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A NEW METHOD FOR SOLVING THE TWO CENTER PROBLEM WITH REALISTIC POTENTIALS

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Новый метод решения задачи двух центров с реалистическими потенциалами

Предложен метод решения задачи двух центров с реалистическими потенциалами, который состоит в том, что одночастичные потенциалы аппроксимируются сепарабельным разложением, а задача с сепарабельными потенциалами решается точно. В качестве примера вычислены энергии и волновые функции нейтрона в поле двух ядер ^{16}O с потенциалами Вудса-Саксона как функции расстояния между ядрами.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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A New Method for Solving the Two Center Problem with Realistic Potentials

A method has been proposed for the solution of the two-center problem with realistic potentials. It consists of two steps: first, we make a separable approximation to the single particle potentials and then the two-center problem with these separable potentials is solved exactly. The only approximations are introduced at the first stage in a well controllable way. As an example, we have calculated the single-particle energies and wave functions in the field of two ^{16}O like Woods-Saxon potentials as functions of their distance **R**.

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

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I. Introduction

For the last few years the quantum mechanical two-center problem is widely discussed in nuclear physics (in atomic physics electron wave functions are successfully used[1,2] which are just the solutions to the two-fixed-center problem). This interest is caused by the vast experimental information on heavy ion reactions and necessity of theoretical description of the existing experimental data. In particular, the studies of the elastic transfer processes[3], potential energy of deformation of colliding nuclei, fission barriers, isomerism of form, etc., [4-8] have shown the usefulness of concepts of the two-center problem.

However, to solve the two-center problem with realistic interactions in practice is quite difficult. Exact solutions are found only for a few special cases, like the oscillator[9], square-well[10] and Coulomb[11] potentials. In refs.[6,12] a rather simple method was proposed for the expansion of single-particle wave functions of the two-center problem with realistic potentials in terms of harmonic oscillator wave functions of the one-center problem. This method, though being easy to handle with in practical calculations, is converging slowly when the distance between nuclei is increased, and the asymptotic behaviour of the wave functions is incorrect. The method[6,12] is valid only for finding the bound single-particle states.

In this paper we develop a method for solving the two-center problem which is based on the expansion of potentials in terms of harmonic oscillator functions $V \to \sum_{ij}^{N} |i\rangle V_{ij} \langle j| \equiv V_{sep}$. In this method the accuracy of the results obtained depends only on the accuracy of the expansion of interaction potentials which can have any form obtained from fitting experimental data or from known potentials. The Schrödinger equation with approximate potentials V_{sep} is solved exactly. Although the calculations were made for bound states ($E(R) < 0$) only, the method is applicable also for finding solutions in the continuous spectrum (e.g., quasistationary states). It is essential that the wave functions obtained by this method have the required asymptotic behaviour. For this reason they can be used as a complete set (like in atomic physics) in studying the heavy ion reactions.

II. General Formulation

The most general spherically symmetric single-particle separable potential can be written as*)

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

where the ket-vectors $|n\ell jm\rangle$ are defined through the form factors: e.g. in momentum representation

$$\langle \underline{k}, s | n\ell jm \rangle = g_{n\ell j}(k) \left[i^{\ell} Y_{\ell}(\hat{k}) \chi_{1/2}(s) \right]^{j}_{m} , \qquad (2)$$

ℓ_{max} defines the number of partial waves in which the potential acts while $N_{\ell j}$ fixes the number of separable terms in each partial wave; $\chi_{1/2}(s)$ is the spin function and $[\ ]^{j}_{m}$ stands for vector coupling. In the treatment of single-particle problems the potential is usually taken to be at the origin of the coordinate system, that is writing the matrix elements $\langle \underline{r} s | \hat{V} | \underline{r}' s' \rangle$ it is understood that the potential is at the point from where $\underline{r}$ and $\underline{r}'$ are measured. If we want to put it to another point, say $\underline{a}$, we have to act on it with the displacement operator:

*) In some cases instead of (1) we have a representation non-diagonal in n; it can be easily reduced to the form (1) by performing a linear transformation upon the indices n and leaving the conserved quantum numbers ℓ, j and m untouched.

$$\hat{V}(\underline{a}) = e^{-i\underline{a}\hat{\underline{p}}}\ \hat{V}\ e^{i\underline{a}\hat{\underline{p}}}, \qquad (3)$$

where $\hat{\underline{p}}$ is the momentum operator. The result is again a separable potential with displaced ket-vectors $e^{-i\underline{a}\hat{\underline{p}}}\,|n\ell_j m\rangle$.

Let us consider now a single particle problem with two potentials of the form (1), one placed at point $\underline{R}_1$ the other at $\underline{R}_2$:

$$H = H_0 + \hat{V}_1(\underline{R}_1) + \hat{V}_2(\underline{R}_2), \qquad (4)$$

where H_0 is the kinetic energy operator: $H_0 = \frac{\hbar^2\hat{\underline{p}}^2}{2m}$.

In order to distinguish between the two potentials $\hat{V}_1$ and $\hat{V}_2$ a further index i $(i = 1,2)$ is introduced for the quantities appearing in eq. (1) and eq. (2): $|n\ell_j m\rangle$, $\lambda_{in\ell_j}$, $g_{in\ell_j}$, $\ell_{max,i}$, $N_{i\ell_j}$ and also for the sums defined by $\ell_{max,i}$ and $N_{i\ell_j}$: $\sum^i$. To simplify this somewhat clumsy way of writing it will be convenient to use abbreviated notation for certain group of indices: $|in\ell_j m\rangle = |I\rangle = |i\alpha\rangle = |i\beta m\rangle$ or $\{in\ell_j m\} = I$, $\{n\ell_j m\} = \alpha$, $\{n\ell_j\} = \beta$.

The Hamiltonian (4) contains two parameters $\underline{R}_1$ and $\underline{R}_2$ and thus its eigenvalues $E(\underline{R}_1,\underline{R}_2)$ and eigenfunctions $|\Psi(\underline{R}_1,\underline{R}_2)\rangle$ obtained from the Schrödinger equation

$$\left[H(\underline{R}_1,\underline{R}_2) - E(\underline{R}_1,\underline{R}_2)\right]|\Psi(\underline{R}_1,\underline{R}_2)\rangle = 0 \qquad (5)$$

also depend on these parameters. To solve (5) we can apply the well known methods developed for separable potentials. For bound state solutions we can rewrite (5) as

$$|\Psi\rangle = G_0(E)\left[\hat{V}_1(\underline{R}_1) + \hat{V}_2(\underline{R}_2)\right]|\Psi\rangle \qquad (6)$$

with the usual notation for the free Green-operator:

$$G_0(E) = (E - H_0)^{-1}. \qquad (7)$$

Using (1) and (3) we get

$$|\Psi\rangle = G_0(E)\Big[\sum_{\alpha}^{1} e^{-i\underline{R}_1\hat{\underline{p}}}\,|1\alpha\rangle\lambda_{1\beta}\langle 1\alpha|\,e^{i\underline{R}_1\hat{\underline{p}}}\,|\Psi\rangle + \sum_{\alpha}^{2} e^{-i\underline{R}_2\hat{\underline{p}}}\,|2\alpha\rangle\lambda_{2\beta}\langle 2\alpha|\,e^{i\underline{R}_2\hat{\underline{p}}}\,|\Psi\rangle\Big] \qquad (8)$$

$$\lambda_{i\beta}\langle i\alpha|\,e^{i\underline{R}_i\hat{\underline{p}}}\,|\Psi\rangle = A_{i\alpha} = A_I \qquad (9)$$

$$\sum_{I'}\left[\lambda^{-1}_{i\beta}\,\delta_{II'} - M^{A}_{II'}(E,\underline{R}_{ii'})\right]A_{I'} = 0 \qquad (10)$$

$$M^{A}_{II'}(E,\underline{R}_{ii'}) = \langle I|\, e^{i\underline{R}_{ii'}\hat{\underline{p}}}\, G_0(E)\,|I'\rangle\ , \quad \underline{R}_{ii'} = \underline{R}_i - \underline{R}_{i'}\ . \qquad (11)$$

In obtaining (11) we made use of the fact, that $[H_0, \hat{\underline{p}}] = 0$ and thus $e^{i\underline{R}_i\hat{\underline{p}}}$ also commutes with $G_0(E)$. The system (10) is homogeneous and its solvability condition

$$\mathrm{Det}\,\|\lambda^{-1}_{i\beta}\,\delta_{II'} - M^{A}_{II'}(E,\underline{R}_{ii'})\| = 0 \qquad (12)$$

defines the exact energy eigenvalues of the Hamiltonian (4). Having obtained the eigenvalues E, we can get the eigenfunction $|\Psi\rangle$ by solving (10) for the coefficients A_I and using (8) for suitable normalization.

The described "algebrazation" of the Schrödinger eq. is a typical way of obtaining exact results for separable potentials[14].

III. Properties of the Solutions

The usual way of obtaining the symmetry properties (and quantum numbers) of the solution $|\Psi\rangle$ to the problem (5) is studying the transformation behaviour of the Hamiltonian (4) and then choosing an appropriate coordinate system, where the symmetries are most apparent. In the case of separable potentials, however, there is another possibility: all features of the solution $|\Psi\rangle$ can be obtained from a detailed study of the linear system (10), and we shall follow this way.

Let us examine the matrix elements (11) in detail. First of all, we see that in the matrix elements diagonal in (ℓ), the exponential factor disappears and they can be written as:

$$M^{A}_{i\alpha,i\alpha'}(E) = \langle i\alpha|\, G_0(E)\,|i\alpha'\rangle = \delta_{jj'}\,\delta_{\ell\ell'}\,\delta_{mm'}\,S_{i\beta,i\beta'}(E) \qquad (13)$$

with

$$S_{i\beta,i\beta'}(E) = -\frac{2m}{\hbar^2}\int_0^\infty \frac{g_{in\ell j}(k)\,g_{i'n'\ell'j'}(k)}{k^2+\gamma^2}\,k^2\,dk\ , \quad \gamma^2 = -\frac{2mE}{\hbar^2}\ .$$

The non-diagonal matrix elements can be obtained using elementary angular momentum algebra as

$$M^{A}_{i\alpha,i'\alpha'}(E,R_{ii'}) = \sum_{LM} i^{L+\ell-\ell'}(-1)^{m'+1/2}\left[\frac{(2\ell+1)(2j+1)(2\ell'+1)(2j'+1)4\pi}{2L+1}\right]^{1/2}\cdot$$
$$\cdot\begin{Bmatrix} L & \ell' & \ell \\ 1/2 & j' & j \end{Bmatrix}(\ell 0\ell' 0|L0)(jmj'-m'|LM)Y^{*}_{LM}(\hat{R}_{ii'})\;Q^{L}_{i\beta,i'\beta'}(E,R_{ii'})$$

with

$$Q^{L}_{i\beta,i'\beta'}(E,R_{ii'}) = -\frac{2m}{\hbar^2}\int_0^\infty \frac{g_{i\ell j}(k)\,g_{i'\ell' j'}(k)\,j_L(kR_{ii'})}{k^2+\gamma^2}\,k^2dk\,. \qquad (14)$$

Using this form of the matrix elements we shall establish several symmetry properties of the solutions $|\Psi\rangle$.

a). Rotation symmetry.

The Hamiltonian (4) is invariant under rotations around the axis connecting the two potentials, or

$$[H,\hat{J}\cdot\underline{n}] = 0\,,$$

where $\underline{n}$ is unit vector in direction $\underline{R}_{12} = \underline{R}_1 - \underline{R}_2$. This means, that the eigenfunctions of $\underline{H}$ can be labelled by the eigenvalues M of $\hat{J}\cdot\underline{n}$. To demonstrate this fact we introduce new unknown numbers B_I instead of A_I by the following orthogonal transformation

$$A_I = A_{i\beta m} = \sum_{m'=-j}^{j} D^{j}_{mm'}(\omega)\,B_{i\beta m'} \qquad (15a)$$

$$B_I = B_{i\beta m} = \sum_{m'=-j}^{j} D^{j*}_{m'm}(\omega)\,A_{i\beta m'}, \qquad (15b)$$

where the $D^{j}_{mm'}(\omega)$ are the rotation matrices and $\omega=(\Phi,\Theta,0)$, Φ and Θ being the polar angles of the vector $\underline{R}_{12}$. Introducing (15) into (10) and using (13) and (14) with the help of some algebraic manipulations on the rotation matrices we obtain the following set of equations for the B_I:

$$\sum_{I'}\left[\lambda^{-1}_{i\beta}\,\delta_{II'} - M^{B}_{I,I'}(E,R_{ii'})\right]B_{I'} = 0 \qquad (16)$$

with

$$M^{B}_{i\alpha,i\alpha'}(E) = \delta_{jj'}\,\delta_{\ell\ell'}\,\delta_{mm'}\,S_{i\beta,i\beta'}$$

and

$$M^{B}_{i\alpha,i'\alpha'}(E,R_{ii'}) = (-1)^{m+1/2}\,\delta_{mm'}\sum_{L} i^{L+\ell-\ell'}\,\frac{4\pi}{2L+1}\,\nu_{ii'}\cdot$$
$$\cdot\left[(2\ell+1)(2j+1)(2\ell'+1)(2j'+1)\right]^{1/2}(\ell 0\ell' 0|L0)(j'mj-m|L0)\cdot$$
$$\cdot\begin{Bmatrix} L & \ell' & \ell \\ 1/2 & j & j' \end{Bmatrix} Q^{L}_{i\beta,i'\beta'}(E,R_{ii'})\,,\quad \nu_{ii'} = \begin{cases} 1 & ii'=12 \\ (-1)^{L} & ii'=21 \end{cases} \qquad (17)$$

The factor $\nu_{ii'}$ comes from the identity:

$$Y^*_{LM}(\hat{R}_{12}) = (-1)^L Y^*_{LM}(\hat{R}_{21})$$

Since the system (16) is diagonal in m, its determinant, which coincides with that of (10), can be written as a product of determinants of sub-matrices with different m. Thus the eigenvalues, the zeros of the total determinant, can be labelled by m showing which of the sub-determinants vanishes. For an eigenvalue E_{m_0} the solutions $B_{i\beta m}$ will be non-zero only for $m = m_0$. Thus we get a classification of the states of the Hamiltonian (4) according to the quantum number $M = m_0$ and (8) can be written as

$$|\Psi M\rangle = G_0(E) \sum_I e^{i\underline{R}_i \hat{\underline{p}}} |I\rangle D^j_{mM}(\omega) B_{i\beta M} \quad . \tag{18}$$

It can be shown that the state $|\Psi M\rangle$ is an eigenfunction of $\hat{\underline{J}}\cdot\underline{n}$ with an eigenvalue M. It is also worth mentioning that the B_I are independent of the angles ω, since the system (16) does not contain them any more, and thus all the angular dependence of the A_I is expressed by eq. (15a).

b). Time reversal symmetry

The Hamiltonian (4) is invariant under time reversal, or

$$[H, \hat{T}] = 0 \quad .$$

Thus if $|\Psi M\rangle$ is an eigenfunction with energy E_M, $\hat{T}|\Psi M\rangle$ must also be an eigenfunction with the same energy. How can we see this from eq. (16)? Writing (16) for $B_{i\beta -m}$ it turns out, that the quantity $\tilde{B}_{i\beta M}$ defined as $\tilde{B}_{i\beta M} = (-1)^{j-\ell-1/2} B_{i\beta -M}$ satisfies the same equations as $B_{i\beta M}$ and therefore $B_{i\beta -m} = (-1)^{j-\ell-1/2} B_{i\beta M}$. Thus we have for the energy eigenvalues $E_{-M} = E_M$ and for the wave function:

$$|\Psi -M\rangle = G_0(E) \sum_I e^{-i\underline{R}_i \hat{\underline{p}}} |I\rangle D^j_{m-M}(\omega) B_{i\beta M} (-1)^{j-\ell-1/2} \quad . \tag{19}$$

It can be shown, that the right-hand side of (18) is proportional to $\hat{T}|\Psi M\rangle$, and thus we have shown that the time-reversed function is also among the solutions given by (16).

c) Permutation symmetry $V_1 \longleftrightarrow V_2$

If the potentials V_1 and V_2 are identical, an additional symmetry of the Hamiltonian (4) arises, namely its invariance under the permutation $\hat{P}_{12}$: $[H, \hat{P}_{12}] = 0$.

A possible realization of $\hat{P}_{12}$ in the single particle Hilbert space is

$$\hat{P}_{12}\,|\underline{r}\,\rangle = |\underline{r}'\rangle = |-\underline{r}+\underline{R}_1+\underline{R}_2\rangle \tag{20}$$

(in the coordinate system $\underline{r}'$ the potential V_1 will be at the point $\underline{R}_2$ and V_2 at the point $\underline{R}_1$). It is clear from eq. (20) that in the special coordinate system, for which $\underline{R}_1+\underline{R}_2 = 0$ the operator $\hat{P}_{12}$ coincides with the space reflection operator.

Let us examine the effect of this additional symmetry on the system (16). Because of the identity of the two potentials the matrix elements Q^L and S are independent of i, i' and symmetric in β,β' :

$$S_{1\beta,1\beta'} = S_{2\beta,2\beta'} = S_{1\beta',1\beta} = S_{2\beta',2\beta} \qquad \text{and}$$

$$Q^L_{1\beta,2\beta'} = Q^L_{1\beta',2\beta} = Q^L_{2\beta,1\beta'} = Q^L_{2\beta',1\beta}$$

For the matrix elements $M^B_{I,I'}$ we get in this case:

$$\begin{aligned} &M^B_{1\beta,1\beta'} = M^B_{1\beta',1\beta} = M^B_{2\beta,2\beta'} = M^B_{2\beta',2\beta} \\ &M^B_{1\beta,2\beta'} = (-1)^{\ell+\ell'} M^B_{1\beta',2\beta} = M^B_{2\beta',1\beta} = (-1)^{\ell+\ell'} M^B_{2\beta,1\beta'} \end{aligned} \tag{21}$$

(we have omitted the index m , which is common for all the matrix elements). If we now introduce new unknown numbers $C_{\Lambda\beta m}$ as

$$\begin{aligned} C_{\Lambda\beta m} &= \frac{1}{\sqrt{2}}\left(B_{1\beta m} + \Lambda(-1)^{\ell} B_{2\beta m}\right), \quad \Lambda = \pm 1 \\ B_{1\beta m} &= \frac{1}{\sqrt{2}}\left(C_{1\beta m} + C_{-1\beta m}\right) \\ B_{2\beta m} &= \frac{1}{\sqrt{2}}(-1)^{\ell}\left(C_{1\beta m} - C_{-1\beta m}\right) \end{aligned} \tag{22}$$

then due to Eqs.(21) we get the following system for them:

$$\sum_{\beta'\Lambda'}\left[\lambda_\beta^{-1}\,\delta_{\beta\beta'}\,\delta_{\Lambda\Lambda'} - M^C_{\Lambda\beta m,\Lambda'\beta' m}\right] C_{\Lambda'\beta' m} = 0 \tag{23}$$

with

$$M^C_{\Lambda\beta m,\Lambda'\beta' m} = \delta_{\Lambda\Lambda'}\left[M^B_{1\beta m,1\beta' m} + \Lambda(-1)^{\ell'} M^B_{1\beta m,2\beta' m}\right]. \tag{24}$$

The new system is diagonal in Λ , and using similar considerations as we did for m , following Eqs. (16) and (18) we get a further classification of states and eigenvalues with quantum number Λ :

$$E_{\Lambda M} \qquad \text{and}$$

$$|\Psi\Lambda M\rangle = G_0(E)\sum_{\alpha}\left[e^{-i\underline{R}_1\hat{\underline{p}}} + \Lambda(-1)^{\ell} e^{-i\underline{R}_2\hat{\underline{p}}}\right]|\alpha\rangle\, D^{j}_{mm}(\omega)\, C_{\Lambda\beta M} \tag{25}$$

(we have omitted the index i from the ket-vectors $|i\alpha\rangle$, since in this case they don't depend on it). Using a simple identity, which immediately follows from (20)

$$\hat{P}_{12}\, e^{-i\underline{R}_1\hat{\underline{p}}}\,|\alpha\rangle = e^{i\underline{R}_2\hat{\underline{p}}}\,|\alpha\rangle = (-1)^{\ell}\, e^{-i\underline{R}_2\hat{\underline{p}}}\,|\alpha\rangle$$

it is easy to show that the wave functions (25) are eigenfunctions of the operator $\hat{P}_{12}$ with eigenvalue Λ .

d). Behaviour for $R_{12}\to 0$ and $R_{12}\to\infty$.

Let us examine the behaviour of our solutions in the two limiting cases: a) the potentials V_1 and V_2 are infinitely far from each other ($R_{12}\to\infty$) ; b) the potentials are at the same place ($R_{12}=0$). In the case a) we have

$$Q^{L}_{i\beta,i'\beta'}(E,R_{12})\longrightarrow 0 \qquad \text{if} \qquad R_{12}\to\infty$$

because of the rapidly varying function $j_L(kR_{12})$ in the integrand of Eq. (14). The matrix $M^{B}_{I,I'}$ of Eq.(16) then can be written as

$$M^{B}_{I,I'}(E,\infty) = \delta_{ii'}\,\delta_{ee'}\,\delta_{jj'}\,\delta_{mm'}\,S_{in\ell_j,in'\ell_j}\,. \qquad (26)$$

The matrix (26) is diagonal in i and its submatrices for $i=1,2$ coincide with those emerging from the single particle problems with potentials V_i alone. Introducing the bound state functions of the potential V_i as

$$(H_0+V_i)\,|\varphi n\ell_j m\rangle_i = \varepsilon_{in\ell_j}\,|\varphi n\ell_j m\rangle_i$$

the solutions of (5) will be of the form

$$|\Psi\rangle = e^{-i\underline{R}_i\hat{\underline{p}}}\,|\varphi n\ell_j m\rangle_i\,,$$

i.e.,the same functions centered around the points $\underline{R}_i$, with the same energies $\varepsilon_{in\ell_j}$. We can see, that in this limit the spherical symmetry (around $\underline{R}_i$) is restored, n,ℓ,j are good quantum numbers and we have $(2j+1)$ - fold degeneracy in m . For identical potentials in this limit the states with $\Lambda=\pm 1$ will be degenerate and therefore it is possible to make linear combinations from them corresponding to the previous case, i.e., the particle being in a bound state around one of the potentials. For the case $R_{12}\to 0$ we have

$$Q^{L}_{i\beta,i'\beta'}(E,0) = \delta_{L0}\,S_{i\beta,i'\beta'}$$

and thus for the matrix $M^{B}_{I,I'}$ in Eq. (16)

$$M^{B}_{i\alpha,i'\alpha'}(E,0) = \delta_{jj'}\,\delta_{ee'}\,\delta_{mm'}\,S_{i\beta,i'\beta'}(E)\,. \qquad (27)$$

It is easy to see, that the matrix (27) corresponds to a single particle problem with the sum of the two potentials. For non-identical potentials this sum corresponds to a new separable potential in which the sum over n in (1) includes both types of form-factors. For identical potentials we shall have a selection rule from (24)

$$\Lambda \cdot (-1)^{\ell} = 1$$

which reflects the trivial fact that in the spherically symmetric case the parity is connected with the value of ℓ: $\Lambda = (-1)^{\ell}$.

IV. Numerical Results

The method developed in the previous section can be applied to realistic (local, short range, finite depth) potentials commonly used in nuclear physics (e.g., Woods-Saxon type) remembering, that under certain quite general mathematical conditions, they can be approximated to any desired accuracy by finite rank operators or, as we call them, separable potentials. There are several possibilities to perform such approximations see, e.g., /14/. We shall follow the one described in /13/ which is based on the use of familiar oscillator wave functions. Let us consider a Woods-Saxon potential, corresponding to the nucleus ^{16}O :

$$V = -V_0 \left(f(r) - \frac{\varkappa}{r} \frac{df}{dr} (\hat{\ell} \cdot \hat{s}) \right), \qquad (28)$$

where $f(r) = [1 + \exp(c(r - R_0))]^{-1}$ and the parameter values are:

$$V_0 = -51.3 \text{ MeV}, \quad \varkappa = .216 \text{ fm}^2, \quad c = 1.59 \text{ fm}^{-1}, \quad R_0 = 1.24 \cdot (16)^{1/3} .$$

If we denote a complete set of harmonic oscillator single particle states by $|\alpha\rangle$: $|\alpha\rangle = |n \ell j m\rangle$, a separable approximation to (28) can be constructed in the following way

$$V \approx V_{sep} = \sum_{\alpha, \alpha'}^{\alpha_{max}} |\alpha\rangle \langle\alpha| V |\alpha'\rangle \langle\alpha'| . \qquad (29)$$

The approximation in (29) consists in cutting the summations over α and α' at a certain "maximal" single particle index α_{max} ; without this truncation, due to the completeness of the states $|\alpha\rangle$, V_{sep} would be identical to V . The validity and the usefulness of approximation (29) for a single Woods-Saxon potential were discussed in detail in /13/. Since V_{sep} of Eq. (29) is of the form (1) (remembering the footnote), the method of the previous section can be applied to it. We have

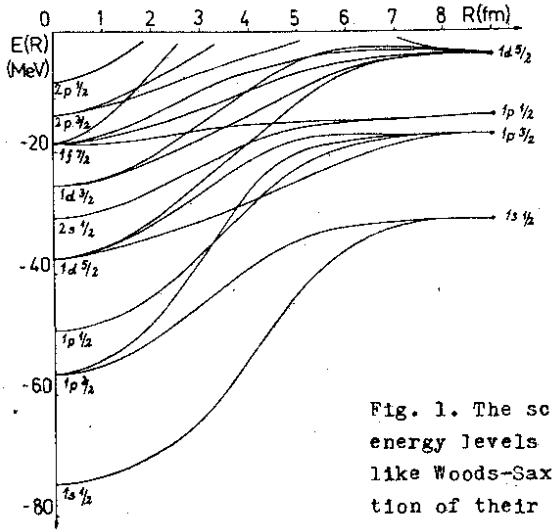

Fig. 1. The scheme of single-particle energy levels in the field of two ^{16}O like Woods-Saxon potentials as a function of their distance $R = |\underline{R}_1 - \underline{R}_2|$.

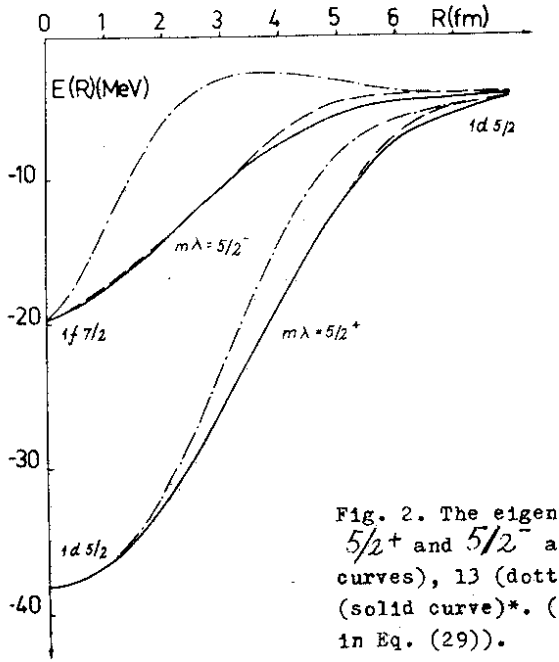

Fig. 2. The eigenvalues $E_{\lambda M}(R)$ for states $5/2^+$ and $5/2^-$ at $\alpha_{max} = 11$ (dash-dotted curves), 13 (dotted curve) and 15 (solid curve)*. (α_{max} is defined in Eq. (29)).

solved the two-center problem for two identical potentials (28) using the approximation (29) for both of them.
For $R_{12} \to 0$ and $R_{12} \to \infty$ the two-center problem is reduced to the one-center problem. Then ℓ and j are proper quantum numbers and we are allowed to study only the convergence in n (n is the radial quantum number of the oscillator wave function). However, the convergence in n for $\ell = 0$ in the one-center problem with potential (28) has been investigated in ref./13/ within the method applied here. Since our numerical results follow exactly those of/13/, we would like only to comment that the method based on separable potentials is more appropriate in describing the wave function asymptotic behaviour than the traditional method of expanding the wave function in the oscillator basis. As it was expected, at small R_{12} the scheme of single-particle energy levels of the two-center well resembles the Nilsson scheme and the splitting of degenerate levels proceeds by the same rules as in the Nilsson model (fig. 1). For large R_{12} the levels become degenerate again at the energies corresponding to the levels of separated potentials. For intermediate R_{12} we have considerable splitting, some of the levels are raised into the continuous spectrum. The overall R_{12}-dependence of the level scheme resembles that obtained from the two-center oscillator-model/9/.

For intermediate R_{12} the quantum numbers ℓ, j are not conserved and in the expansion (29) we should study the convergence in n and ℓ, j. Figure 2 shows the results of calculations of eigenvalues $E_{\Lambda M}(R_{12})$ for states $5/2^+$ and $5/2^-$ (+ means $\Lambda = +1$, - stands for $\Lambda = -1$) at $\alpha_{max} = 11$ (dash-dotted curve), 13 (dotted curve), and 15 (solid curve). From Fig. 2 it is seen that in the case under consideration for $3 \le R_{12} \le 7$ the addition of terms with $\ell = 5$ and $j = 11/2$ to expansion (29) changes the eigenvalues by no more than 0.2 MeV. The terms with $\ell \ge 6$ contribute negligibly. Figures 3 and 4 show the mixing coefficients $C_I(R_{12})$ of the wave function for states $5/2^+$ and $5/2^-$. The rank of determinant equals 15, and for simplicity only the dominating $C_I(R_{12})$ are plotted. It is interesting to trace the change of the coefficients $C_I(R_{12})$ as a function of R_{12}: at small and large R_{12} only one of the $C_I(R_{12})$ differs from

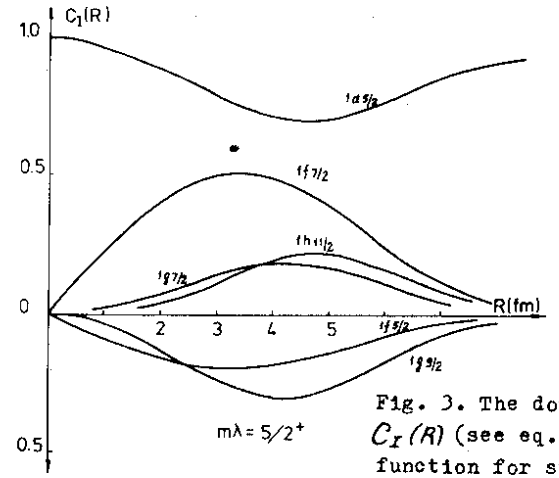

Fig. 3. The dominating coefficients $C_I(R)$ (see eq. (22)) of the wave function for state $5/2^+$.

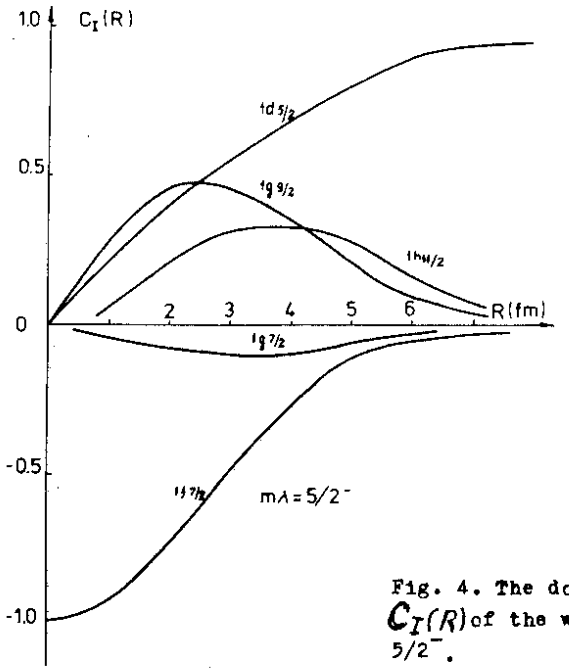

Fig. 4. The dominating coefficients $C_I(R)$ of the wave function for state $5/2^-$.

zero while at intermediate R_{12} a strong mixing of configurations occurs, nevertheless even in this range of R_{12} the convergence in ℓ, j is rapid enough.

V. Conclusion

We have proposed a method for finding the single-particle energies and wave functions of the two-center problem with realistic potentials of finite depth. We have used spherically symmetric potentials for each separated fragment nucleus, however, the method can be extended to deformed potentials, too. Further, the method can be applied to calculate quasistationary states of the two-center problem and their transition to bound states with changing distance between fragment nuclei. It seems to be interesting to employ the single-particle wave functions found by the proposed method as basis functions in heavy ion reactions, where the surface effects are important, since these functions have the required asymptotic behaviour.

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