad (30)$$

we get finally for the functions $u^J_{M\Lambda i}(R)$ the following set of equations:

$$\left[-\frac{1}{2\mu R^2}\left(\frac{d}{dR}R^2\frac{d}{dR} - J(J+1) + 2M^2\right) + v_{aa}(R) + \epsilon_{M\Lambda i}(R) - E\right]u^J_{M\Lambda i}(R) =$$

$$= \frac{1}{2\mu}\sum_{i'}\{(D^{M\Lambda}_{ii'}(R) + B^{M\Lambda}_{ii'}(R)\frac{d}{dR})u^J_{M\Lambda i}(R) + Q^{JM\Lambda+}_{ii'}(R)u^J_{M+1\,\Lambda i'}(R) + \qquad (31)$$

$$+ Q^{JM\Lambda-}_{ii'}(R)u^J_{M-1\,\Lambda i'}(R)\}.$$

For convenience in (31) we have redefined the Q-s as

$$Q^{JM\Lambda\pm}_{ii'}(R) = -\sqrt{(J\mp M)(J\pm M-1)}Q^{M\Lambda\pm}_{ii'}(R). \qquad (32)$$

Using the explicit form of the two-center functions $\Phi_{M\Lambda i}(\vec{p};\vec{R})$ (13) and expanding the product of the two D-functions, it is easy to show that

$$\Phi_{M\Lambda i}(\vec{p};\vec{R})D^J_{-M_J-M}(\Phi,\theta,0) = \sqrt{\frac{4\pi}{2J+1}}\sum_\beta (-1)^{j-M_J}(e^{-\frac{i}{2}\vec{R}\vec{p}} + \Lambda(-1)^\ell e^{\frac{i}{2}\vec{R}\vec{p}})\phi^\beta_{M\Lambda i}(p,R)\times \qquad (33)$$

$$\times \sum_L (jMJ - M\,|L0)\sum_{mM_L}(jmLM_L|JM_J)i^{-\ell}\,\mathcal{Y}^\ell_{jm}(\Omega_p,s)Y_{LM_L}(\Omega_R).$$

This means that due to the angular dependence (29) each term in the expansion (6) has total angular momentum J and projection M_J. In other words, eq. (7) "knows" how to restore the rotation invariance of the problem, "destroyed" by a symmetry - breaking basis set $\Phi_{M\Lambda i}(\vec{p};\vec{R})$.

The next conserved quantum number which has to be reconstructed by studying eq. (7) or (31) is the total parity π. The special feature of eq. (31) that permits us to do so is its property against the substitution $M \to -M$. We have

$$D^{(-M)\Lambda}_{ii'} = D^{M\Lambda}_{ii'};\ B^{(-M)\Lambda}_{ii'} = B^{M\Lambda}_{ii'};\ Q^{J(-M)\Lambda+}_{ii'} = Q^{JM\Lambda-}_{ii'};\ Q^{J(-M)\Lambda-}_{ii'} = Q^{JM\Lambda+}_{ii'}. \qquad (34)$$

In deriving (34) we have used the following property of the coefficients $C^{\beta}_{M\Lambda i}(R)$ of eqs. (10) and (14) [10]

$$C^{\beta}_{(-M)\Lambda i}(R) = (-1)^{j+\ell+\frac{1}{2}}\, C^{\beta}_{M\Lambda i}(R). \qquad (35)$$

Introducting now instead of the pair of functions $u^{J}_{|M|\Lambda_i}(R)$ and $u^{J}_{-|M|\Lambda_i}(R)$ the pair

$$u^{J\nu}_{|M|\Lambda i} = \frac{1}{\sqrt{2}}(u^{J}_{|M|\Lambda i} + \nu u^{J}_{-|M|\Lambda i}); \quad \nu = \pm 1 \qquad (36)$$

the resulting equations will be uncoupled in ν due to eqs. (34) and a new quantum number ν occurred:

$$\left[-\frac{1}{2\mu R^2}\left(\frac{d}{dR}R^2\frac{d}{dR} - J(J+1) + 2M^2\right) + V_{aa}(R) + \epsilon_{M\Lambda i}(R) - E\right] u^{J\nu}_{M\Lambda i}(R) =$$

$$= \frac{1}{2\mu}\sum_{i'}\left\{\left(D^{M\Lambda}_{ii'}(R) + \nu\delta_{M\frac{1}{2}}Q^{J\frac{1}{2}\Lambda-}_{ii'}(R) + B^{M\Lambda}_{ii'}(R)\frac{d}{dR}\right) u^{J\nu}_{M\Lambda i}(R) +\right.$$

$$\left. + Q^{JM\Lambda+}_{ii'}(R)\, u^{J\nu}_{M+1\,\Lambda i'}(R) + Q^{JM\Lambda-}_{ii'}(R)\, u^{J\nu}_{M-1\,\Lambda i'}(R)\right\}. \qquad (37)$$

In eq. (37) $M>0$ and in view of the last term of (37) some special care must be taken for the case $M=\frac{1}{2}$: it was convenient to define $u^{J\nu}_{-\frac{1}{2}\Lambda i'} \equiv 0$ and to incorporate the contribution of the "non-diagonal" $Q^{J\frac{1}{2}\Lambda-}_{ii'}$ term into the diagonal matrix element.

Due to the decoupling in ν in the formal inversion of (36)

$$u^{J}_{|M|\Lambda i} = \frac{1}{\sqrt{2}}\sum_{\nu} u^{J\nu}_{|M|\Lambda i}; \quad u^{J}_{-|M|\Lambda i} = \frac{1}{\sqrt{2}}\sum_{\nu}\nu u^{J\nu}_{|M|\Lambda i}$$

the summation may be omitted since at one time either the $u^{J1}_{|M|\Lambda i}$ or the $u^{J(-1)}_{|M|\Lambda i}$ are different from zero. Using this argument, the total wave function can be written as

$$\Psi^{JM_J}(\vec{p}, \vec{R}) = \sum u^{J}_{M\Lambda i}(R)\Phi_{M\Lambda i}(\vec{p}; \vec{R})\, D^{J}_{-M_J-M}(\Phi, \theta, 0) =$$

$$= \sum_{\substack{M>0\\ i}}\left\{u^{J}_{M\Lambda i}\Phi_{M\Lambda i}D^{J}_{-M_J-M} + u^{J}_{-M\Lambda i}\Phi_{-M\Lambda i}D^{J}_{-M_JM}\right\} = \qquad (38)$$

$$= \sum_{\substack{M>0\\ i}} u^{J\nu}_{M\Lambda i}\left(\Phi_{M\Lambda i}D^{J}_{-M_J-M} + \nu\Phi_{-M\Lambda i}D^{J}_{-M_JM}\right)^{+}.$$

Now we can demonstrate that the quantum number ν arising from the symmetry (34) of the equations (31) is directly associated with the parity π of the total wave function. Using eqs. (13), (35) and (38) we get for the operator $\hat{\pi}$ $(\vec{p}\to-\vec{p};\ \vec{R}\to-\vec{R})$:

$$\hat{\pi}\Psi^{JM_J\nu}(\vec{p}, \vec{R}) = \pi\Psi^{JM_J\nu}(\vec{p}, \vec{R}); \quad \pi = \nu(-1)^{J-\frac{1}{2}} \qquad (39)$$

since

$$\hat{\pi}\Phi_{M\Lambda i}(\vec{p}, \vec{R})D^{J}_{-M_J-M}(\Phi, \theta, 0) = (-1)^{J-\frac{1}{2}}\,\Phi_{-M\Lambda i}(\vec{p};\vec{R})D^{J}_{-M_JM}(\Phi, \theta, 0).$$

Finally, for a three-body wave function with quantum numbers J, M_J and π we have:

$$\Psi^{JM_J\pi}(p, R) = \sum_{\substack{M>0\\ i}} u^{J\pi}_{M\Lambda i}(R)\left(\Phi_{M\Lambda i}D^{J}_{-M_J-M} + \pi(-1)^{J-\frac{1}{2}}\Phi_{-M\Lambda i}D^{J}_{-M_JM}\right) \qquad (40)$$

and the functions $u^{J\pi}_{M\Lambda i}(R)$ satisfy eqs. (37) with label ν replaced by π and the factor ν occuring with the $\delta_{M\frac{1}{2}}$ term by $\pi\cdot(-1)^{J-\frac{1}{2}}$. As soon as the wave function acquired the quantum number π, the Λ becomes unnecessary and can be omitted. Indeed, we have

$$\hat{\pi} = \hat{\pi}_{\vec{r}}\cdot\hat{\pi}_{\vec{R}}; \quad \hat{\pi}_{\vec{R}} = \hat{\pi}\cdot\hat{\pi}_{\vec{r}}$$

and since the wave function is an eigenfunction both of $\hat{\pi}$ and $\hat{\pi}_{\vec{r}}$ with eigenvalues π and Λ, respectively, it will be also an eigenfunction of $\hat{\pi}_{\vec{R}}$ with eigenvalue $\pi_R = \pi\cdot\Lambda$. In our case $\hat{\pi}_{\vec{R}}$ means the interchange of the two α-particles (bosons) and therefore we can have only $\pi_R = 1$ and $\pi = \Lambda$.

Thus we have demonstrated that careful treatment of eq. (7) can provide the necessary quantum numbers for the

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[+] The factor $1/\sqrt{2}$ is irrelevant, since the equations for the $u^{J\nu}_{M\Lambda i}$ are homogeneous.

three-body wave function Ψ. There is, however, another, more heuristic way of deriving the set of equations (38) and (40). Suppose that by some means we could find out that from the two-center functions $\Phi_{M\Lambda i}$ a set of functions $F^{JM_J\pi}_{Mi}(\vec{p};\vec{R})$ can be constructed:

$$F^{JM_J\pi}_{Mi}(p;R)=\sqrt{\frac{2J+1}{8\pi}}\left(\Phi_{M\Lambda i}D^{J}_{-M_J-M}+\pi(-1)^{J-\frac{1}{2}}\Phi_{-M\Lambda i}D^{J}_{-M_JM}\right);M>0 \quad (41)$$

with the following properties:

$$\hat{J}^2F^{JM_J\pi}_{Mi}=J(J+1)F^{JM_J\pi}_{Mi};\ \hat{J}_zF^{JM_J\pi}_{Mi}=M_JF^{JM_J\pi}_{Mi};\ \hat{\pi}F^{JM_J\pi}_{Mi}=\pi F^{JM_J\pi}_{Mi};$$

$$\hat{h}_{t.c.}F^{JM_J\pi}_{Mi}=\epsilon_{M\pi i}(R)F^{JM_J\pi}_{Mi};\ \int F^{JM_J\pi *}_{Mi}F^{J'M'_J\pi'}_{M'i'}\,d\vec{p}\,d\Omega_R=\delta_{JJ'}\delta_{M_JM'_J}\delta_{\pi\pi'}\delta_{MM'}\delta_{ii'}. \quad (42)$$

Noting that these functions form a complete set in the space $(\vec{p},\Omega_{\vec{R}})$ we can expand the three-body wave function in terms of these F-s:

$$\Psi^{JM_J\pi}_{Mi}(\vec{p},\vec{R})=\sum_{\substack{M>0\\ i}}u^{J\pi}_{Mi}(R)\,F^{JM_J\pi}_{Mi}(\vec{p};\vec{R}). \quad (43)$$

In (43) there is naturally no summation over the conserved quantum numbers J, M_J, π. The equations for the $u^{J\pi}_{Mi}(R)$ are obtained in the usual way from the condition:

$$\int F^{JM_J\pi}_{Mi}(\vec{p};\vec{R})^*(\hat{H}-E)\Psi^{JM_J\pi}(\vec{p},\vec{R})\,d\vec{p}\,d\Omega_{\vec{R}}=0. \quad (44)$$

When the expansion (43) is substituted into eq. (44), after performing all the integrations we obtain exactly the system of equations (37). Although this second derivation seems to be simpler, the first one provides some insight into the problem: how the properties of the two-center functions lead inevitably to the basis functions (41) and to the expansion (43).

IV. ADIABATIC ONE-LEVEL APPROXIMATION

After having derived the general system of equations (37) for the functions $u^{J\pi}_{Mi}(R)$ we can ask the question: what is the "minimal extension" of the BOA which preserves the necessary quantum numbers? Since every term in the

expansion (40) possesses the desired quantum numbers, it is sufficient to omit the coupling from the system (37): the summation over i' and the terms with $M\pm1$. There is a further simplification for this case: the coefficient of the first derivative $B^{M\pi}_{ii}(R)$ vanishes, since for $i=i'$ from eqs. (18), (19), (24), (25) and (27) using the properties of the $A^L_{\beta\beta'}$ and $\langle\beta iM|\hat{O}|\beta' i'M'\rangle_p$ of eqs. (21) and (22) we can derive

$$B^{M\pi}_{ii}(R)=\frac{1}{2}\frac{d}{dR}N^{M\pi}_{ii}(R)=0.$$

Thus we are left with the single equation

$$\left[-\frac{1}{2\mu R^2}\frac{d}{dR}R^2\frac{d}{dR}+V_{aa}(R)+\epsilon_{M\Lambda i}(R)+\mathcal{C}^{J\pi}_{Mi}(R)-E\right]u^{J\pi}_{Mi}(R)=0, \quad (45)$$

where the notation

$$\mathcal{C}^{J\pi}_{Mi}(R)=\frac{1}{2\mu}\left[\frac{J(J+1)-2M^2}{R}-D^{M\pi}_{ii}(R)+\delta_{M\frac{1}{2}}\cdot\pi(-1)^{J-\frac{1}{2}}Q^{J\frac{1}{2}\pi-}_{ii}(R)\right] \quad (46)$$

was introduced.

In this case, as in the BOA, we have a single differential equation (45) that governs the relative motion of the two α-particles, but the effective potential has the additional term $\mathcal{C}^{J\pi}_{Mi}(R)$, reflecting the inclusion of the necessary parts of the r.h.s. of eq. (7).

Using the notations of eqs. (41) and (43) the $\mathcal{C}^{J\pi}_{Mi}(R)$ can be written as

$$\mathcal{C}^{J\pi}_{Mi}(R)=-\frac{1}{2\mu}\int F^{JM_J\pi}_{Mi}(\vec{p};\vec{R})^*\Delta_{\vec{R}}F^{JM_J\pi}_{Mi}(\vec{p};\vec{R})\,d\vec{p}\,d\Omega_{\vec{R}}. \quad (47)$$

It is worth mentioning that eq. (45) has no sharply defined centrifugal term of the type const. R^{-2}: this follows immediately from eq. (47) if we write the Laplacian $\Delta_{\vec{R}}$ as

$$\Delta_{\vec{R}}=\frac{1}{R^2}\frac{\partial}{\partial R}R^2\frac{\partial}{\partial R}-\frac{1}{R^2}\hat{L}^2_R$$

and note that the functions $F^{JM_J\pi}_{Mi}(\vec{p};\vec{R})$ are not eigenfunctions of $\hat{L}^2_R$. This feature of eq. (45) reflects the fact

that in a three-body wave function the relative orbital momentum is not a conserved quantum number. In our calculation of ^{9}Be based on eqs. (45) and (46) we have made a further approximation, which - in our opinion - brings it closer in spirit to the BOA: the adiabatic assumption. According to this assumption, calculating the $D_{ii}^{M\pi}(R)$ the matrix elements (22), which contain differentiation of the functions $\phi^{\beta}_{M\Lambda i}(p, R)$ with respect to R, can be neglected. In this approximation we have:

$$\hat{d}(p, R) \sim - f(p,R)\left(\frac{1}{4}p^2 + \frac{1}{R^2}j'(j'+1)\right) + \frac{1}{2R^2}g(p,R)\left(j(j+1)-j'(j'+1)-L(L+1)\right). \tag{48}$$

We do not want to discuss in detal the conditions of the validity of this assumption; its effect for the ^{9}Be case will be considered later.

V. APPLICATION AND RESULTS FOR THE ^{9}Be

Before applying the formalism of the preceding sections to the ^{9}Be, it has to be refined in one aspect. The term $v_{\alpha\alpha}(R)\cdot u^{J\pi}_{Mj}(R)$ in eq. (45) was obtained assuming the simplest (local and central) α–α interaction; in this case the potential depends only on R, and all the manipulations related to the variables $\vec{p}$, s, Ω_R have no effect upon it. The phenomenological α–α potential of Ali and Bodmer /11/, which we have used in /9/ is, however, angular-momentum dependent, or, in other words, it has angular nonlocality. It can be written in the form:

$$\hat{v}^{AB}_{\alpha\alpha} = V_{coul}(R) + \sum_{L=0,2,4} v^{AB}_{L}(R)\cdot \hat{P}_L(\Omega_R). \tag{49}$$

where V_{coul} is the Coulomb interaction of the two α-particles and $\hat{P}_L(\Omega_R)$ is a projection operator onto a state with angular momentum L (in variable $\vec{R}$). The effect of this nonlocality can be evaluated most conveniently using eq. (44). Defining the function $a_L(R)$ as

$$a_L(R) = \int \dot{F}^{JM_J\pi}_{Mi}(\vec{p}, \vec{R})\hat{P}_L(\Omega_R) F^{JM_J\pi}_{Mi}(\vec{p}, \vec{R})\, d\vec{p}\, d\Omega_R \tag{50}$$

the α–α interaction term of eq. (45) is obtained as

$$\left[V_{coul}(R) + \sum_{L=0,2,4} v^{AB}_{L}(R)\, a_L(R)\right] u^{J\pi}_{Mi}(R). \tag{51}$$

Here again we have an effect of L mixing in the three-body wave function, the $a_L(R)$ being the R-dependent mixing coefficients. It can be easily shown by using again eq. (44), that a truly - not only angularly - non-local α–α potential would lead to an integrodifferential equation instead of eq. (45). In the special case when the original α–α potential is non-local but separable, the separability will be, unfortunately, lost during the integrations in eq. (44), and we obtain again an integro-differential equation with a non-separable kernel. In view of this computational difficulty we have not used in the present work the forbidden-state α–α potential /5/, only the Ali-Bodmer one. The n–α interactions of our ^{9}Be three-body model were discussed in detail in /9/; here we only recall their main features:

- the considered partial waves are: $s_{1/2}$, $p_{1/2}$, $p_{3/2}$;
- the form factors are of the form:

$$g_{1\ell j}(p) = \frac{p^{\ell}}{(p^2 + \beta^2_{\ell j})^{\ell+1}} \tag{52}$$

- in p-waves we used single term separable potentials ($N_{1j} = 1$);
- for the $s_{1/2}$ channel we used two types of interaction:

a) attractive one-term potential with form factor (52) with projecting out the Pauli-forbidden bound state; this means a second separable term in this partial wave with form factor

$$g_{201/2}(p) = \frac{1}{(p^2 + \gamma_0^2)(p^2 + \beta^2_{01/2})}$$

and with the strength parameter $\lambda_{201/2} \to \infty$; $\frac{1}{2}(m_\alpha^{-1} + m_n^{-1})\gamma_0^2$ being the binding energy of the forbidden state;

b) repulsive one-term potential.

The interaction parameters are given in the table. The results of the two-center calculation are summarized in fig. 1, where the dominant $\epsilon_{M\Lambda}(R)$[+] eigenvalues are

[+] In our case the additional label i is not needed, the pair MΛ completely specifies the two-center states taken into account.

Table

The parameters of the separable n–α potential. Here μ' denotes the n–α reduced mass and $2\mu'\gamma_0^2$ is the energy of the Pauli-forbidden bound state (for the attractive potential)

	$s_{1/2}$ (attractive)	$s_{1/2}$ (repulsive)	$p_{1/2}$	$p_{3/2}$
β	1.494 fm^{-1} (γ_0 =.835 fm^{-1})	.7 fm^{-1}	1.177 fm^{-1}	1.499 fm^{-1}
$2\mu'\lambda$	-9.283 fm^{-3}	3.770 fm^{-1}	-13.873 fm^{-5}	-60.708 fm^{-5}

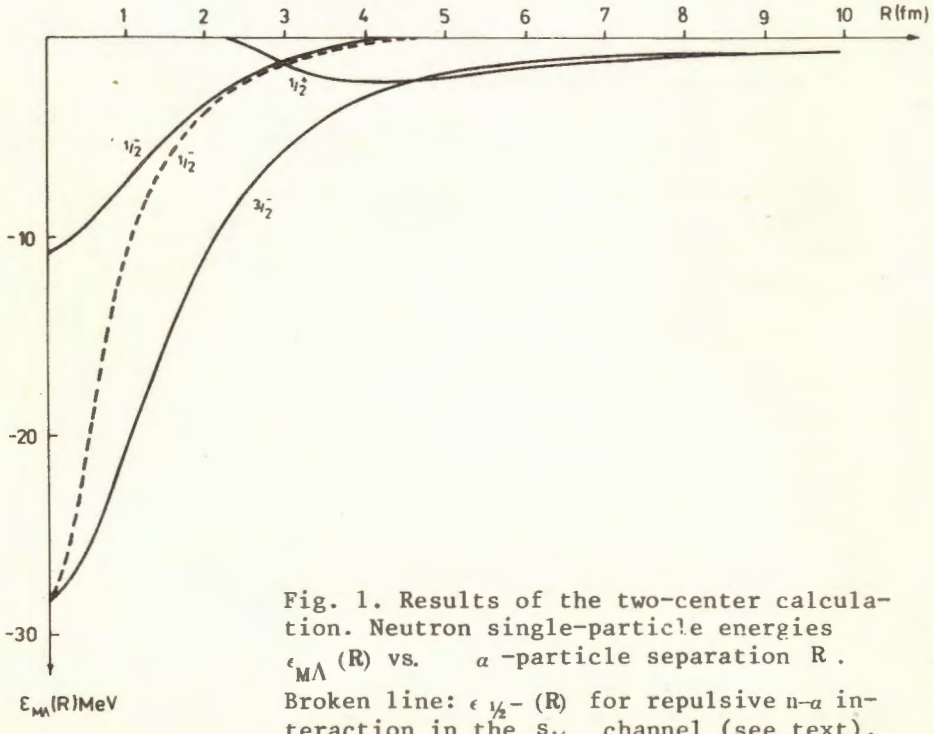


Fig. 1. Results of the two-center calculation. Neutron single-particle energies $\epsilon_{M\Lambda}(R)$ vs. α-particle separation R. Broken line: $\epsilon_{1/2^-}(R)$ for repulsive n–α interaction in the $s_{1/2}$ channel (see text).

plotted against R. As it was pointed out in [9], a significant difference between the case a) and b) of the s-wave interaction was observed only for the $M\Lambda = 1/2^-$ case.

The calculation of the ^{9}Be spectrum along the lines of eqs. (45), (46) and (48) based on the two-center states of fig. 1 starts with the evaluation of the additional potentials (46). The results are displayed in figs. 2a,2b,2c for the cases $M\pi = 3/2^-$, $1/2^+$ and $1/2^-$ ($s_{1/2}$-attraction), respectively. In these figures we have plotted for different J and fixed $M\pi$ the effective potential term $V_M^{J\pi}(R)$ of eq. (45):

$$V_M^{J\pi}(R) = V_{coul}(R) + \epsilon_{M\pi}(R) + \sum_{L=0,2,4} v_L^{AB}(R) a_L(R) + \mathcal{C}_M^{J\pi}(R). \qquad (53)$$

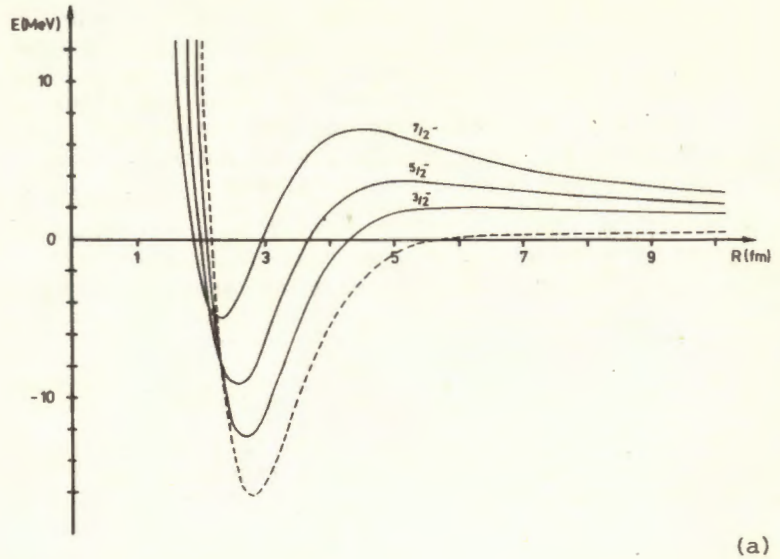
For comparision the Born-Oppenheimer effective potential $v_0^{AB}(R) + \epsilon_{M\pi}(R)$ is also shown (broken line). It has to be noted that since for the case $M\pi = 1/2^+$ the two-center solutions do not exist for $R < R_0 = 2.05$ fm, the curves for this case were obtained by extrapolating from $R > R_0$. We used the following procedure: having observed that for $R \to R_0$ the coefficients $a_L(R)$ and the additional potentials $\mathcal{C}_{1/2}^{J+}(R)$ have the property:

$$a_L(R) \to \delta_{LL(J)}$$
$$\mathcal{C}_{1/2}^{J+}(R) \to \frac{1}{2\mu} \frac{L(J)\cdot(L(J)+1)}{R^2} \qquad \text{for} \quad R \to R_0 \qquad (54)$$

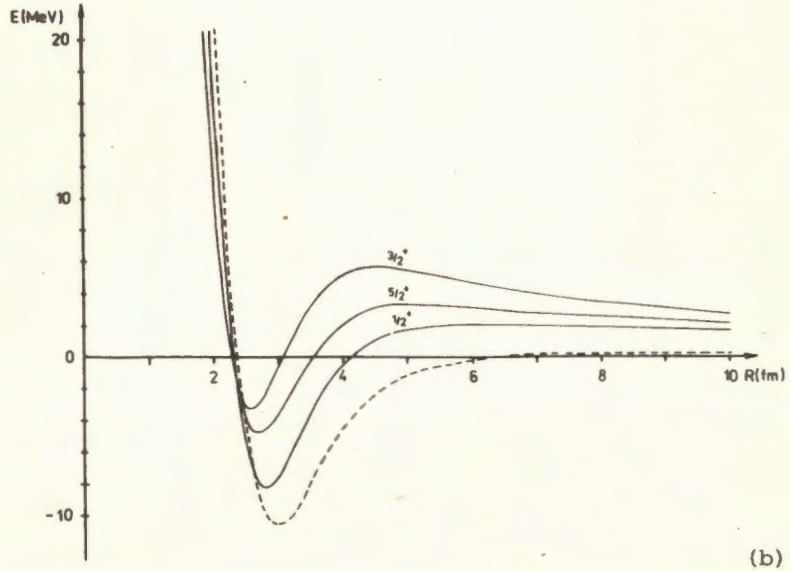
for $R < R_0$ we assumed:

$$V_{1/2}^{J+}(R) = V_{coul}(R) + v_{L(J)}^{AB}(R) + \frac{1}{2\mu} \frac{L(J)\cdot(L(J)+1)}{R^2}. \qquad (55)$$

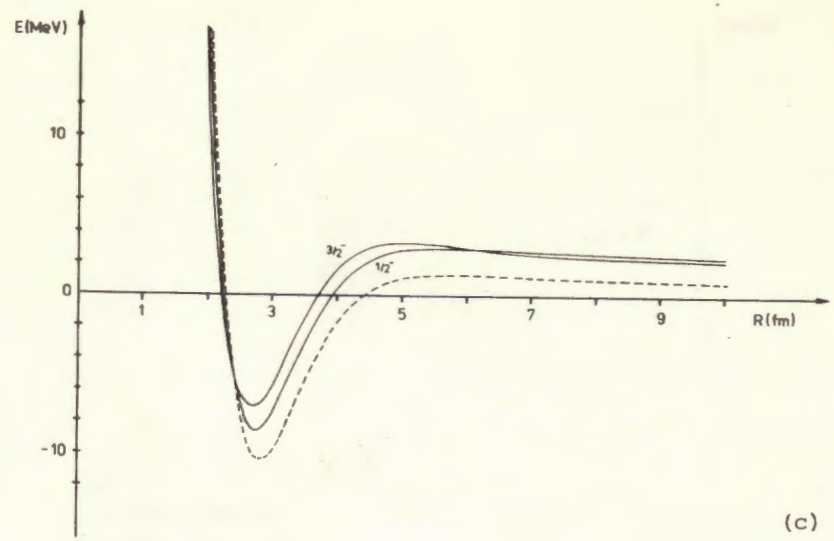
The L(J) values are the following: $L(1/2) = 0$, $L(3/2) = L(5/2) = 2$. This procedure is by no means rigorous; strictly speaking, the one-level approximation of the three-body wave function is not valid in this case for $R < R_0$; in a correct treatment the continuum two-center states should be also included in the expansion (6) to account for the possibility of the neutron escape if the two α-particles are too close. We still expect



(a)



(b)



(c)

Fig. 2. The effective potentials $V_M^{J\pi}(R)$ obtained from the different two-center states (see eq.(53)).
(a) $M\pi = 3/2^-$
(b) $M\pi = 1/2^+$
(c) $M\pi = 1/2^-$

for the few lowest total angular momentum values J . Broken lines: the corresponding Born-Oppenheimer effective potentials.

that the error, introduced this way, does not break down completely the applicability of our simple approach, since the incorrectly treated region ($R<R_0$) is almost fully covered by the strong Pauli repulsion of the two α-particles, which does not allow them to spend too much time in this region.

After having obtained the potentials (53), the eigenvalue equation (45) was solved to obtain the spectrum of ^{9}Be. The results are shown in fig. 3. Like in the experimental spectrum, we got only one true bound state below the $\alpha+\alpha+n$ threshold, the $J\pi = 3/2^-$ ground state. All the other states of the spectrum are above the threshold, and thus the corresponding eigenvalues are complex. The widths of the lower-lying states are very small ($\Gamma \leq .001$MeV)

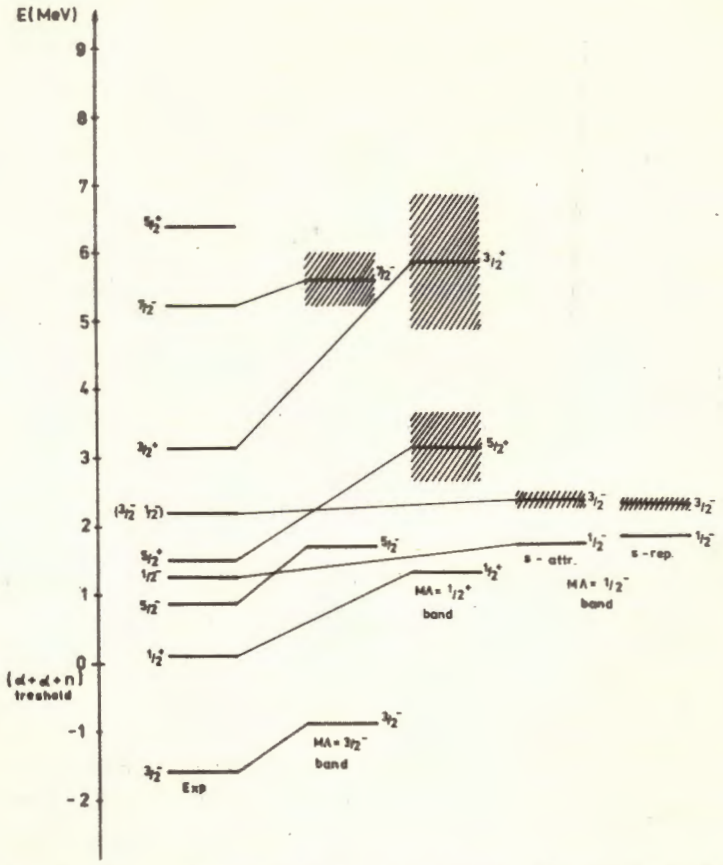


Fig. 3. Comparison of the calculated and experimental spectrum of ^{9}Be.

so we did not plot them. The spectrum is naturally divided into "rotational bands" based on the different intrinsic states $M\pi$. The $M\pi = 1/2^-$ band has been calculated with both versions of the s-wave potential; the difference is quite small. We have also checked the validity of the adiabatic assumption (48). It turned out that the inclusion of the differentiation with respect to R has a negligible effect upon the ^{9}Be spactrum, except for the case of $M\pi = 1/2^+$, where the derivatives are pathologically great around R_0, again indicating a certain instability of the model in that region.

VI. CONCLUSIONS

The qualitative agreement of our calculated spectrum with the experimental one is satisfactory, especially in view of the no-adjustable-parameter character of the calculation. The negative parity states are slightly underbound, while the positive parity band is shifted upwards more considerably. At this point we have to face the age-old question of nuclear physics : who is responsible for the discrepancy, the assumptions of the model and the built in approximations or the input interactions?

It is known that the phenomenological α–α potential of Ali and Bodmer always gives underbinding for bound systems containing α-particles [7]. This underbinding is explained by the failure of the AB-potential to reproduce the correct short-distance behaviour of the α–α relative wave function (inner oscillations) required by the Pauli principle. It is argued [12] that the underbinding effect increases with decreasing average relative distance of the α-particles in a certain system. Thus, for ^{12}C it is quite strong (~ 5-7 MeV), for ^{8}Be it is negligible, and therefore for the weakly bound ^{9}Be we can also expect a small effect. Hence, in our opinion, the small underbinding of the negative parity states is most likely due to this effect. We plan to check this statement by a similar calculation using an α–α force correctly taking into account the Pauli princuple. As far as the positive-parity band is concerned, we are less sure about the conceptual correctness of the model; the expansion is based in this case on a very weakly bound two-center state (even ceasing for $R<R_0$) and the closeness of the neglected continuum states may be responsible for the more important discrepancy.

ACKNOWLEDGEMENT

The authors are deeply indebted to Dr. T.Vertse (Research Institute for Nuclear Physics, Debrecen, Hungary) for supplying them with his excellent resonant-state-calculating program.

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Received by Publishing Department
April 17 1979.