BOUND STATES OF A NONLOCAL SEPARABLE POTENTIAL

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A theory of the bound states of a nonlocal separable potential is developed using the exact expression for the partial amplitudes of the S matrix. It is shown that the number of bound states does not exceed the number of "attractive" terms in the potential function, and that the energy levels depend monotonically on the common coupling constant and on the partial coupling constants characterizing each interaction term. The number of bound states and the position of the lowest energy level are estimated.

In a previous paper,[1] an exact expression for the partial amplitudes of the S matrix was obtained for the nonrelativistic scattering from a nonlocal separable potential proposed by Yamaguchi,[2] and its analytic structure in the k plane was investigated. It was shown, in particular, that besides the poles corresponding to bound states, other singularities are possible in the upper half-plane, which give rise to cuts along the lines Re K = const; the poles lie along the positive imaginary axis, as is to be expected. The aim of the present paper is to present a detailed analysis of the bound states, to obtain their possible number for a given interaction and to determine the characteristics of the energy levels.

We shall follow the notation of the previous paper;[1] the number of terms in the sum over j in the Schrödinger equation

$$-(\Delta+k^2)\psi(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{j=1}^{N}\beta_j^l f_j^l(r)\int f_j^{l*}(r')\psi(\mathbf{r}')P_l\left(\frac{\mathbf{rr}'}{rr'}\right)d\mathbf{r}' \tag{1}$$

will be called the order of the nonlocal separable potential. The functions $f_j^l(r)$ are assumed to be linearly independent (if there is linear dependence, the corresponding terms must be reduced). The function $rf_j^l(r)$ is absolutely integrable for $r \geq \gamma > 0$, with a possible singularity of the type

$$O(r^{-3/2+\mu}),\quad \mu>0$$

at $r = 0$.

The bound states are connected with the zeroes of the determinant

$$D_l(k)=\det{}_N[\delta_{ij}-a_{ij}^l(k)]; \tag{2}$$

$$a_{ij}^l(k)=\frac{4\beta_j^l}{2l+1}\int_{-\infty}^{\infty}\frac{B_i^{l*}(q)B_j^l(q)}{q^2-k^2}dq; \tag{3}$$

$$B_j^l(k)=(-i)^l\int_0^{\infty}kf_j^l(r)r^2j_l(kr)dr. \tag{4}$$

As already mentioned, all zeroes of $D_l(k)$ lie on the imaginary half-axis $k = ip$ $(p > 0)$.

We shall investigate the equation

$$\det{}_N\left[\lambda\delta_{ij}-\frac{4\beta_j^{l*}}{2l+1}\int_{-\infty}^{\infty}\frac{B_i^{l*}(q)B_j^l(q)}{p^2+q^2}dq\right]=0, \tag{5}$$

whose solutions for $\lambda = 1$ describe the bound states. We note that λ^{-1} is proportional to the strength of the interaction: if we replace everywhere $f_j^l(r)$ by $\lambda^{-1/2}f_j^l(r)$, we obtain (5) from (2). Equation (5) is the characteristic equation for the matrix.

$$T=(a_{ij}^l(k))=\left(\frac{4\beta_j^l}{2l+1}\int_{-\infty}^{\infty}\frac{B_i^{l*}(q)B_j^l(q)}{p^2+q^2}dq\right). \tag{6}$$

First we consider the case where all $\beta_j^l = \beta$ and thus all have the same sign, i.e., the interaction gives pure attraction or pure repulsion. Then the matrix (6) is hermitian, and from its elements one can construct the quadratic form

$$Q_T(x,x;p^2)=\sum_{ij}a_{ij}^l x_i x_j^* =\frac{4\beta}{2l+1}\int_{-\infty}^{\infty}\left|\sum_{j=1}^{N}x_jB_j^l(q)\right|^2\frac{dq}{a^2+p^2}, \tag{7}$$

which has a definite sign identical with that of β. It follows that all N solutions $\lambda_n(p^2)$, $n = 1, 2, \ldots, N$, of (5) are positive for $\beta = 1$ and negative for $\beta = -1$. We are, of course, only interested in the positive solutions. Here ($\beta = 1$, attraction) $Q_T(x,x;p^2)$ decreases monotonically as p^2 increases:

$$Q_T(x,x;p^2)>Q_T(x,x;p'^2),\quad p'^2>p^2.$$

Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$ be the canonical coefficients of the quadratic form $Q_T(x,x;\, p^2)$. They are simultaneously the eigenvalues of the matrix T and the solutions of (5). The latter is an algebraic equation with continuous functions as coefficients, so that all $\lambda_n(p^2)$ are also continuous. By the theorem on the coefficients of congruent quadratic forms[3] we have

$$\lambda_n(p^2) > \lambda_n(p'^2), \quad n = 1, 2, \ldots, N.$$

Going to the limit $p' \to p$, we obtain

$$d\lambda_n / dp^2 < 0. \tag{8}$$

Eq. (7) immediately leads to

$$\lim_{p^2\to\infty} Q_T(x, x; p^2) = 0$$

and hence the limit

$$\lim_{p^2\to\infty} \lambda(p^2) = 0 \tag{9}$$

also exists.

Let us show that relations equivalent to (8) and (9) are valid for any choice of β_j^l. For convenience, we number the f_j^l in the following way: the first M numbers are assigned to the terms with positive sign ($\beta_j^l = 1$), and the following numbers correspond to $\beta_j^l = -1$. We also change the notation somewhat:

$$a_{ij}^l(k) = \begin{cases} a_{ij}, & i, j \leqslant M \\ b_{ij}, & M < i, j \leqslant N. \\ c_{ij} & \text{in the intermediate regions.} \end{cases} \tag{10}$$

The equation $D_l(ip) = 0$ is now written in the form

$$|E - T| = \begin{vmatrix} 1 - a_{1,1} & \ldots & -a_{1,M} & c_{1,M+1} & \ldots & c_{1,N} \\ \vdots & & \vdots & \vdots & & \vdots \\ -a_{M,1} & \ldots & 1 - a_{M,M} & c_{M,M+1} & \ldots & c_{M,N} \\ -c_{M+1,1} & \ldots & -c_{M+1,M} & 1 + b_{M+1,M+1} & \ldots & b_{M+1,N} \\ \vdots & & \vdots & \vdots & & \vdots \\ -c_{N,1} & \ldots & -c_{N,M} & b_{N,M+1} & \ldots & 1 + b_{N,N} \end{vmatrix} = 0 \tag{11}$$

(E is the unit matrix).

First of all we note that $\det_{N-M}[\delta_{ij} + b_{ij}]$ is a positive definite quantity. Indeed, every determinant of the form (5) can be written as a polynomial

$$\sum_{m=0}^{N} (-\lambda)^{N-m} A_m(p^2); \tag{12}$$

where $A_m(p^2)$ is the sum of all principal minors M_m of order m of the matrix T. For $\beta_j^l = \beta$ the minors M_m have the same sign as β^m:

$$M_m = \left(\frac{4\beta}{2l+1}\right)^m \det_m\left[\int_{-\infty}^{\infty} \frac{B_{i_s}^{l*}(q)\, B_{i_t}^l(q)}{p^2 + q^2}\, dq\right]. \tag{13}$$

The determinant on the right-hand side of (13) is a Gram determinant and, hence, positive. From this follows that

$$|B| = \det[\delta_{ij} + b_{ij}] \geqslant 1, \tag{14}$$

since $|B|$ can be written in the form (12) for $\lambda = 1$ and $\beta = -1$.

The fact that $|B|$ is positive can also be established in another way. We can always construct functions $\sigma_i(q,p)$ such that

$$\delta_{ij} + b_{ij} = \int_{-\infty}^{\infty} \frac{\sigma_i(q,p)\,\sigma_j^*(q,p)}{p^2 + q^2}\, dq. \tag{15}$$

Then $|B|$ is a Gram determinant. The functions σ_i can be constructed in the following way. Expression (4) shows that all functions $B_j^l(q)$ have a definite parity which is identical for functions with the same l. Let us choose an orthogonal system of functions $u_j(q,p)$ which are normalized with weight $(p^2+q^2)^{-1}$ and have the opposite parity of $B^l(q)$. Then one easily sees that

$$\sigma_i(q,p) = B_i^l(q) + u_i(q,p) \tag{16}$$

satisfies (15).

In studying the roots of (11) one cannot go directly to the investigation of the form corresponding to the matrix T, since it is not hermitian. In order to amend this, we multiply each of the last N−M columns of the determinant (11) by −1 and consider the equation

$$|\lambda' E - T'| = \begin{vmatrix} \lambda' - a_{1,1} & \ldots & -a_{1,M} & -c_{1,M+1} & \ldots & -c_{1,N} \\ \vdots & & & \vdots & & \vdots \\ -a_{M,1} & \ldots & \lambda' - a_{M,M} & -c_{M,M+1} & \ldots & -c_{M,N} \\ -c_{M+1,1} & \ldots & -c_{M+1,M} & \lambda' - 2 - b_{M+1,M+1} & \ldots & -b_{M+1,N} \\ \vdots & & \vdots & \vdots & & \vdots \\ -c_{N,1} & \ldots & -c_{N,M} & -b_{N,M+1} & \ldots & \lambda' - 2 - b_{N,N} \end{vmatrix} = 0, \tag{17}$$

whose solutions coincide for $\lambda' = 1$ with the solutions of (11) and, hence, describe the bound states; but λ' no longer has the meaning of an inverse coupling constant.

The matrix T' is hermitian, and the quadratic form corresponding to it has the form

$$Q_{T'}(x,x;p^2)=\frac{4}{2l+1}\int_{-\infty}^{\infty}\left|\sum_{i=1}^{N}B_i^l(q)x_i\right|^2\frac{dq}{p^2+q^2}+2\sum_{n=M+1}^{N}|x_n|^2. \tag{18}$$

From this we easily obtain (8). In the following, however, we shall almost never consider T' and the quadratic form $Q_{T'}$. Instead, we shall obtain another matrix in which the attractive part of the interaction is explicitly separated.

Assuming first that $N - M \geq 2$, we multiply (11) by $|B|^{M-1}$ and, using the Sylvester identity for determinants,[4] obtain

$$\det_M[\delta_{ij}-h_{ij}]=0, \tag{19}$$

where

$$h_{ij}=\frac{1}{|B|}\begin{vmatrix} a_{i,j} & c_{i,M+1} & \dots & c_{i,N}\\ c_{M+1,j} & 1+b_{M+1,M+1} & \dots & b_{M+1,N}\\ \vdots & \vdots & & \vdots\\ c_{N,j} & b_{N,M+1} & \dots & 1+b_{N,N}\end{vmatrix}. \tag{20}$$

The matrix $H = (h_{ij})$ will play the role of T for a purely attractive interaction. Equations (19) and (20) are also true for $N - M = 1$. This is easily seen by extracting the N-th row and column of (11) in the usual procedure for lowering the order of a determinant.

We note that on the imaginary axis $k = ip$

$$|a_{ij}|^2\leqslant a_{ii}a_{jj}, \tag{21}$$

which follows from the Schwarz inequality. The same inequality for h_{ij} is obtained from the Sylvester identity:

$$|B|\times\begin{vmatrix} a_{i,i} & a_{i,j} & c_{i,M+1} & \dots & c_{i,N}\\ a_{j,i} & a_{j,j} & c_{j,M+1} & \dots & c_{j,N}\\ c_{M+1,i} & c_{M+1,j} & & & \\ \vdots & \vdots & & B & \\ c_{N,i} & c_{N,j} & & & \end{vmatrix} = |B|^2(h_{ii}h_{jj}-|h_{ij}|^2), \tag{22}$$

for the second determinant on the left-hand side of (22) is positive since it can be written as a Gram determinant with the help of (16).

The determinant

$$\begin{vmatrix} a_{i,i} & c_{i,M+1} & \dots & c_{i,N}\\ c_{M+1,i} & & & \\ \vdots & & B & \\ c_{N,i} & & & \end{vmatrix}, \tag{23}$$

can also easily be reduced to the form of a Gram determinant. By the generalized Hadamard inequality for positive definite matrices[5] we then obtain an estimate for h_{ii}:

$$h_{ii}\leqslant a_{ii}. \tag{24}$$

After these remarks, we shall, as before, consider the equation

$$\det_M[\lambda\delta_{ij}-h_{ij}]=0, \tag{25}$$

whose solutions for $\lambda = 1$ will give the bound states. Let us write the quadratic form corresponding to the matrix H:

$$Q_H=\sum_{i,j=1}^{M}h_{ij}x_ix_j^*=\frac{1}{|B|}\begin{vmatrix} P & Y_{M+1} & \dots & Y_N\\ Y_{M+1}^* & & & \\ \vdots & & B & \\ Y_N^* & & & \end{vmatrix}. \tag{26}$$

Here

$$P=\int_{-\infty}^{\infty}\left|\sum_{j=1}^{M}B_j^l(q)x_j\right|^2\frac{dq}{p^2+q^2},$$

$$Y_n=\int_{-\infty}^{\infty}B_n^{l*}(q)\sum_{j=1}^{M}B_j^l(q)x_j\frac{dq}{p^2+q^2}.$$

With the help of the generalized Hadamard inequality we obtain at once

$$Q_H\leqslant P. \tag{27}$$

The quadratic form Q_H is positive definite just like the determinant (23). It follows that all M solutions $\lambda_n(p^2)$ of (25) are positive and we find from (27)

$$\lim_{p^2\to\infty}Q_H(x,x;p^2)=0. \tag{28}$$

Let us now show that $Q_H(x,x;p^2)$ is a monotonically decreasing function of p^2, which will then constitute the proof of (8). After some transformations we find

$$|B|^2\frac{dQ}{dp^2}=-\int_{-\infty}^{\infty}\frac{dq}{(p^2+q^2)^2}U(p,q,x); \tag{29}$$

$$\begin{aligned}U(p,q,x)&=|B|^2\left|\sum_{j=1}^{M}B_j^l(q)x_j\right|^2\\&-2|B|\,\mathrm{Re}\left\{\sum_{n,m=M+1}^{N}B_{nm}B_n^{l*}Y_m^*\sum_{j=1}^{M}B_j^lx_j\right\}\\&+\sum_{n,m}\sum_{s,t}Y_nY_m^*B_{nm}B_s^{l*}B_t^lB_{st}\\&-\sum_{n,m}|B|Y_nY_m^*\sum_{\substack{s\neq n\\t\neq m}}B_s^{l*}B_t^lB_{nmst},\end{aligned} \tag{30}$$

where B_{nm}, B_{nmst} are the cofactors of the determinant $|B|$. Let us again use the Sylvester identity in its simplest form

$$|B|B_{nmst}=B_{nm}B_{st}-B_{nt}B_{sm}. \tag{31}$$

As a result

$$U(q,p,x)=\left|\,|B|\sum_{j=1}^{M}B_j{}^l x_j-\sum_{n,m}B_n{}^l Y_m B_{nm}\right|^2 \tag{32}$$

and hence,

$$dQ\,/\,dp^2<0. \tag{33}$$

Let us introduce the common coupling constant ρ for all functions $f_j^l(r)$. For pure attraction we obtain at once from (7) ($\beta = 1$)

$$\rho\frac{\partial Q_T}{\partial\rho}=Q_T>0;\qquad \frac{\partial\lambda}{\partial\rho}>0. \tag{34}$$

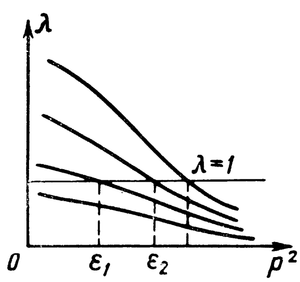
For mixed forces, (18) allows us to write

$$\frac{\partial Q_{T'}}{\partial\rho}>0,\qquad \frac{\partial\lambda'}{\partial\rho}>0. \tag{35}$$

Let $\epsilon = p^2$ be the energy of the bound state $\lambda(\epsilon, \rho) = 1$. Then

$$\frac{\partial\lambda}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial\rho}+\frac{\partial\lambda}{\partial\rho}=0,\qquad \frac{\partial\varepsilon}{\partial\rho}=-\frac{\partial\lambda}{\partial\rho}\Big/\frac{\partial\lambda}{\partial\varepsilon}>0. \tag{36}$$

The energy levels increase monotonically with increasing coupling constant. An illustration of the dependence of the solutions of the equation (5) on p^2 shows N curves which approach zero monotonically (see the figure). Each curve can intersect the line $\lambda = 1$ only once, so that for a purely attractive nonlocal potential of order N there are no more than N bound states.



For mixed forces, Eq. (25) yields only M curves $\lambda_i(p^2)$, where by (33) and (28),

$$\frac{\partial\lambda_i}{\partial p^2}<0,\ \lim_{p^2\to\infty}\lambda_i=0$$

no more than M bound states can exist. Thus the number of bound states of a nonlocal separable potential cannot exceed the number of "positive" terms in the sum (1).

Using the known properties of eigenvalues and the inequality (24), we find

$$\sum_{i=1}^{M}\lambda_i(p^2)=\operatorname{Sp}H=\sum_{i=1}^{M}h_{ii}\leqslant\sum_{i=1}^{M}a_{ii}$$
$$=\frac{4}{2l+1}\int_{-\infty}^{\infty}\left|\sum_{i=1}^{M}B_i{}^l(q)\right|^2\frac{dq}{p^2+q^2} \tag{37}$$

The equality sign applies only when M = N. Expression (37) allows one at once to obtain a crude estimate of the number of bound states (in addition to the relation $n \le M$ already found):

$$n_l<\sum_{i=1}^{M}\lambda_i(0)=\frac{4}{2l+1}\int_{-\infty}^{\infty}\left|\sum_{i=1}^{M}B_i{}^l(q)\right|^2\frac{dq}{q^2}$$
$$=\frac{4\pi}{(2l+1)^2}\int_0^\infty\int_0^\infty F^l(r)F^{l*}(r')\,r_<^{l+2}r_>^{\prime\,1-l}dr\,dr'$$
$$<\frac{4\pi}{(2l+1)^2}\left|\int_0^\infty r^{3/2}F^l(r)\,dr\right|^2,$$
$$F^l(r)=\sum_{i=1}^{M}f_i{}^l(r). \tag{38}$$

Moreover, (37) leads to an estimate of the energy $\epsilon_0 = p_0^2$ of the lowest bound state with the help of the equation

$$\sum_{i=1}^{M}\lambda_i(p_0{}^2)=1,\ \text{i.e.}\ \int_{-\infty}^{\infty}\left|\sum_{i=1}^{M}B_i{}^l(q)\right|^2\frac{dq}{\varepsilon_0+q^2}=\frac{2l+1}{4}. \tag{39}$$

We note that the estimate (38) is valid only if a stronger restriction is imposed on the tail of the function $f_j^l(r)$, viz.,

$$f_j{}^l\underset{r\to\infty}{=}o(r^{-5/2}).$$

We can further determine the type of motion of the energy levels of the bound states as the coupling constants of the different interaction terms for example, ρ_i^+ and ρ_j^- are varied (the upper indices indicate whether they belong to the attractive or repulsive parts of the interaction). We show that the following inequalities hold for all levels:

$$\frac{\partial\varepsilon}{\partial\rho_i{}^+}\geqslant0,\ \frac{\partial\varepsilon}{\partial\rho_j{}^-}\leqslant0. \tag{40}$$

To find the bound states we must solve the equation

$$|E-H|=\begin{vmatrix}1-h_{1,1} & -h_{1,2} & -h_{1,3} & \ldots & -h_{1,M}\\ -h_{2,1} & 1-h_{2,2} & -h_{2,3} & \ldots & -h_{2,M}\\ -h_{3,1} & -h_{3,2} & 1-h_{3,3} & \ldots & -h_{3,M}\\ \vdots & \vdots & \vdots & & \vdots\\ -h_{M,1} & -h_{M,2} & -h_{M,3} & \ldots & 1-h_{M,M}\end{vmatrix}=0, \tag{41}$$

which reduces to the following form by an identity transformation:

$$|E-H'|$$

$$=\begin{vmatrix} 1-h_{1,1} & h_{1,2} & h_{1,3} & \dots & h_{1,M} \\ h_{2,1} & 1-h_{2,2} & -h_{2,3} & \dots & -h_{2,M} \\ h_{3,1} & -h_{3,2} & 1-h_{3,3} & \dots & -h_{3,M} \\ \vdots & \vdots & \vdots & & \vdots \\ h_{M,1} & -h_{M,2} & -h_{M,3} & \dots & 1-h_{M,M} \end{vmatrix}=0. \quad (42)$$

From the matrices H and H′ we construct the quadratic forms Q_H and $Q_{H'}$ [cf. (26)]:

$$Q_H(x,x)=h_{11}|x_1|^2 + \sum_{i=2}^{M} h_{i1}x_ix_1^* + \sum_{j=2}^{M} h_{1j}x_1x_j^* + \sum_{i,j=2}^{M} h_{ij}x_ix_j^*, \quad (43)$$

$$Q_{H'}(x,x)=h_{11}|x_1|^2 - \sum_{i=2}^{M} h_{i1}x_ix_1^* - \sum_{j=2}^{M} h_{1j}x_1x_j^* + \sum_{i,j=2}^{M} h_{ij}x_ix_j^*. \quad (44)$$

Since both quadratic forms are positive definite, they can be reduced simultaneously to canonical form and hence, will simultaneously assume their extremal values. Let us introduce the vector $\{x^0\}$ such that

$$Q_H(x^0, x^0) = \lambda_i(p^2), \quad Q_{H'}(x^0, x^0) = \lambda_i'(p^2).$$

If we consider an eigenvalue λ_i such that $\lambda_i(0) > 1$, we will have $\lambda_i(p^2) = 1$ for some value of the argument p^2. Evidently $\lambda_i'(p^2)$ is also equal to unity for the same value of the argument, for $\lambda_i(p^2) = 1$ means that (41) is an identity for this value of p^2, and (42) becomes an identity together with (41). Thus

$$Q_H(x^0, x^0;\ p^2) = Q_{H'}(x^0, x^0;\ p^2),$$

i.e.,

$$\sum_{j=2}^{M} h_{1j}x_1^0x_j^{0*} + \sum_{i=2}^{M} h_{i1}x_i^0x_1^{0*} = 0. \quad (45)$$

Introducing the coupling constant ρ_1^+ for $f_1^l(r)$, we obtain from (43)

$$\rho_1^+\frac{\partial Q_H}{\partial \rho_1^+} = h_{11}|x_1|^2 + \frac{1}{2}\sum_{j=2}^{M} h_{1j}x_1x_j^* + \frac{1}{2}\sum_{i=2}^{M} h_{i1}x_ix_1^*. \quad (46)$$

Let us take the vector $\{x^0\}$ as the argument of Q_H. Then we find from (45) and (46)

$$\rho_1^+\frac{\partial \lambda_i}{\partial \rho_1^+} = h_{11}|x_1|^2 \geqslant 0. \quad (47)$$

The same result can also be obtained for any $\rho_j^+ (j = 1, 2, \dots, M)$.

The derivative with respect to ρ_N^- can be obtained by taking the derivative of (25). After some transformations using (31) we have

$$\rho_N^-\frac{\partial Q_H}{\partial \rho_N^-} = -\frac{1}{|B|^2}\begin{Vmatrix} Y_{M+1} & Y_{M+2} & \dots & Y_N \\ 1+b_{M+1,M+1} & b_{M+1,M+2} & \dots & b_{M+1,N} \\ \vdots & \vdots & & \vdots \\ b_{N-1,M+1} & b_{N-1,M+2} & \dots & b_{N-1,N} \end{Vmatrix} < 0. \quad (48)$$

Equations (47) and (48) together with (36) yield (40). This result allows us to investigate the appearance of new levels and the motion of the old ones.

For a given nonlocal separable potential of order N with M attractive terms there are $n_l \leq M$ bound states. Let us add still another term (with $\beta = 1$) and let us raise the value of its coupling constant ρ^+ from zero. All levels of the system begin to drop monotonically, and as ρ^+ is increased, new bound states will appear (if $n_l < M$); in the limit, the number of bound states will reach M + 1. Increasing the partial coupling constants ρ^- will raise the energy levels, and the problem whether the system may in the end have no bound states at all, requires further investigations.

Our results show that a nonlocal separable potential may be very convenient for many practical calculations. If the forces acting in the system are not sufficiently known, as is the case in the theory of the nucleus, it is most reasonable to test models which lead to a closed solution of the problem, and the nonlocal separable potential is just such a model. This applies in particular to systems with a limited and known number of bound states. Our model is the simpler for calculations, the less levels there are in the system; the position of the levels is determined by an algebraic equation. Here the results of Yamaguchi[6] deserve attention, where the model of a nonlocal separable potential was successfully applied to the study of a single-level system, the deuteron. This leads us to hope for good results also in the case of more complicated systems.

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15