Interaction of composite particles and the Pauli principle

V. I. Kukulin, V. G. Neudachin, and Yu. F. Smirnov

Scientific-Research Institute of Nuclear Physics, Moscow State University
Fiz. Elem. Chastits At. Yadra **10**, 1236–1293 (November–December 1979)

Modern approaches to the interaction of composite particles in nuclear and, partly, atomic physics are reviewed. The main attention is devoted to the effects of the Pauli principle in systems of two and three composite particles. Modified Faddeev equations are derived for a system of three composite particles, and the construction of variational bases for such systems is discussed in detail. The general concepts of ghost channels and ghost states, which are eigenstates of the total Hamiltonian with symmetry forbidden by the Pauli principle, are introduced. Some model examples are investigated for systems of three and four particles, in which a rigorous microscopic treatment is possible, and these examples are used to illustrate the meaning of the forbidden states and the optical potentials for scattering of composite particles. The structure of the carbon nucleus in the 3α model is discussed as an example.

PACS numbers: 21.40. + d, 31.10. + z

INTRODUCTION

The present review is devoted to describing the dynamics of systems of two and three composite particles consisting of fermions (nucleons in nuclear physics and electrons in atomic physics), particular attention being paid to the effects of the Pauli principle. It is well known that the requirement of complete antisymmetry (under all permutations) of the total wave function of such a system of several composite particles leads to computational schemes of great complexity even in simple approaches such as the resonating-group method and the generator-coordinate method-the two most widely used microscopic methods for analyzing composite systems. For example, a direct resonating-group method calculation of the spectrum of a system of three α particles requires calculation of a huge number (about 10^{12}) exchange integrals and takes ~150 h of computing time on a large computer.[1] At the same time, the simplifications that must be made in such a calculation to obtain the final results are sometimes so appreciable that exact allowance for all exchange effects cannot be achieved at all within the accuracy of the employed model. In addition (and this is the most important thing), such a calculation (which includes several successive programs) is a kind of black box—its output data are not correlated in a physically perspicuous manner with the values of the input parameters (say, the parameters of the NN interaction, etc.). Similar problems arise in attempts at a complete microscopic description of the (d, p) stripping reaction on a magic nucleus or in the description of reactions with clusters of the type $^7\mathrm{Li}(\alpha, t)^8\mathrm{Be}$, etc.

It is therefore worth attempting to formulate simpler and physically well-grounded approaches to these problems. Several such approaches have been proposed, and a detailed description of them is the aim of this review.

In each approach of this kind, the antisymmetrization effect is included in one way or another in the effective interaction between the composite particles; moreover, in contrast to the resonating-group method, this effective interaction of two composite particles is constructed in a fairly simple manner such that one could use such an interaction to treat systems of three or more clusters. This is a common philosophy in theoretical physics in the treatment of systems of several particles. For example, in the study of $3N$ and $4N$systems on the basis of the Faddeev–Yakobovskiĭ equations, the complicated NN potential is very often replaced by a simplified separable interaction, which correctly reproduces the main features of the true potential and at the same time leads to a numerically solvable scheme.

The simplest model for the interaction of two clusters is obviously a local potential. However, if it is to be an adequate model, it must lead to scattering wave functions (and phase shifts) "similar" to those obtained in a microscopic approach such as the resonating-group method. It has been found that this can be achieved by introducing states into the potential model that are forbidden by the Pauli principle. These states, as will be shown play a fundamental part in the problems considered here, and their presence and structure will reflect the influence of the Pauli principle.[2-7]

The concept of a forbidden state appeared in quantum mechanics in connection with the Pauli principle. In his theory of the relativistic electron, Dirac made the assumption that solutions with negative mass are not manifested physically under ordinary conditions because all positions for particles with negative mass are occupied in the vacuum state. This problem became relevant in nuclear physics too when the nuclear shell model was formulated and the optical potential introduced; this was the case not only in problems relating to scattering theory, where it is necessary to modify the formulation of Levinson's theorem, but also in the theory of reactions or, more generally, in an investigation of systems of several composite particles off the mass shell.

1. FORBIDDEN STATES IN COMPOSITE SYSTEMS

Qualative Treatment of Forbidden States in Systems of Two Clusters. If both parts of a system $A+B$ are composite, it is to be expected that a part of the Hilbert space of the wave functions of this system will not be accessible to the system, i.e., will be forbidden by the Pauli principle, as is the case in a system con-

 0090-4759/79/060492-24$02.80

sisting of nucleon and closed shells. However, in the case of two composite particles $A+B$ it is much harder to establish which states are allowed and which forbidden. In addition, one can have more complicated situations, when some states are partly allowed and partly forbidden.

But in problems in nuclear physics concerning the interaction of clusters oscillator wave functions can be used with reasonable accuracy. Under these circumstances, it is fairly easy to see how the Pauli principle will be manifested in the interaction of composite nuclear systems. Let us take the system $\alpha+\alpha$. In its lowest state, it forms the nucleus ^{8}Be with shell configuration $(0s)^4(1p)^4$. The antisymmetric oscillator shell wave function of this configuration $|s^4p^4; L, M, S=0, T=0\rangle$, can be rewritten in the cluster form[8-10]

$$\begin{aligned}&|s^4p^4: L, M, S=0, T=0\rangle\\&=N^{-1}\{\hat{A}\varphi_\alpha(1,2,3,4)\varphi_\alpha(5,6,7,8)\Phi_{sh}(\rho)\}\Psi_{000}(\mathbf{R}_0).\end{aligned}\tag{1}$$

Here,

$$\varphi_\alpha(1,2,3,4)=\exp\Big[-\frac{1}{2}a\sum_{i=1}^{4}(\mathbf{r}_i-\mathbf{R}_{\alpha i})^2\Big]\chi_{S_i=0,\,T_i=0}(1,2,3,4)\tag{2}$$

is the internal wave function of the α cluster, $\mathbf{R}_{\alpha i}$ is the c.m.s. coordinate of the i-th α cluster, $\varkappa_{ST}$ is the spin–isospin part of the function, $\rho=\mathbf{R}_{\alpha1}-\mathbf{R}_{\alpha2}$ is the relative coordinate of the two α clusters, and $\Phi_{sh}(\rho)\equiv\Phi_{NLM}(\rho)$ is the oscillator wave function of the relative motion of the clusters with angular momentum L and projection M of it. The last factor $\Psi_{000}(\mathbf{R}_0)$ is the oscillator function of the zero-point vibrations of the overall center of mass of the system $\mathbf{R}_0=(\mathbf{R}_{\alpha1}+\mathbf{R}_{\alpha2})/2$. It must necessarily be present in the shell wave function in accordance with Elliott and Skyrme's theorem.[11]

Since the shell configuration s^4p^4 contains four oscillator quanta, and the internal functions of the clusters do not contain oscillator quanta, all four quanta of this configuration are transferred to the wave function $\Phi(\rho)\equiv\Phi_{4LM}(\rho)$ of the relative motion of the clusters. Thus, for the ground state of the nucleus ^{8}Be the wave function $\Phi(\rho)$ is equal to the function $|4s\rangle$, i.e., it has two nodes. States with fewer than four quanta are not realized in a system of eight nucleons (they would correspond to the configurations s^8, s^7p, s^6p^2, and s^5p^3 forbidden by the Pauli principle), and, therefore, states of the relative motion $\Phi_{NLM}(\rho)$ of two α clusters with $N<4$ quanta are forbidden. In other words, if we replace $\Phi(\rho)$ in (1) by the function $\Phi_{NLM}(\rho)$ with $N=0,1,2,3$, the antisymmetrization operator makes the right-hand side of (1) vanish identically. Thus, in the $\alpha+\alpha$ system we have identified the following forbidden states with respect to the relative motion of the clusters: $0s, 2s, 2d$; as regards the states $1p, 3p, 3f$, they should be rejected immediately, since the wave function $\Phi(\rho)$ of their relative motion must be even on account of the Bose statistics for α particles. Generalizing the arguments given above, we can give a qualitative definition of forbidden states and describe a method for identifying them. Forbidden states in the system of clusters A_1+A_2 can be defined as the states $\Phi_{NLM}(\rho)$ of their relative motion on the substitution of which the cluster function $A\{\varphi_{N_1}(A_1)\varphi_{N_2}(A_2)\Phi(\rho)\}$ of the system vanishes identically. Here, $\varphi_{N_1}(A_1)$ is the internal function of the cluster A_1, which contains N_1 oscillator quanta. It is assumed that the oscillator parameters $\hbar\omega$ of the clusters A_1 and A_2 are the same. The frequency $\hbar\omega$ is related to the parameter a in the function (2) by $a=r_0^{-2}=m\omega\hbar^{-1}$, where m is the nucleon mass. It is clear that if states with number of quanta $N\geq N_{\min}$ are allowed for a system of A_1+A_2 nucleons, the allowed states of Φ_{NLM} must have $N\geq N_{\min}-N_1-N_2$ quanta, and all states with $N<N_{\min}-N_1-N_2$ will be forbidden. The values of $N_{\min}$ can be readily calculated by summing the oscillator energies of the A_1+A_2 nucleons when they are put in the lowest possible shell levels. If $A_1+A_2\leq4$, then $N_{\min}=0$; if $A_1+A_2\leq16$, then $N_{\min}=A_1+A_2-4$; if $A_1+A_2\leq40$, then $N_{\min}=12+2(A_1+A_2-16)$, etc. Thus, we have obtained a fairly simple method for identifying forbidden states. However, it has the shortcoming of being valid only for oscillator cluster functions $\varphi(A_1)$ and $\varphi(A_2)$, and, moreover, these must be characterized by the same "radius" r_0. In addition, the method must be made more precise even in this idealized case. For example, for the system ^{16}O + ^{16}O, where $N_1=N_2=12$ and $N_{\min}=2\times32-20=44$, all that one can say definitely is that states with $n<20$ are forbidden. However, a more detailed investigation[12] shows that in this system all states up to $n=24$ are forbidden. It is therefore desirable to have a well-defined quantitative method for identifying forbidden states. One variant was proposed by Feshbach,[13] and also by Kerman *et al.*,[14] and in recent years has been widely used by many authors[2,15-18] to study different cluster systems. The general definition of forbidden states was proposed in Ref. 19 (see also Ref. 20) and is discussed below.

Forbidden States in Feshbach's Scheme. Suppose the nuclei A_1 and A_2 collide. For simplicity, we shall restrict ourselves to one elastic channel and consider the scattering of these nuclei in the framework of the resonating-group method.[1] If $\varphi(A_1)$ and $\phi(A_2)$ are the wave functions of the colliding nuclei, the wave function of the complete system in the resonating-group method has the form

$$\Psi\sim\hat{A}\{\varphi(A_1)\varphi(A_2)\Phi(\rho)\},\tag{3}$$

where $\Phi(\rho)$ is the wave function of the relative motion of the fragments A_1 and A_2. Substituting the function (3) in the Schrödinger equation and multiplying it scalarly from the left by the vector $\langle\varphi(A_1)\varphi(A_2)|$, we obtain the well-known equation of the resonating-group method for the function $\Phi(\rho)$:

$$\langle\varphi(A_1)\varphi(A_2)|H-E|\hat{A}\varphi(A_1)\varphi(A_2)\Phi(\rho)\rangle=0.\tag{4}$$

This equation is a special case of the equations of Feshbach's so-called unified theory of nuclear reactions,[13] if the coupling of the elastic channel with all the remaining channels is ignored in that theory.

In Eq. (4), the internal antisymmetric functions of the free clusters are assumed to be known, and they are generally taken in the Gaussian form (2) or in the form of the lowest oscillator shell functions if the mass of the cluster is >4. The antisymmetrization operator is $\hat{A}=\sum(-1)^{P^*}P^*$, where P^* are permutations that inter-

change one, two, etc., nucleons between the clusters A_1 and A_2. Within each cluster, the numbers of the particles after the interchange must be arranged in natural order. The number of such permutations is $(A_1+A_2)!/A_1!A_2!$; for even permutations $P^*(-1)^{P^*} = +1$ and -1 for odd. Note that because of the presence of these permutations, and also because of the contribution of the exchange forces, Eq. (4) contains nonlocal terms and is an integrodifferential equation. The presence of the nonlocal terms can be readily confirmed by considering the second term in the expression (4):

$$\langle \varphi(A_1)\varphi(A_2) \mid \hat{A}\varphi(A_1)\varphi(A_2)\Phi(\rho)\rangle \equiv (1-\hat{K})\Phi(\rho), \tag{5}$$

where $\hat{K}$ is the integral overlap kernel and has the form

$$\hat{K}(\rho,\rho') = \int d\tau \sum_{k=1}^{\min(A_1,A_2)} (-1)^{k+1} \binom{A_1}{k}\binom{A_2}{k} \times \langle \varphi(A_1)\varphi(A_2) \mid P_{A_1, A_1+A_2}P_{A_1-1, A_1+A_2-1}\cdots \cdots P_{A_1-k+1, A_1+A_2-k+1} \mid \varphi(A_1)\varphi(A_2)\rangle. \tag{6}$$

Here, $P_{r,s}$ is a permutation of the particles with the numbers r and s. The integration over τ is performed as follows. The complete set of coordinates of the system consists of the Jacobi coordinates for cluster A_1; $\xi_1, \xi_2, \ldots, \xi_{A_1-1}$, for cluster A_2: $\eta_1, \eta_2, \ldots, \eta_{A_2-1}$ and the coordinate $\rho = A_1\Sigma r_i - A_2{}^1\Sigma r_j$. We transform this set, introducing the coordinate

$$\rho' = P_{A_1, A_1+A_2}\cdots P_{A_1-k+1, A_1+A_2-k+1}\rho$$

[i.e., ρ' is the distance between the nucleon groups A_1 and A_2 after exchange of k nucleons between them and in general for each term in the sum (6) there is a corresponding coordinate ρ'], and also retaining from the set ξ_i, η_i the A_1+A_2-3 Jacobi coordinates that together with ρ and ρ' form a complete set of A_1+A_2-1 linearly independent coordinates for the system A_1+A_2. In (6), it is assumed that integration is performed over the coordinates $\xi_1 (1=1,2,\ldots,A_1+A_2-3)$ and the resulting kernel K depends on the two variables ρ and ρ'. The action of the operator $\hat{K}$ on $f(\rho)$ is defined in the usual manner:

$$\hat{K}f(\rho) = \int d\rho' K(\rho,\rho') f(\rho'). \tag{7}$$

The overlap kernel K is of independent interest and it will be considered in more detail below.

In conclusion, we note that for two identical clusters, $A_1 = A_2$, the expression (6) and Eq. (4) as a whole simplify, since the exchange of all nucleons in this case is equivalent to the identity permutation [if $f(\rho)$ has the necessary parity: + for even A_1 and − for odd A_1], exchange of one nucleon is equivalent to exchange of $A_1 - 1$ nucleons, etc. Thus,

$$\langle \varphi(A_1)\varphi(A_1) \mid \hat{A}\varphi(A_1)\varphi(A_1)\Phi(\rho)\rangle = 2(1-\hat{K})\Phi(\rho). \tag{8}$$

The expression for the integral kernel $\hat{K}$ is similar to (6), except that the summation index k takes values from 1 to $[A/2]$ ($[s]$ is the integral part of the number s).

According to Feshbach,[13] the overlap integral K for two-cluster systems has the following general properties: 1) K is Hermitian; 2) K is a positive-definite kernel; 3) $1-K$ is also a positive-definite kernel; 4) the kernel K is bounded, i.e., $\int\int d\rho d\rho' |K(\rho,\rho')|^2 \leqslant \text{const}$ 5) the trace of the kernel is finite.

We introduce the eigenfunctions $\Phi_n(\rho)$ and the eigenvalues λ_n of K:

$$\hat{K}\Phi_n(\rho) = \lambda_n\Phi_n(\rho). \tag{9}$$

Then K can be represented in the form

$$K(\rho,\rho') = \sum_n \lambda_n\Phi_n(\rho)\Phi_n^*(\rho') = \sum_n \lambda_n P_n, \tag{10}$$

where $P_n = \Phi_n\rangle\langle\Phi_n$ is the projection operator onto the state $\Phi_n(\rho)$. Naturally, the expansion (10) of the kernel contains only those eigenvectors $\Phi_n(\rho)$ that correspond to nonzero eigenvalues.

The eigenvalues of the kernel $1-K$ are equal to $1-\lambda_n$:

$$(1-\hat{K})\Phi_n(\rho) = \mu_n\Phi_n(\rho), \quad \mu_n = 1-\lambda_n. \tag{11}$$

It is interesting to discuss the meaning of the eigenvalues and eigenfunctions of the overlap kernel. Feshbach[13] considered the simple example of nucleon scattering by a magic nucleus A, which is described by a wave function in the form of a Slater determinant:

$$\varphi(A) = (A!)^{-1/2}\hat{A}\{\varphi_1(\mathbf{r}_1)\varphi_2(\mathbf{r}_2)\cdots\varphi_A(\mathbf{r}_A)\}. \tag{12}$$

Substituting this function in (6) and noting that $A_2 = 1$ and $\varphi(A_2) = 1$ and that the integration is performed over the nucleon coordinates $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{A-1}$, and that the coordinates ρ and ρ' are identical in this case with the nucleon coordinates $\rho = \mathbf{r}_{A-1}$ and $\rho' = \mathbf{r}_A$ (we ignore for the moment the problem of the center of mass of the nucleus), we obtain

$$K = \sum_{i=1}^{A} \varphi_i(\rho)\varphi_i^*(\rho'). \tag{13}$$

It can be seen from this that the eigenfunctions of $\hat{K}$ are the wave functions φ_i, $i = 1, 2\ldots$, A, of the occupied states of the nucleus A and that they all correspond to the same eigenvalue $\lambda = 1$. The wave functions of the states φ_j, $j = A+1, A+2, \ldots$, that are not occupied can also be regarded as eigenfunctions of $\hat{K}$, but corresponding to zero eigenvalues. The eigenvalues $\lambda = 1$ require a special analysis. For them,

$$(1-\hat{K})\Phi_n = 0, \tag{14}$$

i.e.,

$$\langle \varphi(A_1)\varphi(A_2) \mid \hat{A}\{\varphi(A_1)\varphi(A_2)\Phi_n\}\rangle = 0.$$

Therefore, we also have

$$\langle \hat{A}\{\varphi(A_1)\varphi(A_2)\Phi_n\} \mid \hat{A}\{\varphi(A_1)\varphi(A_2)\Phi_n\}\rangle = 0$$

or

$$\hat{A}\varphi(A_1)\varphi(A_2)\Phi_n(\rho) = 0. \tag{15}$$

Thus, the states $\varphi(A_1)\varphi(A_2)\Phi_n(\rho)$ vanish identically as a result of antisymmetrization when one of the eigenfunctions corresponding to $\lambda = 1$ is taken as the wave function $\Phi(\rho)$ of the relative motion. Therefore, such states are forbidden by the Pauli principle. We shall therefore call eigenfunctions of the overlap kernel K corresponding to its eigenvalue $\lambda = 1$ forbidden states. If the eigenvalue is zero, $\lambda = 0$, we shall say that the

corresponding state is completely allowed, since for it the operator $1-\hat{K}$ containing the exchange terms is simply equivalent to the identity operator. If $0<\lambda<1$, such states can be said to be partly allowed or half-forbidden. The example of a nucleon on a magic nucleus shows that in this case the eigenvalues λ for single-particle states are equal to the occupation numbers: Occupied states of the nucleus A are forbidden and states that are not occupied are completely, allowed in agreement with the intuitive definition of forbidden states given earlier, but the introduction of the overlap kernel K makes it possible to introduce a clearer gradation of the different states of the relative motion of the fragments A_1 and A_2. Thus, the key element in the identification of the forbidden states in Feshbach's approach is the determination of the eigenvalues and eigenfunctions of the overlap kernel K. It is therefore worth considering this question in more detail.

To elucidate the meaning of the eigenvalues and the method for calculating them, let us consider the case when the nuclei A_1 and A_2 are characterized by the wave functions of the translationally invariant shell model[8]; $|A_iN_i\alpha_iL_iS_iT_i\rangle$, $i=1,2$, with the same frequency $\hbar\omega$ (α stands for all the additional quantum numbers that characterize the state).

For simplicity, we take $L_1=L_2=0$ and consider the expression

$$(1-\hat{K})\,\Phi_{NLM}(\rho)\equiv\langle A_1N_1\alpha_10S_1T_1;$$
$$A_2N_2\alpha_20S_2T_2:ST\,|\quad\hat{A}\,|\,A_1N_1\alpha_10S_1T_1,\ A_2N_2\alpha_20S_2T_2,\ NL(\rho):LST\rangle, \tag{16}$$

where $\Phi_{NLM}(\rho)\equiv|NLM(\rho)\rangle$ is the oscillator wave function of the relative motion of the fragments A_1 and A_2 with the same parameter $\hbar\omega$ as for the nuclei A_1 and A_2. The operator $\hat{A}$ is diagonal with respect to the quantum numbers L, S, and T and, in addition, it does not change change the total number of quanta $N^*=N_1+N_2+N$ in the system. Therefore, after integration over all the variables except ρ, we must also obtain on the right-hand side of (16) an oscillator function of ρ with $N'=N^*-N_1-N_2=N$ quanta and angular momentum $L'=L$, i.e.,

$$(1-\hat{K})\,\Phi_{NLM}(\rho)=(1-\lambda)\,\Phi_{NLM}(\rho), \tag{17}$$

and the eigenfunctions of K are the oscillator functions $\Phi_{NLM}(\rho)$. To obtain the eigenvalue λ, we must use the relation[8]

$$\hat{A}\,|\,A_1N_1\alpha_10S_1T_1,\ A_2N_2\alpha_20S_2T_2,\ NL:LST\rangle$$
$$=(A_1+A_2)!\,(A_1!\,A_2!)^{-1}\sum_{\alpha}\langle A_1+A_2N^*\alpha LST\,|\,A_1N_1\alpha_10S_1T_1;$$
$$A_2N_2\alpha_20S_2T_2,\ NL\rangle\,|\,A_1+A_2N^*\alpha LST\rangle. \tag{18}$$

Combining (16) and (18), we find

$$1-\lambda=\sum_{\alpha}S^{\alpha}_{A_1A_2}, \tag{19}$$

where

$$S^{\alpha}_{A_1A_2}=(A_1+A_2)!\,(A_1!\,A_2!)^{-1}\langle A_1+A_2N^*\alpha LST\,|\,A_1N_1\alpha_10S_1T_1,$$
$$A_2N_2\alpha_20S_2T_2,\ NL\rangle^2 \tag{20}$$

is the spectroscopic factor for the virtual breakup of the composite nucleus into the state $|A_1+A_2N^*\alpha LST\rangle$ through the channel A_1+A_2 (Ref. 8). A method for calculating the coefficients of fractional parentage $\langle|\rangle$ in the translationally invariant shell model which occur on the right-hand sides of (18) and (19) was developed in Ref. 8, and therefore Eqs. (19) and (20) make it possible to find the eigenvalues λ of K. In Ref. 2 these results are generalized for $L_1, L_2\neq0$, and also to the case of coupled channels and many-cluster systems.
K. In Ref. 2 these results are generalized for $L_1, L_2\neq0$, and also to the case of coupled channels and many-cluster systems.

Ghost States as a Generalization of the Concept of Forbidden States. Although the theory of forbidden states in nuclear systems developed by Feshbach[13] and Kerman *et al.*[14] proved to be very helpful, subsequent investigations showed that such an approach also has serious shortcomings due to the occurrence of almost forbidden ($\lambda_n\sim1$) and half-forbidden states. In particular, it was found[15-18] that the presence of almost forbidden states leads to the appearance at very high energies $E_{cms}\sim40$ MeV of unusual resonances that do not have a clear physical interpretation and strongly resemble the well-known spurious resonances that arise when the Kohn–Hulthén variational principles are applied to scattering problems.[19] However, a much more serious shortcoming is the fact that the Feshbach–Kerman theory is entirely based on the resonating-group method or on the cluster approximation for the total wave function of a system of the form (1), i.e., essentially on the adiabatic model (with exchange), whereas the concept of forbidden states (forbidden by the Pauli principle) is much wider and should not, in general, be restricted to particular approximations for the wave functions.

It is therefore of great interest to establish what the forbidden states in the resonating-group method correspond to in a rigorous theory of many-particle systems. There is such a possibility and it is based on the rigorous Faddeev–Yakubovskiĭ theory of many-particle systems. Namely, one must take a problem for three or four nucleons and establish in the framework of a rigorous theory what kind of forbidden states appear in such systems. The correspondence found in this (i.e., rigorous) manner can then be extended to other nuclear systems. Such an investigation was made made[20,21] for *nd* scattering (in the channel with $S=3/2$) and for *dd* scattering in the channel with $S=2$. Below, we shall briefly present the main results.

We consider first *nd* scattering in the quartet channel. Since the spins of all three nucleons are here parallel, the orbital wave function must be antisymmetric under transposition of the two neutrons, i.e., in the interaction of the two neutrons one must take into account only the odd partial waves, and, as is well known, this interaction can be ignored at low energies. The remaining two *np* interactions will be triplet ^3S. Under these conditions, the total orbital wave function decomposes into a sum of two Faddeev components (in accordance with the two *np* interactions),

$$\Psi_{S,a}=\psi^{(1)}_{S,a}\pm\psi^{(2)}_{S,a}, \tag{21}$$

where the plus sign corresponds to a spatially symmetric orbital function (physically unrealizable), and the

minus sign to the antisymmetric function; the indices s and a correspond to these signs.

An important feature of the Faddeev approach is that for the symmetric $\psi_s^{(i)}$ and antisymmetric $\psi_a^{(i)}$ Faddeev components the equations are different (the kernels for the symmetric and antisymmetric cases differ in sign).

We shall call the physically unrealizable channel with the symmetric orbital wave function a ghost channel, and the bound states in this channel ghost bound states, or simply ghosts. In the framework of the Faddeev–Yakubovskiĭ theory (or any other mathematically correct theory of many-particle scattering) the problem of permutational symmetry has some specific features. The point is that although the total Schrödinger wave function Ψ has a particular permutational symmetry, its Faddeev components $\psi^{(i)}$—and a decomposition of Ψ similar to (21) into channel components exists in any "good" theory—do not have a definite permutational symmetry. In fact, the type of permutational symmetry of the solutions is determined in such a theory by the structure of the integral kernel, and the procedure for finding the kernel corresponding to a solution of given symmetry includes the decomposition and reduction of the matrix integral kernel into submatrices corresponding to irreducible representations of the group of permutations. In the general case, such an analysis has not yet been made, but for the special cases considered here it can be carried out without difficulty.[20,21]

Thus, the system of Faddeev equations for the components $\psi_{s,a}^{(i)}$ has the form

$$\psi_{s,a}^{(i)} = \varphi^{(i)} \pm G_0 T_i P_{12} \psi_{s,a}^{(i)}, \quad i = 1, 2, \tag{22}$$

where $\psi_{s,a}^{(2)} = \pm P_{12}\psi_{s,a}^{(1)}$, and the plus sign in (21)–(22) corresponds to the ghost channel; and the minus sign to the physical channel; P_{12} is the operator of transposition of two identical neutrons, $G_0 \equiv (E - H_0)^{-1}$ is the free Green's function, and T_i is the t matrix of the triplet interaction in channel i, with $T_2 = P_{12}T_1P_{12}$. The wave function of the initial state is $\varphi^{(i)} = \varphi_{23}(\mathbf{p})\delta(\mathbf{q} - \mathbf{q}_0)$, where φ_{23} is the deuteron wave function, and $\mathbf{q}_0$ is the momentum of the incident neutron.

Further, of great importance for the scattering problem are the sign and norm of the kernel $K = G_0 T_i P_{12}$, which determines the intensity of the interaction. In its turn, the norm of the kernel depends on the values of its eigenvalues, which are determined by the matrix equation

$$\hat{K}_2(E)\,\hat{\chi}_n^{s,a} = \pm \alpha_n(E)\,\hat{\chi}_n^{s,a}, \tag{23}$$

where the matrix kernel $\hat{K}_2$ of the system (23) is[46] the operator

$$\hat{K}_2(E) = \begin{pmatrix} 0 & G_0(E)T_1(E) \\ G_0(E)T_2(E) & 0 \end{pmatrix},$$

and $\chi_n^{c,a}$ are two-component columns, the plus sign in (23) corresponding to the index s and the minus sign to the index a. To bound states in the physical channel (a channel) there correspond the eigenvalues $\alpha_n(E) = -1$, and to those in the ghost channel (s channel) there correspond $\alpha_n(E) = +1$. Indeed, an actual calculation in Ref. 20 made it possible to identify in the ghost channel a bound state with energy $E_G \approx -5.5$ MeV, which is none other than the quartet triton with spin 3/2 and symmetric spatial part of the wave function forbidden by the Pauli principle. In the physical channel (where the sign of the kernel corresponds to repulsion) there are no bound states, i.e., the kernel $K = G_0T_1P_{12}$ does not have large negative eigenvalues. But since the system of Faddeev equations (22) is equivalent to the original Schrödinger equation, the appearance of an eigenvalue of the Faddeev kernel in the ghost channel means that in the total Hamiltonian of the system there is a bound (eigen) state of forbidden symmetry, a ghost, which could have been predicted without any calculations. Indeed, if we consider the system $p + 2n$ in a symmetric spatial state with two triplet ^3S interactions, it is perfectly clear that in this system there is a bound state with energy $E_G \sim 2\varepsilon_d$, where ε_d is the deuteron binding energy (the equality $E_G = 2\varepsilon_d$ would hold if the proton were infinitely heavy).

What is the importance of the ghost states in scattering theory?

First, from the point of view of the influence on the scattering problem the ghosts play the same part as the physical bound states. In particular, ghosts give rise to the same divergence of the Born series (for the Faddeev–Yakubovskiĭ equations) as the physical bound states, and the scattering wave function in the physical channel must be orthogonal to the wave functions of both the physical bound states and the ghosts.

Second, it is preferable to use precisely the ghost states or their form factors (the overlap integrals with the cluster functions) in approximate approaches such as the orthogonality-condition model instead of the Feshbach-forbidden states, and this will probably make it possible to avoid a number of difficulties and obscurities encountered in the elimination of half-forbidden and almost forbidden states from the scattering problem.[15-18]

The same treatment can be given for dd scattering in the quintet channel in the framework of the Yakubovskiĭ equations, where again there is a ghost bound state (possibly, not only one) with symmetric orbital wave function and energy $E_G \approx -15$ MeV (ghost α particle), which leads to a divergence of the Born series for the Yakubovskiĭ equations, etc.[20,21] The generalization to an arbitrary number of particles is obvious, since the N-particle Faddeev–Yakubovskiĭ equations are dynamically equivalent to the N-particle Schrödinger equation, and the spectrum of the kernels of the N-particle Faddeev–Yakubovskiĭ equations must correspond exactly to the spectrum of the N-particle Hamiltonian, as was shown above for the $3N$ system. It is therefore clear that in a rigorous many-particle theory true bound states of the total Hamiltonian with symmetry forbidden by the Pauli principle correspond to the forbidden states that appear in the resonating-group method. And in such a definition, all dependence on the actual approximations made for the scattering wave function disappears. Of course, in actual calculations (with $(N \geq 5)$ some approximations are necessary.

Let us now compare the Feshbach definition (9) of forbidden states with what follows from the rigorous theory (23) with $\alpha_n(E) = \pm 1$. In both cases, the forbidden states are defined as eigenfunctions corresponding to unit eigenvalues [$\lambda_n = 1$ in the first case and $\alpha_n(E) = 1$ in the second] of some integral kernel. However, these states are defined in accordance with the resonating-group method purely by the structure overlap kernel, which depends neither on the energy nor on the dynamics of the interaction (let us say, on the nature of the forces between the particles, the positions of the thresholds, etc.). But in the rigorous theory we have the eigenfunctions of the Faddeev kernels, which depend on both the energy and the actual dynamical factors, which is much better, though harder to implement. Therefore, in the rigorous theory no half-forbidden states occur, since the total Hamiltonian either does or does not contain bound states of forbidden symmetry. Only virtual or resonance forbidden states are possible; but, strictly speaking, they belong to the continuum and not the discrete spectrum. The appearance in a number of cases of a rich spectrum of half-forbidden states in the Feshbach scheme is probably due to the attempt to treat the problem of many-particle scattering in a finite-dimensional space of square-integrable functions, which always leads to the appearance of singularities, whose number is equal to the dimension of the model space. Indeed, if we write the representation for the scattering wave function in the Kohn–Hulthén variational principle[19] in the form

$$\Psi = \Psi_{\text{asympt}} + \sum_{i=1}^{N} a_i \varphi_i, \tag{24}$$

where φ_i are square-integrable functions, and Ψ_{asympt} is the asymptotic part of the wave function, the scattering amplitude found from (24) will have unphysical singularities at the energies corresponding to the eigenvalues of the Hamiltonian matrix: $\langle \varphi_i | H | \varphi_j \rangle$, $i, j = 1, 2, \ldots, N$ (Ref. 19). Entirely similar singularities arise in the attempt to treat half-forbidden states as truly forbidden states.[15,18]

In conclusion, we point out that the introduction of ghost states in the theory of many-particle scattering is also very fruitful from the practical point of view, since it makes it possible to explain scattering for systems of the type *nd*, *dd*, n^3He, etc., in the channels in which the Pauli principle is dominant by unitary orthogonalization of a plane wave (see below) to the ghost bound state.[20,21] In these cases, one can even write down a simple analytic expression for the scattering amplitude on and off the mass shell.[20,21]

2. DESCRIPTION OF THE INTERACTION OF COMPOSITE PARTICLES IN THE ORTHOGONALITY-CONDITION MODEL

Orthogonality-Condition Model. In 1969, Saito[22] proposed the orthogonality-condition model to replace the very complicated exchange terms that appear in the resonating-group method. He was guided by the following considerations. Let us consider again the basic equation in the resonating-group method for the scattering wave function $\chi(\mathbf{R})$ of two clusters:

$$(T_D + V_D - E)\chi(\mathbf{R}) = \langle \varphi_a \varphi_b | T + \sum_{i>j} V_{ij} - E \Big| \frac{1}{N!} \sum_P (-1)^P P(\varphi_a \varphi_b \chi(\mathbf{R})) \rangle, \tag{25}$$

where the right-hand side is the exchange kernel due to the antisymmetrization of the total wave function. It is on account of these exchange terms in Eq. (25) that the so-called spurious solutions $\chi_\alpha(\mathbf{R})$, corresponding to eigenvalues of the overlap kernel $K(\mathbf{R}, \mathbf{R}')$ with unit eigenvalues, appear. We have said above that these spurious solutions correspond to the states forbidden by the Pauli principle. Saito, and also others,[23] established that the characteristic shell oscillations of the radial wave functions in the region of overlapping of the clusters arise when these spurious solutions are eliminated from the scattering problem, i.e., when the scattering wave function is orthogonalized with respect to all $\chi_\alpha(\mathbf{R})$. The next step made by Saito then appears natural; he proposed that the right-hand side in (25) should be removed altogether and replaced by the additional condition that the solution of (25) with vanishing right-hand side should be orthogonal to all χ_α, i.e., (25) should be replaced by the equation

$$(T_D + V_D - E)\chi(\mathbf{R}) = 0 \tag{26}$$

with the additional orthogonality condition

$$\langle \chi_\alpha | \chi \rangle = 0, \quad \alpha = 1, \ldots, n. \tag{27}$$

The system (26)–(27) is Saito's orthogonality-condition model. The solutions (26)–(27) should be understood, not as the choice of all solutions of the homogeneous equation (26) satisfying the orthogonality condition, but as the solution of Eq. (26) in the subspace orthogonal to the vectors χ_α, $\alpha = 1, \ldots, n$, i.e., as the solution of the equation

$$Q(T_D + V_D - E)Q\chi = 0, \tag{28}$$

where $Q = 1 - \Gamma$ is the projection operator onto the subspace of allowed states, and $\Gamma = \sum_{\alpha=1}^{n} |\chi_\alpha\rangle\langle\chi\alpha|$ is the projection operator onto the forbidden subspace.

To solve (28), Saito proposed the use of the method of Lagrange multipliers, which reduces here to the replacement of (28) by a corresponding equation with right-hand side

$$(T_D + V_D - E)\chi = \sum_\alpha \lambda_\alpha | \chi_\alpha \rangle, \tag{29}$$

where the Lagrange multipliers λ_α must be chosen to make the solutions (29) satisfy the required conditions of orthogonality to χ_α. This led Saito to the result

$$\lambda_\alpha = \langle \chi_\alpha | T_D + V_D | \chi \rangle; \tag{30}$$

and finally he obtained for the orthogonality-condition model an equation of the form[22]

$$(T_D + V_D - E)\chi = \sum_\alpha | \chi_\alpha \rangle \langle \chi_\alpha | T_D + V_D | \chi \rangle. \tag{31}$$

It is easy to see that for $E \neq 0$ any solution of (31) satisfies the required orthogonality condition. However, for $E = 0$ there can be a problem, since at this point one can have admixing (with arbitrary weights) of spurious solutions χ_α (forbidden states) to the solution χ. This means that at zero energy the solution of Satio's equation (31) is not orthogonal to the forbidden states. We shall see below that this is a reflection of a deeper fact, namely, that Saito's equation is not valid off the

mass shell and that the method of Lagrange multipliers is inconvenient for the systematic and complete allowance for the orthogonality conditions. For the solution of this last problem, the method of orthogonalizing pseudopotentials proposed in Ref. 24 is very effective. But before we explain the technique of orthogonal projection, we shall briefly discuss the results obtained by means of the orthogonality-condition model.

αα Scattering. Application of the orthogonality-condition model to αα scatttering is effective for the following reasons: First, the α particle is very stable, and therefore application to the αα system of the resonating-group method, which is the basis of Saito's model, is physically justified; second, the spectrum of eigenvalues of Feshbach's overlap kernel for the αα system (see §2) is very well suited for using the orthogonality-condition model, since in this system there are eigenvalues that are strictly unity, and the remaining eigenvalues are small; third, there are here no spin effects complicating the treatment. The experimental values are compared with those calculated in the orthogonality-condition model for the αα phase shifts with $l = 0, 2, 4$ in Fig. 1 (Ref. 25), from which it can be seen that the orthogonality-condition model gives a very good description of the phase shifts and also the scattering wave functions, the simplicity and perspicuity of the description being incomparably better than that of the resonating-group method.

We may add that the good accuracy achieved by the orthogonality-condition model in the αα problem even made it possible to consider extraction of the coupling constant of the σ-meson–nucleon interaction from the data on αα scattering.[25] Subsequently, the model was also used for other two-cluster systems[23] of the type $\alpha^{12}C$, $\alpha^{16}O$, etc., and also for three-cluster systems, in particular, for the 3α system.[2] We discuss this case in Sec. 5. However, the use of the model for systems of the type $\alpha^{12}C$, $\alpha^{16}O$, and others encounters some difficulties, in contrast to the αα system. These are due to the nature of the spectrum of eigenvalues γ_α of the overlap kernel. As was shown in Refs. 16, 17, and 23, for a system of two clusters with mass numbers $A > 4$ or with significantly differing oscillator radii (which is the case for systems such as $\alpha^{16}O$) the eigenvalue spectrum of the kernel $K(\mathbf{R}, \mathbf{R}')$ is smooth (see, for example, Fig. 2, which shows the spectrum of of eigenvalues γ_N for the system $^{16}O + ^{16}O$). In this spectrum, there are no strictly forbidden or strictly

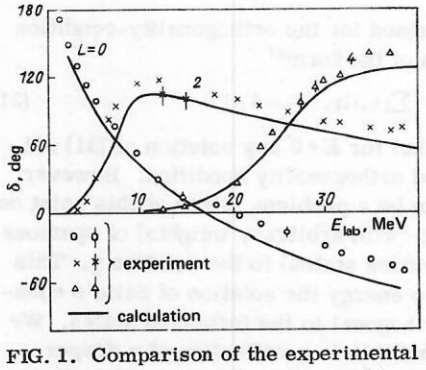

FIG. 1. Comparison of the experimental αα phase shifts with calculations based on the orthogonality-condition model.

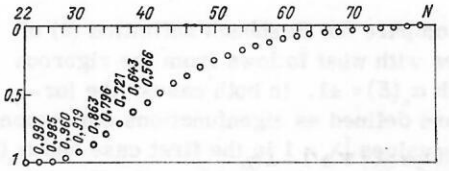

FIG. 2. Eigenvalue spectrum of the antisymmetrization kernel, γ_N, for the system $^{16}O + ^{16}O$ (N is the number of the eigenvalue).

allowed states, and all eigenfunctions correspond to the so-called half-forbidden states, which in shell language correspond to partly filled states. Unfortunately, for these cases the orthogonality-condition model is inapplicable in its original form, and it would seem that one must return to the cumbersome resonating-group method. However, a more detailed and rigorous analysis based on the exact many-particle Faddeev and Faddeev–Yakubovskiĭ integral equations shows that this is not so, and it has proved possible to generalize and make more precise the orthogonality-condition model for the majority of cases of scattering of two and also more clusters,[7,21,28]

Orthogonal Projection Method Based on Orthogonalizing Pseudopotentials. The idea of the method of orthogonalizing pseudopotentials is very simple and is intimately related to the concept of penalty functions in the theory of dynamic programming. Suppose a part of a space (in our case, this part of the Hilbert space, and in optimization theory it is part of the parameter space in which the optimization is performed) is forbidden (or inaccessible to the dynamical system). Then, instead of directly solving the problem in the orthogonal subspace $\mathcal{H}_Q$ of the total space $\mathcal{H} = \mathcal{H}_\Gamma \oplus \mathcal{H}_Q$, it is more convenient to introduce into the equation a penalty function, which, when the equation is solved, "forces" the dynamical system into the allowed subspace H_Q. For the Schrödinger equation (26) with the additional conditions (27), a convenient penalty function is a repulsive separable addition to the Hamiltonian $\lambda\Gamma$, where the projection operator $\Gamma = \sum_{\alpha=1}^{n} |\chi\alpha\rangle\langle\chi\alpha|$ contains a sum over the forbidden states, and the constant λ must tend to infinity in the final result. In the limit $\lambda \to \infty$, we obtain a solution that is strictly orthogonal to the forbidden subspace. $\mathcal{H}_\Gamma$. Implementing now this program, we introduce the pseudo-Hamiltonian

$$\tilde{H} = H + \lambda\Gamma$$

and find the solution of the Schrödinger equation

$$(\tilde{H} - E)\,\tilde{\Psi}_E = 0. \tag{32}$$

It is easy to obtain

$$\tilde{\Psi}_E = \Psi_E + c(\lambda)\,G(E)\,\chi_0, \tag{33}$$

with the constant

$$c(\lambda) = \lambda\langle\chi_0 | \Psi_E\rangle / (1 - \lambda\langle\chi_0 | G(E) | \chi_0\rangle),$$

where $G(E) = (E - H)^{-1}$ is the Green's function of the original Hamiltonian; for simplicity, we consider the case when there is only one forbidden state χ_0. The generalization for several forbidden states is obvious. The function Ψ_E is a solution of the original Schrödin-

ger equation. In the limit $\lambda \to \infty$, we find

$$\lim_{\lambda\to\infty} c(\lambda) = -\langle\chi_0 \mid \Psi_E\rangle/\langle\chi_0 \mid G \mid \chi_0\rangle,$$

and the admixture of the function χ_0 to the solution $\tilde{\Psi}_E$:

$$\lim_{\lambda\to\infty} \langle\chi_0 \mid \tilde{\Psi}_E\rangle = \lim_{\lambda\to\infty} \langle\chi_0 \mid \Psi_E\rangle (1-\lambda\langle\chi_0 \mid G(E) \mid \chi_0\rangle)^{-1} = 0, \quad (34)$$

i.e., in the limit $\lambda \to \infty$ we obtain the required orthogonality of the solution $\tilde{\Psi}_E$ to χ_0. Then the solution of (32) can be written in the explicit form

$$\tilde{\Psi}_E = \Psi_E - G \mid \chi_0\rangle\langle\chi_0 \mid \Psi_E\rangle/\langle\chi_0 \mid G \mid \chi_0\rangle = \Psi_E - G\Gamma(\Gamma G\Gamma)^{-1}\Gamma\Psi_E. \quad (35)$$

It is easy to see that Saito's equation for $E \neq 0$ gives the same solution for the scattering wave function as (35). However, if the corresponding operators are considered off the mass shell, the projection technique by means of the orthogonalizing pseudopotentials leads to results that differ from those of the Saito equation (31).

As an example, let us consider the projection of the Green's function for Eq. (32):

$$\tilde{G}_\lambda(E) = (E-\tilde{H})^{-1} = (E-H-\lambda\Gamma)^{-1}.$$

Using the further the standard resolvent identities, we find

$$\tilde{G}_\lambda = G + \lambda G\Gamma\tilde{G}_\lambda. \quad (36)$$

In the limit $\lambda \to \infty$,

$$\tilde{G} = \lim_{\lambda\to\infty} \tilde{G}_\lambda = G - G\Gamma(\Gamma G\Gamma)^{-1}\Gamma G, \quad (37)$$

where the inverse operator $(\Gamma G\Gamma)^{-1}$ is defined only in the subspace $\mathcal{H}_\Gamma$.

It is easy to see that the projected $\tilde{G}$ has the required orthogonality property, since $\Gamma\tilde{G} = 0$, and in the limit $\lambda \to \infty$ it has no spurious poles in the physical region. However, if the original Hamiltonian $\mathcal{H}$ is projected onto the allowed subspace $\mathcal{H}_Q$, as is done in Satio's approach, the corresponding resolvent

$$G_S = (E-QHQ)^{-1} \quad (38)$$

satisfies the different equation

$$G_S = G - G(\Gamma H + H\Gamma - \Gamma H\Gamma)G_S,$$

from which we obtain

$$G_S = G - G\Gamma(\Gamma G\Gamma)^{-1}\Gamma G + \Gamma/E = \tilde{G} + \Gamma/E,$$

i.e., the resolvent of Saito's equation differs from the one found by means of the orthogonalizing pseudopotentials by the additional term Γ/E, which for $E = 0$ destroys the property of orthogonality to $\mathcal{H}_\Gamma$. However, if we invert, not (38), but the operator $Q(E-H)Q$, i.e., we invert the operator $(E-H)$ in the orthogonal subspace (and the technique with orthogonalizing pseudopotentials makes it possible to do this easily), we readily find

$$\left.\begin{aligned} &\tilde{G} = Q[Q(E-H)Q]^{-1}Q; \\ &\tilde{G}[Q(E-H)Q] = Q. \end{aligned}\right\} \quad (39)$$

This last equation is the analog of the ordinary identity

$$(E-H)G = I$$

in the orthogonal subspace $\mathcal{H}_Q$. Thus, the proposed technique of orthogonal projection gives (in contrast to Feshbach's projection formalism) a convenient means for finding the inverse operators in the orthogonal subspace. The further generalization of this approach to the many-particle case is given in the following sections.

The Pauli Principle and Reduction of the Interaction. Allowance for the Pauli principle in the problem of the scattering of composite particles leads to an interesting physical consequence—a kind of reduction of the interaction. This reduction is manifested in two important aspects: First, the effective interaction in the system is significantly weakened; second, and this is intimately related to the first point, there is a significant reduction in the sensitivity of the results (i.e., the phase shifts, wave functions, etc.), to the details of the interaction potential between the particles, especially in the inner region, i.e., where this interaction is least well known and, generally, only an effective description is meaningful. In particular, for the orthogonality-condition model the detailed behavior of the direct interaction potential V_D in the inner region has very little influence on the results. Essentially, both these consequences are a manifestation of the well-known fundamental fact that in a system of fermions the Pauli principle greatly enhances the importance of the kinetic energy and accordingly reduces the significance of the interaction potential energy. It is this circumstance in particular that underlies the model of almost free electrons in the theory of metals. The same fundamental fact was made the basis of the approaches of Lippmann and Schey[29] and Burke and Chandra[30] to the description of electron scattering by atoms and molecules. In the problem of the scattering of two composite nuclear particles discussed here, this very important consequence of the Pauli principle can be illustrated best as follows.

We write down the Lippmann-Schwinger equation corresponding to the Schrödinger equation (32) for the projected wave function $\tilde{\Psi}$,

$$\tilde{\Psi} = \tilde{\Psi}_0 + \tilde{G}_0 V\tilde{\Psi}, \quad (40)$$

where

$$\tilde{\Psi}_0 = \Psi_0 - G_0 \mid \chi_0\rangle\langle\chi_0 \mid \Psi_0\rangle/\langle\chi_0 \mid G_0 \mid \chi_0\rangle$$

is a solution of the free Schrödinger equation in the orthogonal subspace $\mathcal{H}_Q$, and

$$\tilde{G}_0 = G_0 - G_0 \mid \chi_0\rangle\langle\chi_0 \mid G_0\rangle/\langle\chi_0 \mid G_0 \mid \chi_0\rangle = G_0 - G_0\Gamma(\Gamma G_0\Gamma)^{-1}\Gamma G_0 \quad (41)$$

is the free Green's function corresponding to $\tilde{\Psi}$. Note that the last expression for $\tilde{G}_0$ is valid in the general case, i.e., when the projection operator Γ has any dimension. As a calculation shows,[27,31] the zeroth approximation $\tilde{\Psi}_0$ and its corresponding amplitude

$$\tilde{A}_0 = \Gamma/\Gamma G_0\Gamma \quad (42)$$

already describe the exact resonating-group method phase shifts and the corresponding wave functions satisfactorily in a number of cases. In addition, the amplitude A_0 is unitrary, and the function $\tilde{\Psi}_0$, being orthogonal to all the forbidden states (included in Γ), has the necessary number of nodes in the inner region, and the

phase shift calculated for it corresponds to the amplitude $\tilde{A}_0$. Since both $\tilde{\Psi}_0$ and A_0 correspond to scattering induced by the imposition of the orthogonality conditions, they were called,[31] respectively, the wave function and the amplitude of orthogonal scattering. If now the amplitude $\tilde{A}_0$, *which is entirely due to the Pauli principle*, includes an appreciable fraction of the total amplitude, the remainder, which depends on the dynamics, i.e., the difference $A - A_0$ between the exact amplitude and the orthogonal scattering amplitude, will make a relatively small contribution and, as a result, the exact amplitude will depend much less strongly on the details of the interaction potentials than the corresponding amplitude without allowance for the orthogonalization conditions. It is important that the outer part of the effective interaction, which is not strongly affected by the orthogonalization, can be calculated with sufficient accuracy in both atomic and nuclear physics (see the following section). Note further that since the scattering wave functions for a Hermitian Hamiltonian are always orthogonal to the wave functions of the discrete spectrum irrespective of whether forbidden or allowed states are under consideration, the same technique of orthogonal projection will be effective if the known (for example, from the shell model) *physically observed bound states* are included in the projection operator Γ. In this case, the sensitivity of the scattering problem (for composite particles) to the uncertainties in the choice of the optical potential is reduced even more significantly.

Thus, we arrive at a new picture of the interaction of composite particles (or of a nucleon with a nucleus) and a corresponding new approach, which makes it possible to clarify and make more precise the intuitive phenomenological models used in this field. To some extent, this new approach has already been implemented in atomic physics to solve the problem of electron scattering by atoms and molecules.

Electron Scattering by Atoms and Molecules. In 1960, Lippmann and Schey[29] proposed an optical model for the scattering of electrons by atoms[1)] analogous to Saito's model for nuclear particles. In their paper, they formulated a general view of the problem of electron scattering by composite particles that is somewhat more general than the approach of the orthogonality-condition model and has served as the basis for a number of more recent investigations into more complicated problems such as, for example, the scattering of electrons on molecules (see below). Lippmann and Schey proceeded from the same considerations as we have discussed above in this section. Namely, they assumed that the long-range part of the electron–atom atomic potential is known and equal to

$$V_l(r) = V_C(r) + V_p(r), \tag{43}$$

where

$$V_C(r) = -e^2(1/a_0 + 1/r)\exp(-2r/a_0)$$

is the screened Coulomb potential (a_0 is the Bohr radius), and $V_p(r)$ is the polarization potential

$$V_p(r) = -\alpha/2r^4, \tag{44}$$

where α is the experimentally known dipole polarizability.[2)] The polarization potential (44) is the asymptotic part ($r \to \infty$) of the first-order correction (in perturbation theory) to the electron–atom potential calculated in the adiabatic approximation. In the inner region, the behavior of the optical potential is unknown and in fact, in this region, a precise concept of an optical potential is hardly meaningful, except perhaps for an effective description of the wave function of the relative motion of the fragments in the inner region. Therefore, instead of constructing an optical potential in this region, it is more expedient to impose on the scattering wave function the condition of orthogonality to the exact many-particle states of the discrete spectrum, it being necessary to take into account both the allowed (i.e., physically realized) and the forbidden states. For example, for s-wave eH scattering, it is necessary to orthogonalize the scattering wave function in the triplet channel to the $1s$-occupied orbital of the hydrogen atom, and in the singlet channel to the unique bound state of the ion H^-. Scattering in the higher partial waves "feels" only the tail of the optical potential, which is adequately described by a construction of the type (43). Thus, we arrive at a very perspicuous and simple procedure for constructing an approximate optical potential. In such an approach, the important thing is not so much the optical potential itself as the construction of the approximate scattering wave function. If necessary, and this is very important, the obtained function (of the corresponding scattering amplitude) can be made more precise by means of an appropriate variational principle,[3)] in order to take into account the polarization of the system and nonadiabatic effects. In Fig. 3, we give the results of calculations for eH scattering and compare these results with the experimental data; we also show the variational corrections to the obtained scat-

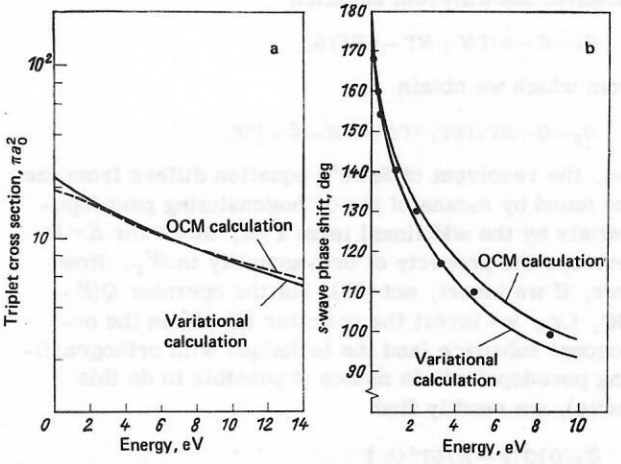

FIG. 3. Cross section of eH scattering in the triplet channel (a) and comparison of the theoretical (curves) and experimental s-wave phase shifts (points) of triplet eH scattering (b).

[1)] Specifically, they considered the scattering of electrons by hydrogen atoms.

[2)] For the hydrogen atom, $\alpha = 4.5$.

[3)] Lippmann and Schey used Kohn's principle.

tering function (and amplitude). It can be seen that the corrections are small and that the result of the orthogonality-condition model makes the main contribution.

In the case of electron scattering by molecules, it is absolutely necessary to take into account the Pauli principle by means of orthogonalization with respect to the occupied molecular orbitals, since even when exchange effects are ignored the problem is much more complicated than in the atomic case. Therefore, the appreciable complication of the equations through the rigorous treatment of the exchange effects leads in the majority of cases to excessively cumbersome equations even for modern high-speed computers. This difficulty is usually circumvented as follows. The exact treatment of the exchange effects is used only in one or two of the most important channels. In the remaining channels, these effects are treated approximately, i.e., by means of orthogonalization. After expansion of all the interaction potentials (of the electron and the molecule) and the corresponding scattering wave functions with respect to partial waves, we obtain the system of equations

$$\left(\frac{d^2}{dr^2}-\frac{l_i(l_i+1)}{r^2}+k^2\right)\mathcal{U}_{l_il_j}(r) - \sum_{l_j} V_{l_il_j}(r)\,\mathcal{U}_{l_il_j}(r)=\sum_{\alpha}\gamma_\alpha\Phi_{l_i}^{(\alpha)}(r), \tag{45}$$

where the right-hand side is the orthogonalizing correction to the original Schrödinger equation for the wave function $\mathcal{U}_{l_il_j}(r)$ of the scattered electron in the molecular field $V_{l_il_j}$; $\Phi_{l_i}^{(\alpha)}(r)$ are the wave functions of the occupied orbitals, and the constants γ_α must be chosen on the basis of the orthogonality conditions

$$\langle\Phi_{l_i}^{(\alpha)}\mid\mathcal{U}_{l_il_j}\rangle=0,\quad \alpha=1,\ \ldots,\ n.$$

The second index l_j of the solution refers to the variable describing the orientation of the molecule in the laboratory coordinate system. For scattering on atoms, the orthogonalizing correction simplifies and in the case of a single occupied orbital Φ_l) is equal to $\gamma\Phi_l(r)$. It is easy to see that the above method of orthogonalization using orthogonalizing pseudopotentials leads to exactly the same form of the orthogonalizing correction. Indeed, in the approach of the orthogonalizing pseudopotentials, the correction is

$$\lambda\mid\Phi_l\rangle\langle\Phi_l\mid\mathcal{U}_l\rangle,$$

where $\lambda\to\infty$ and U_l is the solution of the equation with the orthogonalizing correction. It can easily be seen from (34) that the overlap is

$$\langle\Phi_l\mid\mathcal{U}_l\rangle=\langle\Phi_l\mid\chi_l\rangle/(1-\lambda\langle\Phi_l\mid G\mid\Phi_l\rangle)\sim 0(1/\lambda),$$

where χ_l is the solution of the original Schrödinger equation (without allowance for orthogonalization).

Thus, in the limit $\lambda\to\infty$ the parameter λ cancels strictly, and we arrive at the following form of the orthogonalizing correction:

$$-\mid\Phi_l\rangle\langle\Phi_l\mid\chi_l\rangle/\langle\Phi_l\mid G\mid\Phi_l\rangle\equiv\gamma(E)\mid\Phi_l\rangle,$$

i.e., we arrive at exactly the same form as was used in the calculations of Refs. 32 and 33. In addition, it is now easy to write down a general expression for the Lagrange multiplier $\gamma(E)$:

$$\gamma(E)=-\langle\Phi_l\mid\chi_l\rangle/\langle\Phi_l\mid G\mid\Phi_l\rangle.$$

The generalization to the case of many occupied orbitals is obvious. Very complete calculations were made in recent years for eN_2 scattering.[30,32,33] These calculations showed that in the states $^2\Sigma_g$, $^2\Sigma_\mu$, $^2\Pi_\mu$, in which there are occupied orbitals of the N_2 core, approximate treatment of the Pauli principle by means of orthogonal projection leads to results that are close to the exact results,[4)] whereas in the state $2\Pi_g$, in which there is a well-known and important resonance at $E_e\approx 2.5$ eV, occupied orbitals of the core are absent and the exchange effects must be taken into account by complete antisymmetrization.

3. OPTICAL POTENTIALS WITH FORBIDDEN STATES FOR DESCRIBING THE INTERACTION OF THE LIGHTEST NUCLEI

Phenomenological Analysis. It is well known that the optical model in nuclear physics has proved to be very successful and fruitful for describing numerous phenomena associated with scattering of nucleons by nuclei. The optical potential is usually assumed to be the local equivalent of the self-consistent nonlocal potential of the nuclear field, which can be found from a microscopic approach of the Hartree–Fock type. It has been shown (see, for example, Ref. 34) that if a phase-shift equivalent potential is constructed for the nonlocal interaction of a neutron with the ^{16}O nucleus calculated in Hartree–Fock theory, this potential virtually coincides with the standard Woods–Saxon potential used in the optical model for scattering of neutrons by ^{16}O.

We now consider the scattering of composite particles by composite particles, in particular, the best studied case of $\alpha\alpha$ scattering. Already in the fifties, there were constructed for this system (see the digression into the history of the $\alpha\alpha$ problem and the complete bibliography in the review of Ref. 35) several phenomenological local potentials giving a good description of the $\alpha\alpha$ phase shifts at low energies (up to 10 MeV). However, all these local potentials differed strongly from the potentials of the optical model, since they contained a hard core of appreciable radius and their parameters depended strongly on the angular momentum l. The standard motivation for including the hard core was the argument that the Pauli principle prevents the particles from penetrating each other. However, subsequent investigations showed that arguments of this kind are too simplified even for heavy particles such as ^{12}C and ^{16}O, while for the light cluster systems such as $\alpha\alpha$, αt, and n^3He, etc., they are simply false. The point is that the local repulsive core simulating the effect of the Pauli principle is merely a quasiclassical image, which is valid when the nucleons

[4)] By exact, we mean calculations in which the identity of the particles and the Pauli principle are taken into account by complete antisymmetrization of the wave function of the system with respect to all the electrons.

with respect to which the antisymmetrization is performed have large radial quantum numbers, i.e., this picture is more or less suitable for medium and especially heavy nuclei. But in the case of light nuclei such as ^{7}Li, and *a fortiori* for the very large class of nuclear processes in which deuterons, tritons, and α particles participate, the notion of a local Pauli-repulsive core is simply false.

This is already indicated by the traditional optical model, which successfully describes the scattering of deuterons, tritons, and α particles by means of the smooth attractive Woods–Saxon potential with appreciable depth $V_0 \approx 80$–100 MeV. Therefore, the phenomenological potentials with repulsive core for the interaction of light clusters (for example, for the $\alpha\alpha$ system) that were proposed and widely used in the fifties and sixties already appear inadequate from this point of view. As we have already said, the main ideas about the nature of these interactions were deduced on the basis of calculations by means of the resonating-group method, especially those from the pioneering work of Okai and Park.[36] They were the first to point out the importance of taking into account the spurious solutions of the equations of the resonating-group method and the close correspondence between the scattering wave functions (i.e., the wave functions of the relative motion) and the shell model. It also became clear from their paper that in systems such as the $\alpha\alpha$ system (and ones like it) the Pauli principle is manifested, not through damping of the wave function in the region of overlap of the particles (as simulated by a replusive core), but through the shell nature of the oscillations of this function. Moreover, the characteristic oscillations appear only after the elimination of the so-called spurious (or redundant) solutions of the resonating-group equations, these spurious solutions being the states forbidden by the Pauli principle. Bringing together all these ideas about the interaction of composite particles (including the orthogonality-condition model), we succeeded in 1971 in formulating a simple and physically perspicuous approach to the description of the interaction of light composite particles on the basis of a microscopically derived optical potential with forbidden states.[37,38]

The idea of this approach is based on the well-known fact that for Hermitian Hamiltonians the scattering wave functions are orthogonal (at all energies) to the functions of the discrete spectrum. Therefore, if one constructs a sufficiently deep local potential whose lower states correspond to the states forbidden by the Pauli principle, i.e., correspond to eigenfunctions of the antisymmetrization kernel, the required orthogonality of the scattering functions to the forbidden states will be ensured automatically.

And since the structure of the forbidden states can be extracted readily from the shell model, *bypassing the resonating-group method*, the actual procedure for constructing the optical potential with forbidden states includes the following elements: 1) analysis of the forbidden states in the given system on the basis of the shell model; 2) construction of the corresponding local potential containing these states as its bound states; 3) refinement of the parameters of the potential by fitting to the experimentally known phase shifts.

We shall now illustrate how this approach is realized for specific cases. For example, let us again take the $\alpha\alpha$ system. In shell language, the lowest forbidden configurations are s^8 ($L = 0$) and s^6p^2 ($L = 0, 2$),[5)] zero oscillator quanta corresponding to the s^8 configuration and two to s^6p^2. Therefore, the lowest allowed configuration, corresponding to the ground state of the ^{8}Be nucleus, is the configuration $s^4p^4(L = 0, 2, 4)$ with four excitation quanta. When such a configuration is broken up into two unexcited α particles (each having the configuration s^4) the excitation energy $E^* \sim 4\hbar\omega \sim 60$–$70$ MeV goes over into the kinetic energy of the relative motion of the α clusters in their overlap region. It is therefore clear that the local potential simulating the shell picture described above must be sufficiently deep and broad to accommodate the $0S$, $2S$, and $2D$ forbidden states (the last two are degenerate in the oscillator potential) and the $4s$ allowed state corresponding to the ^{8}Be ground state. Simple estimates immediately give the following parameters of the potential: depth $V_0 \approx$ 120 MeV, width $R \approx 1.7$ F. Subsequent improvement of the parameters on the basis of the observed $\alpha\alpha$ phase shifts leads to the following parameters of the potential in the Woods–Saxon form:

$$V_0 = 125 \text{ MeV}; \quad R = 1.78 \text{ F}, \quad a = 0.66 \text{ F}. \tag{46}$$

The theoretical and experimental $\alpha\alpha$ phase shifts are compared in Fig. 4. The corresponding elastic scattering cross sections are shown in Fig. 5. It can be seen that the very simple l-independent three-parameter potential describes well the five phase-shift curves in a wide energy range, and also the energy of the 0^+ ground state of ^{8}Be (96 keV). Figure 6 shows

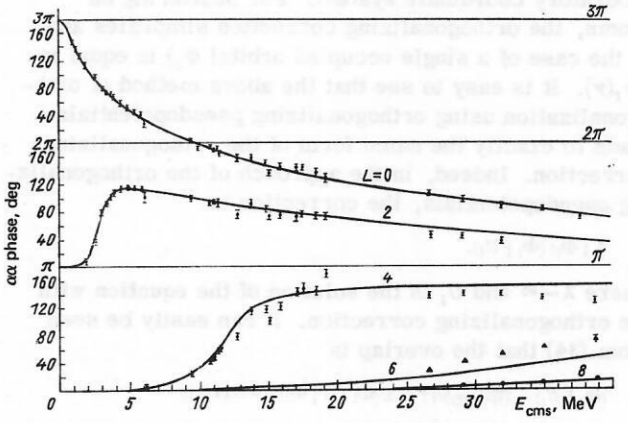

FIG. 4. Comparison of theoretical and experimental $\alpha\alpha$ phase shifts for $L = 0$, 2, 4, 6, 8. Along the ordinate, we have used the calibration that follows the generalized Levinson theorem (with allowance for forbidden states). The theoretical phase shifts are the phases for the $\alpha\alpha$ optical potential with forbidden states (46).

[5)]Because the two α particles are identical and have zero spin, only even angular momenta $L = 0, 2\ldots$, are allowed in the $\alpha\alpha$ system.

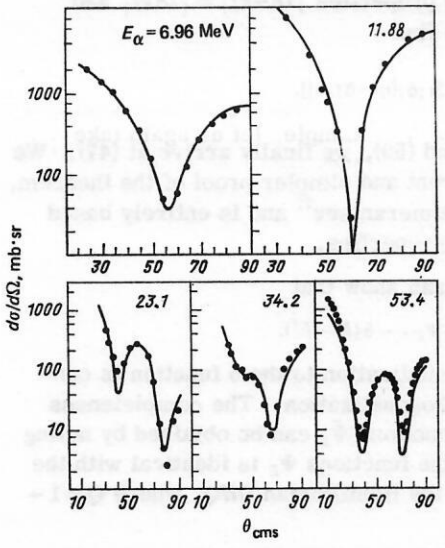

FIG. 5. Differential cross sections of $\alpha\alpha$ scattering at different energies calculated with the potential (46). At $E_\alpha = 53.4$ MeV there is added a volume absorbing potential with the same geometrical parameters as for the real part and depth $W = 5$ MeV.

the potential well of the optical potential with forbidden states, and its levels. It can be seen that the states $2S-2D$ are almost degenerate and that the distance between the levels $2S$ and $0S$, $\Delta E \approx 36$ MeV, agrees well with the excitation energy $2\hbar\omega = 18$ MeV, which is characteristic of the free α particles, i.e., taken as whole, the picture of the potential levels agrees well with the oscillator shell model. It remains to add that the parameters were fitted by means of the phase shifts, *and the structure of the discrete spectrum was obtained automatically*. This shows that the described potential approach to the scattering of clusters leads, in contrast to the standard phenomenological fits in nuclear physics, to an internally consistent physical picture in good agreement with the shell model. We mention one further important aspect

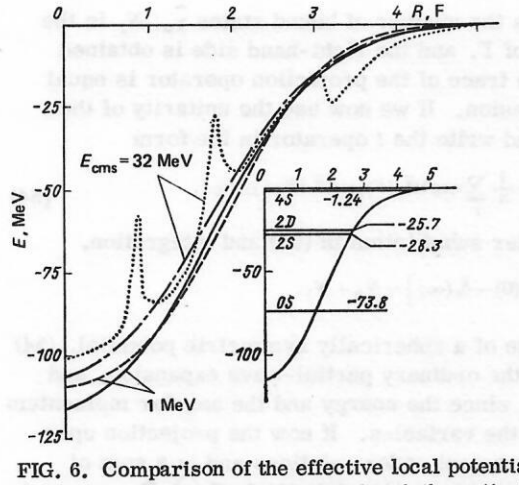

FIG. 6. Comparison of the effective local potentials derived from the resonating-group method with the optical $\alpha\alpha$ potential (46) for two energies in the center-of-mass system. The continuous curve is the Woods–Saxon potential with the parameters (46); the remaining curves are effective local resonating-group potentials. The insertion in the lower right shows the position of the $\alpha\alpha$ forbidden states.

of the use of such microscopically derived potentials which is related to Levinson's theorem (for details, see the following section). The point is that optical potentials with forbidden states automatically lead to a generalization of Levinson's theorem with allowance for the forbidden states, since they occur here on an equal footing with the allowed states, and the fact that the forbidden states are physically unrealizable must be taken into account only off the mass shell.

A similar analysis was made for the majority of light-particle pairs αd, t^3He, dt, etc., and optical potentials were obtained that give a very good description (with a small number of parameters) of the experimental phase shifts and cross sections (for the details, see Refs. 37–40); moreover, the structure of the scattering wave functions and the discrete spectrum is in complete agreement with the shell model for all the considered systems. Subsequent investigations[6,41] revealed that the microscopically derived interaction potentials found in this manner are phase-shift-equivalent to the nonlocal interactions that are used in the resonating-group method and the orthogonality-condition model.

We should, however, point out that this correspondence ence is good only for light cluster systems such as $\alpha\alpha$ and the like, whereas for the scattering of heavy ions for example, $^{12}C + {}^{12}C$, $^{16}O + {}^{12}C$, an optical potential of this kind has little meaning for two reasons. The point is that in the rigorous theory of phase-shift-equivalent optical potentials[34] these potentials must depend on the energy (even if the original nonlocal potential is static) And the weak energy dependence found for the light systems probably reflects the fact that the nonlocality of the potential is very slight. This is also indicated by comparison of the wave functions in the region of overlapping of the particles, i.e., the slight difference of the suppression factor $A(k, r)$ from unity.[42] This last is not the case for scattering of heavy ions, which is indicated in the first place (and also by general physical considerations) by the strong suppression of the scattering wave functions in the inner region.[42] Under these conditions, and bearing in mind the important circumstance that the imaginary part of the potential is no longer small (essentially, the imaginary part screens the entire inner region), so that the nature of the oscillations of the scattering wave function in the inner region is no longer particularly significant, it is expedient to give up a local potential consistent with the shell model and go over to a phenomenological potential that describes satisfactorily the experimental data and leads to smooth solutions (without frequent oscillations due to the Pauli principle in the overlap region) which are damped in the inner region. There is no need to say that such optical potentials must be shallow. Such shallow potentials are usually employed to describe scattering of heavy ions such as $^{16}O + {}^{16}O$. From the point of view of the correspondence with the true phase-shift-equivalent potentials, these phenomenological shallow potentials are typical model pseudopotentials and are very similar to the ones used in solid-state theory to calculate band structure.[43]

Generalization of Levinson's Theorem to Scattering of Composite Particles. In any microscopic approach to the interaction of composite particles, the interaction potential is nonlocal (and, in general, energy dependent). Since the most general case of a nonlocal, energy-dependent interaction is too complicated for analytic treatment, the results given below apply, strictly speaking, to models for which an analytic investigation is possible. Swan[44] was the first to suggest a generalization of Levinson's theorem to composite particles (in both atomic and nuclear physics). Taking the example of a particular form of the exchange potentials in the framework of the resonating-group approach, he showed that the forbidden states must be included in Levinson's theorem on an equal footing with the physically observed allowed bound states, so that the generalized Levinson theorem must have the form

$$\delta_l(0)-\delta_l(\infty)=\pi(n+m), \tag{47}$$

where n is the number of allowed bound states and m is the number of forbidden states in the l-th partial wave. Chronologically, the latest proof is due to Glockle and Le Turneux,[45] who proved Eq. (47) for the orthogonality-condition model. Their proof is a direct generalization of the standard proof of this theorem based on the analytic behavior of the Jost function of the problem in the upper half-plane, Im $k \geq 0$.[46]

Briefly, their proof is as follows. Let $G(E)$ be the Green's function corresponding to the left-hand side of Eq. (31); $f_0(k)$ is the corresponding Jost function. Then the function

$$D(k)=f_0(k)\det[G_{\alpha\beta}(E)]\equiv f_0(k)\,g(k)$$

($[G_{\alpha\beta}(E)]$ is the matrix composed of the elements $\langle\chi_\alpha|G(E)|\chi_\beta\rangle$) is the Fredholm determinant of the integral equation corresponding to the Schrödinger equation (31). Further, one can show that the zeros of $D(k)$ are directly related to the poles of the total S matrix, and the argument of $D(k)$ is equal to the phase shift $\delta(k)$ in the orthogonality-condition model, i.e.,

$$D(k)=|D(k)|\exp[-i\delta(k)];$$

$D(k)$ is not equal to the total Jost function of the problem, but differs from it by a factor $\Delta(k^2)$. Considering then the analytic properties of the matrix elements $G_{\alpha\beta}(k)$ in the upper half-plane, Glockle and Le Turneux show that

$$g(k)\underset{k\to\infty}{\Rightarrow}(1/k^{2n})[1+O(1/k^2)],\qquad \operatorname{Im}k>0, \tag{48}$$

where n is the number of states forbidden by the Pauli principle. But since the original Jost function satisfies $f_0(k)\to 1$ as $k\to\infty$, $D(k)\to g(k)$ in this limit. If now there are on the upper k half-axis m zeros of $D(k)$ corresponding to physical bound states, we have the standard contour integral[46]

$$\frac{1}{2\pi i}\int\frac{1}{D(k)}\frac{dD}{dk}\,dk=m. \tag{49}$$

But because of the property (48), the integral over the upper semicircle is

$$\int_C -\frac{2n}{k^{2n+1}}\left(\frac{1}{k^{2n}}\right)^{-1}dk=-2\pi i n. \tag{50}$$

Using further the properties $|D(-k)|=|D(k)|$ and $\delta(-k)=-\delta(k)$, we find

$$\int_{-\infty}^{\infty}dk\,\frac{d\ln D(k)}{dk}=2i[\delta(0)-\delta(\infty)],$$

and, using (49) and (50), we finally arrive at (47). We give here a different and simpler proof of the theorem, which is due to Pomerantsev[27] and is entirely based on completeness properties.

Using (35), we can show that

$$\langle\tilde\Psi_E|\tilde\Psi_{E'}\rangle=\langle\Psi_E|\Psi_{E'}\rangle\sim\delta(E-E'),$$

i.e., that the normalization to the δ function is conserved by the orthogonalization. The completeness relation for the functions $\tilde\Psi_E$ can be obtained by noting that the basis of the functions Ψ_E is identical with the eigenfunctions of the Hamiltonian QHQ, where $Q=1-\Gamma$. Therefore

$$\int|\tilde\Psi_E\rangle\langle\tilde\Psi_E|\,dE+\tilde P_B=1-\Gamma, \tag{51}$$

where $\tilde P_B=\sum_\alpha|\tilde\chi_\alpha\rangle\langle\tilde\chi_\alpha|$ is the projection operator onto the bound states of the pseudo-Hamiltonian $\tilde H=H+\lambda\Gamma$, and $|\tilde\chi_\alpha\rangle$ are also eigenfunctions of QHQ. Since $\Gamma\tilde P_B=\tilde P_B\Gamma=0$, it follows that $\tilde P_B+\Gamma$ is the total projection operator onto the complete discrete spectrum of the operator QHQ. It is then necessary to introduce the Møller operator

$$\tilde\Omega=\int_0^\infty dE\,|\tilde\Psi_E\rangle\langle\Psi_{0_E}|,$$

which maps the continuum of the Hamiltonian H_0 isometrically onto the continuum of $\tilde H$ (or QHQ, which is the same). From (51), we deduce

$$\tilde\Omega^*\tilde\Omega-\tilde\Omega\tilde\Omega^*=\tilde P_B+\Gamma. \tag{52}$$

Further following Jauch's method,[47,48] we take the trace of Eq. (52) and express the trace of the left-hand side in terms of the t matrix on the mass shell:

$$i\pi\int_0^\infty dE\,\mathrm{Sp}\left\{\tilde t^*\frac{\partial\tilde t}{\partial E}-\tilde t\frac{\partial\tilde t^*}{\partial E}\right\}=\tilde N_B+N_\Gamma, \tag{53}$$

where $\tilde N_B$ is the number of bound states $\tilde\chi_\alpha$; N_Γ is the dimension of Γ, and the right-hand side is obtained because the trace of the projection operator is equal to its dimension. If we now use the unitarity of the t operator and write the t operator in the form

$$\tilde t(E)=-\frac{1}{\pi}\sum_l\exp[i\tilde\delta_l(E)]\sin\tilde\delta_l(E)\,|\chi_l\rangle\langle\chi_l|, \tag{54}$$

we find, after substitution in (53) and integration,

$$\frac{1}{\pi}\left[\sum_l\tilde\delta_l(0)-\tilde\delta_l(\infty)\right]=\tilde N_B+N_\Gamma.$$

In the case of a spherically symmetric potential, (54) reduces to the ordinary partial-wave expansion, and $|\chi_l\rangle\langle\chi_l|=1$, since the energy and the angular momentum exhaust all the variables. If now the projection operator Γ is invariant under rotations and is a sum of projection operators with definite l, $\Gamma=\sum\Gamma_l$, we readily obtain

$$(1/\pi)[\delta_l(0)-\delta_l(\infty)]=\tilde N_{B_l}+N_{\Gamma_l}.$$

It is easily seen that the proof does not use explicitly

the analytic properties of the solutions for complex k, but is entirely based on the unitarity of the t matrix and the completeness properties of the basis in the truncated space. We add that when an optical potential with forbidden states is used the generalized Levinson theorem is satisfied automatically. As regards the practical value of the theorem, it consists in predicting large elastic phase shifts at high energies for the systems in which there are many forbidden states but the number of allowed bound states is usually small. In particular, large elastic phase shifts were predicted in Refs. 37 and 39 for $\alpha\alpha$ scattering at energies $E_{\mathrm{rel}} \approx 200-400$ MeV in the center-of-mass system. To test these predictions, elastic scattering in the $\alpha\alpha$ system at $E_{\alpha\ \mathrm{lab}} \approx 600-800$ MeV was studied in the experiments of Ref. 49. An appreciable elastic cross section of nondiffraction nature was found. However, if final conclusions are to be drawn, we require a theory (not yet developed) of the interaction of composite particles at intermediate energies $E_\alpha \approx 0.5$ GeV.

Model System of the Interaction of Two Clusters. Resonating-group method equation for the 2+2 system. We analyze how the general features of the interaction of composite systems of fermions are manifested for the example of a model system consisting of two identical clusters. Each cluster is, in its turn, composed of two particles with masses M and m. We shall call it a 2+2 system. The advantage of this model system is that it is sufficiently simple for one to be able to calculate all the integral kernels of the resonating-group method and investigate their properties. At the same time, it is sufficiently complicated to have nontrivial properties and be of physical interest.

The $m+M$ cluster can be regarded as, for example, consisting of a nucleon m and a heavy core M. The distinctive feature of the system is that for $M=m$ it is identical with the bineutron–bineutron system, which is a system of two clusters with closed shells, i.e., it is similar to the $\alpha\alpha$ system. In the limit $M \gg m$, it becomes similar to the hydrogen molecule. This model problem is convenient in that, by varying the mass ratio $y=M/m$, one can follow in detail the evolution of the system and understand at the microscopic level how the Pauli principle is manifested in different limiting cases. Direct comparison of the cumbersome equations of the resonating-group method for $\alpha\alpha$ and $^{16}O^{16}O$, for example, would be not very effective.

We shall consider the state of the 2+2 system in which the spatial wave function is antisymmetric under transposition of the two particles with mass M (numbered 1 and 3) and also of the pair of particles with mass m (numbered 2 and 4), i.e., the system has a structure like that of orthohydrogen in the triplet state. To simplify the calculations, we use a wave function of the form

$$\varphi(\mathbf{r}_{12}) = (\alpha/\pi)^{3/4} \exp(-\alpha r_{12}^2/2) \tag{55}$$

to describe each cluster ("hydrogen pseudoatom") and a Gaussian interaction between all four particles:

$$V_{ij} = -V_0 \exp(-\gamma r_{ij}^2). \tag{56}$$

We shall solve the problem of the scattering of such clusters in the single-channel approximation of the resonating-group method. The wave function of the system is sought in the form

$$\Psi = (1-P_{13})(1-P_{24})\varphi(\mathbf{r}_{12})\varphi(\mathbf{r}_{34})\Phi(\boldsymbol{\rho}), \tag{57}$$

where $\boldsymbol{\rho} = (y\mathbf{r}_1 + \mathbf{r}_2 - y\mathbf{r}_3 - \mathbf{r}_4)/(y+1)$, $y = M/m$. The equation for the wave function $\Phi(\boldsymbol{\rho})$ of the relative motion of the clusters is written in the form

$$\langle \varphi(\mathbf{r}_{12})\varphi(\mathbf{r}_{34}) \mid H-E \mid (1-P_{13})(1-P_{24})\varphi(\mathbf{r}_{12})\varphi(\mathbf{r}_{34})\Phi(\boldsymbol{\rho})\rangle = 0. \tag{58}$$

Bearing in mind that the cluster $m+M$ as a whole is a boson, we require $\Phi(\boldsymbol{\rho})$ to be an even function of $\boldsymbol{\rho}$. Equation (58) then takes the form

$$(T + V_D - K - E)\Phi(\boldsymbol{\rho}) = 0. \tag{59}$$

Here, V_D is the direct interaction of the clusters, and the integral exchange kernel $K = K_T + K_V + EK_0$ includes contributions from the kinetic, K_T, and potential, K_V, energies and the integral overlap kernel K_0. The explicit form of the nonlocal terms K_0, K_T, K_V and the direct interaction V_D is given in Ref. 50.

In accordance with the results of the preceding subsection, the eigenfunctions of the overlap kernel

$$K_0 = (\alpha/2\pi)^{3/2}(1+y)^6(2y)^{-3} \times \exp\{-[\alpha(y+1)^2/8y^2][y^2(\boldsymbol{\rho}-\boldsymbol{\rho}')^2 + (\boldsymbol{\rho}+\boldsymbol{\rho}')^2]\} \tag{60}$$

are the wave functions $\Phi_{nlm}(\boldsymbol{\rho})$ of a three-dimensional harmonic oscillator, and we have the eigenvalue[50]

$$\lambda_n = (y-1)^n/(y+1)^n \approx \exp[-2n/(y+1)], \quad n \text{ even}. \tag{61}$$

It is clear from this that in the 2+2 system at all values of y there is only one truly forbidden state $0s(n=l=0)$. The spectrum of the eigenvalues λ_m is interesting. For $y=1$, only one state is forbidden, the remaining values $\lambda_m = 0$ corresponding to allowed states. For $y \neq 1$, instead of an abrupt change of λ_n from 1 to 0 there is a smooth exponential transition between these limiting values. The states with $0 < \lambda_n < 1$ in this transition region can be called half-forbidden.

The limiting case $y \gg 1$ is interesting. In this case, the integral kernels of the resonating-group method in (59) become almost local. A measure of the nonlocality is the width of the spread of the kernels with respect to the variable $\boldsymbol{\rho} - \boldsymbol{\rho}'$. It can be seen from (60) that at large y we can write for the kernel K_0

$$K_0 f(\boldsymbol{\rho}) \approx \exp[-(\alpha/2)\rho^2] f(\boldsymbol{\rho}). \tag{62}$$

The remaining kernels of the resonating-group method can be reduced similarly to a local form. If this procedure is carried out, it is found that all the kernels acquire the form characteristic of the exchange terms in the Heitler–London method.[51] In this method, the distance between the heavy particles 1 and 3 is fixed, and the wave function of the light particles is composed of the orbitals φ relative to the two heavy centers 1 and 3:

$$\Psi \sim (1/\sqrt{2})[\varphi_1(\mathbf{r}_2)\varphi_3(\mathbf{r}_4) - \varphi_3(\mathbf{r}_2)\varphi_1(\mathbf{r}_4)], \tag{63}$$

where

$$\varphi_1(\mathbf{r}_j) = (\alpha/\pi)^{3/4} \exp[-(\alpha/2)(\mathbf{r}_j - \rho/2)^2];$$
$$\varphi_3(\mathbf{r}_j) = (\alpha/\pi)^{3/4} \exp[-(\alpha/2)(\mathbf{r}_j + \rho/2)^2].$$

Direct calculation of the overlap integral gives

$$S(\rho) = \int d\mathbf{r}_1 d\mathbf{r}_2 \varphi_1(\mathbf{r}_2)\varphi_3(\mathbf{r}_4)\varphi_3(\mathbf{r}_2)\varphi_1(\mathbf{r}_4) = \exp\left(-\frac{\alpha}{2}\rho^2\right), \quad (64)$$

which agrees with the local form (62) of the kernel K_0. Similarly, we find that the expectation value of the operator $H - E$ with respect to the function (63) is equal to the left-hand side of the resonating-group equation (58) in the limit of large y. Thus, we have shown that when one of the particles M of the cluster is much heavier than the second particle m, i.e., when we approach the situation characteristic of molecules, the resonating-group equation goes over naturally into the equation of the Heitler–London method based on the Born–Oppenheimer adiabatic approximation. This equation has the form

$$[1 - S(\rho)]^{-1} \langle \varphi_1(\mathbf{r}_2)\varphi_3(\mathbf{r}_4)|H - E| \times |\varphi_1(\mathbf{r}_2)\varphi_3(\mathbf{r}_4) - \varphi_3(\mathbf{r}_2)\varphi_1(\mathbf{r}_4)|\rangle f(\rho) = [-(\hbar^2/M)\Delta_\rho + V_T(\rho) + V_L(\rho) + V_{13}(\rho) - E] f(\rho) = 0. \quad (65)$$

Here,

$$V_T(\rho) = \hbar^2\alpha\rho^2 \exp(-\alpha\rho^2/2)/4m\,[1 - \exp(-\alpha\rho^2/2)]$$

is the repulsive potential that reflects the increase in the kinetic energy of the light fermions in the overlap region of the clusters. As $\rho \to 0$, $V_T(\rho) \to \hbar\alpha/2m = \hbar\omega/2$, which is equal to the excess kinetic energy of the light fermions in the combined system, in which they occupy the oscillator orbits $1s$ and $1p$, as compared with their kinetic energy at large distances ρ, where they are each in the $1s$ orbit around their respective centers. The potential $V_L(\rho)$ is due to the interaction of the light particles with the heavy particles and with each other; $V_{13}(\rho)$ is the direct interaction of the heavy particles 1 and 3. Of course, the above treatment is schematic and reflects only the behavior of the contributions to the interaction potential between the heavy ions that correspond to the exchange of a small number of nucleons between the colliding particles. (However, such exchanges are evidently the most important.)[52] Nevertheless, the results of Refs. 41 and 50 quoted above indicate (and similar conclusions are drawn in Ref. 53) why the scattering of sufficiently heavy ions can be reproduced by optical potentials with repulsion of the type of the interatomic potentials in a molecule[54-57] and why methods like the molecular orbital–linear combination of atomic orbitals (MO-LCAO) method are effective in the theory of heavy ions.[58]

The situation is different for $y \sim 1$, when the nonlocality of the potential cannot be ignored. Below, we shall consider this case in more detail.

The bineutron-bineutron system. We investigate a model system in which there are only forbidden and allowed states ($y = 1$). Half-forbidden states (including the case of the 2+2 system) are analyzed in Refs. 18 and 59–62. We consider the scattering of a bineutron (with spin $S = 0$) by a bineutron. As a whole, this system in the lowest state corresponds to the shell configuration s^2p^2 and has the one forbidden state

$$\Phi_0(\rho) = (2\alpha/\pi)^{3/4} \exp(-\alpha\rho^2). \quad (66)$$

As usual in the resonating-group method, we take the effective interaction of the nucleons in the form[63]

$$V(\mathbf{r}) = -V_0(W + MP^x)\exp(-\gamma r^2). \quad (67)$$

The direct potential V_D in (59) has the form

$$V_D(\rho) = -V_0[2\alpha/(2\alpha+\gamma)]^{3/2}(4W - 2M)\exp(-2\alpha\gamma\rho^2/(2\alpha+\gamma)), \quad (68)$$

and the exchange kernel $K(\rho, \rho')$ includes several terms the exchange integrals for the kinetic and the potential energy and the overlap integral K_0. The S-wave solution of Eq. (59) is not necessarily orthogonal to the function Φ_0. However, physical meaning attaches to only the projected function $\tilde{\Phi}(\rho)$, which is orthogonal to $\Phi_0(\rho)$, i.e.,

$$\tilde{\Phi}(\rho) = P_0\Phi(\rho), \quad (69)$$

where the projection operator $P_0 = 1 - |\Phi_0\rangle\langle\Phi_0|$ separates only the allowed states of the system. We shall therefore investigate the resonating-group equations on the basis of the functions $\tilde{\Phi}(\rho)$.

Using the operator P_0, we can rewrite the Schrödinger equation (59) for our system in the form

$$P_0(T_\rho + V_D + V_N - E)P_0\Phi(\rho) = 0, \quad (70)$$

with the nonlocal exchange correction

$$V_N\Phi(\rho) = -V_0(4M - 2W)(2\alpha/\pi)^{3/2} \times \int d\rho' \exp\left[-2\alpha\left(\frac{\rho+\rho'}{2}\right)^2\right] \times \exp\left[-\left(\frac{\alpha}{2} + \gamma\right)(\rho - \rho')^2\right]\Phi(\rho'). \quad (71)$$

It follows from (70) that on the transition from a function tion Φ of arbitrary form to the orthogonalized functions $\tilde{\Phi} = P_0\Phi$ all the nonlocal kernels (except V_N) are annihilated. In a more complicated system, of course, this will not occur, but some of the nonlocal kernels will undoubtedly disappear. Equation (70) can be rewritten in the form

$$(T_\rho + V_D + V_N - E)\tilde{\Phi}(\rho) = 0 \quad (72)$$

with the additional condition

$$\langle\Phi|\Phi_0\rangle = 0. \quad (73)$$

The relation (72) shows that the neglect of several nonlocal kernels in (59) is compensated by the orthogonality condition (73). From the energy point of view, this last means that the contribution of these terms of the Hamiltonian is transformed into the extra kinetic energy corresponding to the oscillating function $\tilde{\Phi}$.

It can be seen from (71) that for $\alpha \gg \gamma$, when the radius of the clusters is much less than the range of the NN forces, and when allowance is made for the orthogonality condition (73), the contribution of the integral kernel V_N is zero, since $V_N \to K_0$ for $\gamma \ll \alpha$.

In the opposite case $\gamma \gg \alpha$, the exchange correction V_N is transformed into the local potential

$$U_N(\rho) = -V_0(4M - 2W)(2\alpha/\gamma)^{3/2}\exp(-2\alpha\rho^2),$$

and, as a whole, the sum $U_{\text{eff}} = V_D + U_N$ appears as the effective local potential

$$U_{\text{eff}} = -2V_0 (2\alpha/\gamma)^{3/2} \exp(-2\alpha\rho^2).$$

Despite the fact that V_D can be repulsive for $M > 2W$, U_{eff} is an attractive potential and does not depend on the ratio of the forces in the even and odd orbital states.[64] Thus, already our simplest schematic examples show that the potential U_{eff} can differ strongly from the potential V_D. In the general case, when $\gamma \sim \alpha$, the potential V_N is essentially nonlocal and plays an appreciable part. However, under these conditions too one can construct a local, E-dependent optical potential $U_{\text{opt}}(\rho)$ equivalent to the nonlocal potential U_{eff} both from the point of view of the phase shifts and the point of view of the number of nodes of the function $\tilde{\Phi}(\rho)$ and their positions. When this potential is used, Eq. (70) takes the form

$$P_0 (T + U_{\text{eff}} - E) P_0 \Phi(\rho) = 0. \tag{74}$$

For the 2 + 2 system, it is the exact equivalent of the equations of the resonating-group method. However, as is shown in Secs. 2 and 5, it is a good approximation to these equations in more complicated cases as well. In practical calculations in accordance with the orthogonality-condition model, one frequently uses V_D instead of U_{eff}, which is not always justified, as can be seen from our investigations.

Calculation of Equivalent Local Potentials by the Buck-Perey Method. It was shown above that in the resonating-group method the Schrödinger equation for the relative motion of the clusters contains, in addition to the direct local interaction V_D, nonlocal terms. Unfortunately, the scattering problem for nonlocal potentials has not been studied nearly as well as for local potentials. Therefore, the concepts deduced from the experience with local potentials are more familiar and one is naturally led to attempt to replace a nonlocal potential by a local one that is equivalent in, for example, the sense of describing the phase shifts. Of course, this equivalent local potential cannot be an ordinary local potential; it will necessarily depend on the energy E and probably also on the angular momentum l. The eigenfunctions of the equivalent local potential and the nonlocal potential need not be identical in the whole of space (the Perey effect).[65] Therefore, equivalent local potentials have limited value and do not give a complete picture of the properties of the system. However, they are very helpful for understanding qualitative features. Moreover, in nuclear physics the experimental data on the scattering of clusters by clusters and by heavier nuclei are usually interpreted by means of local optical potentials.

There exists a rigorous method for constructing an equivalent local potential for a given nonlocal interaction; it was developed by Coz, Arnold, and McKellar.[34] However, it suffers from the shortcoming that before one obtains the equivalent local potential it is necessary to solve a complicated Schrödinger equation with the nonlocal potential. But then the equivalent local potential is actually no longer necessary and can serve only for illustrative purposes. It is much more important to develop an approach that makes it possible to find at least approximately the equivalent local potential directly from the nonlocal potential without solving the Schrödinger equation for the latter. Such methods exist, though they are approximate. As an example, we can take the method of Buck and Perey,[64,65] who showed that if there is a system described by the Schrödinger equation

$$\left[\frac{\hbar^2}{2\mu}\nabla^2 - V_D + E\right]\psi_N(\mathbf{R}) = \int U_N\left(\frac{\mathbf{R}+\mathbf{R}'}{2}\right)\frac{\exp[-(\mathbf{R}-\mathbf{R}')^2\beta^2]}{\pi^{3/2}\beta^3}\psi_N(\mathbf{R}')\,d\mathbf{R}', \tag{75}$$

then when $U_N(\mathbf{R})$ varies smoothly and the derivatives of the potential can be ignored compared with the derivatives of $\Psi_N(\mathbf{R})$ (we recall that in problems of cluster scattering we encounter rapidly oscillating functions $\Psi(\mathbf{R})$ which are orthogonal to the forbidden states, and therefore such an assumption is perfectly reasonable), Eq. (75) can be reduced approximately to the form

$$[(\hbar^2/2\mu)\nabla^2 + E - V_D]\psi_N(\mathbf{R}) = V_L'\psi_N(\mathbf{R}), \tag{76}$$

where V_L' is obtained from the transcendental equation

$$V_L'(R) = \exp[(\mu\beta^2/2\hbar^2)(V_L' + V_D - E)]\,U_N(R). \tag{77}$$

The total equivalent local potential for (75) is

$$V_L = V_D + V_L'. \tag{78}$$

Of course, the Buck–Perey procedure is not at all rigorous, since it is assumed that $\Psi_N = \Psi_L$ (neglect of the Perey suppression factor) and that the gradients of the potentials $U_N(R)$ and $V_L'(R)$ are small. Therefore, it probably cannot reproduce fine details of the true equivalent local potential. However, it gives the correct result $V_L'(R) \approx U_N(R)$ in the limit of a short nonlocality range β and is very effective in practical calculations (see Ref. 64, in which equivalent local potentials were found for scattering of 14-MeV neutrons by ^{56}Fe). In Eq. (75), a nonlocality of a special Gaussian form is chosen. This is convenient for treating cluster systems, in which integral kernels of Gaussian type are encountered. However, the Buck–Perey procedure can be generalized to more complicated systems. For example, in Ref. 67 the Buck–Perey method was successfully used to obtain an equivalent local potential for scattering of an electron by the hydrogen atom. We shall apply the Buck–perey method to the potential V_N for the bineutron–bineutron system. This can be done, since the potential V_N in (71) corresponds to the type of potential treated in this method. It is important to know that the local potential V_L equivalent to V_N, being E-dependent, is the same for all the four values of the orbital angular momentum l of the clusters that we consider. We use the customary[62] parameters of the NN forces:

$$V_0 = 73 \text{ MeV}; \quad \gamma = 0.46 \text{ F}^{-2} \quad ; \quad W = M = 0.5 \tag{79}$$

and $\alpha = 0.22$ F^{-2}, which corresponds approximately to the minimal internal energy of a cluster for the interaction (67). Then the Buck–Perey procedure (77)–(78) in conjunction with the functions

$$V_D(R) = -V_{0D}\exp(-\varkappa_1 R^2); \quad U_N(R) = -U_{0N}\exp(-\varkappa_2 R^2)$$

leads to the phase-shift-equivalent local potential $V_L(R)$, which can be approximately represented by the

Woods–Saxon potential with the parameters

$$V_0 = 50 \text{ MeV}; \quad R_0 = 1.5 \text{ F}; \qquad a = 0.6 \text{ F}.$$

In this potential, there is a forbidden $0S$ state with binding energy ~9 MeV. If we take the Gaussian $\exp(-\delta R^2)$ as the trial function of this state, a minimum of the energy is attained at $\alpha = 0.20$ F^{-2} for the wave function (66) of the forbidden state. Therefore, the orthogonality condition (73) is satisfied automatically. Such a situation is found for all optical potentials of cluster–cluster scattering of the type $\alpha\alpha$, αt, αd, etc.[38]

For the energy dependence of the phase-shift-equivalent potential V'_L at low energies, we obtain

$$V'_{0L}(E) \approx V'_{0L}(E=0)\exp(-E/E_0),$$

where $E_0 = 84$ MeV. For the optical potential $V(R) = V_D(R) + V'_L(R)$, the energy dependence of the well depth V_0 in the region of comparatively low energies $E < E_0$ has the form

$$V'_0(E) \approx V_0 - (1/4)E,$$

which is close to that usually employed in the nuclear optical model and which we obtained from analysis of the E dependence of the optical potentials for different pairs of clusters.[37,38]

In Ref. 41, an equivalent local potential was obtained for the bineutron–bineutron system for the Brink–Boiker NN forces, which contain repulsion at short distances. The obtained equivalent local potential was found to be very close to the one described above for the equivalent local potential between clusters was noted by Tamagaki[63] in an investigation of the $\alpha\alpha$ system. This property is apparently a general property of cluster systems. In Ref. 41, the S-wave phase shift was also calculated for the obtained equivalent local potential of the bineutron–bineutron system, and the result is in reasonable agreement with the results of exact calculations in the resonating-group method for the same system.[42] In calculations by the Buck–Perey method, no allowance is made for the Perey suppression factor. It can be estimated in accordance with a simple formula obtained for potentials of the type (75)–(78) by Fiedeldey[70]; $A(\rho) \approx \exp[-(m\beta^2/8\hbar^2)V_L]$, which for our system gives $A(\rho) \sim 0.8$ near $\rho = 0$. Therefore, the suppression factor can be ignored in our case in a first approximation.

4. APPLICATION OF THE FORMALISM OF THE FADDEEV EQUATIONS TO A SYSTEM OF THREE COMPOSITE PARTICLES

We point out first that a system of three composite particles is a convenient model for the entire theory of direct nuclear reactions, in which one or even two particles can be elementary (for example, in dp reactions), or all three particles composite [for example, in reactions of the type (^{7}Li, α) with lithium ions]. In addition, light nuclei such as ^{6}Li, ^{9}Be, ^{12}C, ^{24}Mg, and others can be handled with great success in the framework of a three-particle model of the type $^6\text{Li} \to \alpha np$, $^9\text{Be} \to \alpha\alpha n$, $^{12}\text{C} \to 3\alpha$, etc., where at least one of the particles is composite. And if the discrete spectrum in such systems can also be calculated by means of variational methods, the most reliable basis for treating a structurally rich continuum (and quasidiscrete spectrum) is provided by the Faddeev integral equations, which have already been used more than once for this purpose.[71]

Review of Results so Far Obtained. We note first of all the pronounced discrepancy in this region between the generality of the proposed three-body approaches (generalized Faddeev equations) and the extent to which they can be realized in practice. In this respect, the problem of three composite particles lags far behind the three-nucleon problem, in which virtually all the so far proposed methodological treatments have been exploited in practice and there are in addition several three-particle calculations with complete allowance for all the physically important states of the $3N$ system and all components of the NN potential (up to angular momentum value $J = 2$).[6)]

In the problem of three composite particles, all the necessary generalizations of the three-particle formalism have been implemented theoretically. In particular, in the first of the papers of Ref. 71, modified Faddeev equations are derived with allowance for the complex form of the interaction potential between the composite particles (i.e., allowance is made for the imaginary part of the two-body interaction potential). Subsequently, Lovas[71] generalized the three-particle equations to take into account internal excitations of the composite particles (for example, excitation of the target in a dp reaction). Interesting three-particle effects then arise that are associated with the excitation and de-excitation of the core (or simply the composite particles participating in the reaction) in the intermediate states.

Finally, the last important missing link—allowance for the Pauli principle in the system of three composite particles—was supplied in Refs. 28 and 79. Here too, we encounter specific three-particle effects such as deuteron disintegration only "subject to the orthogonality condition." However, the level of practical application of the three-particle model of nuclear reactions remains relatively "low," corresponding to the level in the three-nucleon problem in the middle of the sixties. We shall here devote our main attention to allowance for the Pauli principle in a system of three composite particles.

The standard approach with the Faddeev equations consists of using separable potentials, which are constructed with the same Yamaguchi-type form factors as for the NN interaction, the parameters being fitted to the experimental phase shifts. This approach is a mechanical generalization of the formalism developed for $3N$ systems, but, although simple, does not appear to us to be physically justified, since, as we have shown above, the interaction of composite particles is to a large extent determined by the Pauli principle and the

[6)] In particular, in Ref. 100, a system of (18) (!) two-dimensional (!) Faddeev equations was solved.

corresponding exchange effects, and the nature of, for example, the $\alpha\alpha$ potential is not similar to that of the NN potential. Nevertheless, a considerable number of calculations of light nuclei have already been performed on the basis of this formalism. The general scheme is as follows. In the partial waves in which there are near-threshold bound states or resonances of the two-particle subsystems, ordinary separable attractive potentials (of Yamaguchi type) are used. We give examples:

$n\,(p)\,\alpha$	in the states $P_{3/2}$, $P_{1/2}$;
^{3}H (^{3}He) α	in the states $P_{3/2}$, $F_{5/2}$, $F_{7/2}$;
$\alpha\alpha$	in the states D_2, G_4 ,

etc.

In the partial waves in which there are no such definite near-threshold singularities of where the phase shifts "change sign," a separable repulsive potential is taken. Here are some typical examples:

$n(p)\alpha$ in the state $S_{1/2}$;

^{3}H(^{3}He)α in the states with even orbital angular momenta S, D, etc.

The same applies to the application of the formalism of the Faddeev equations to the investigation of three-particle models of direct nuclear reactions of the dp type,[71] in which an approach of this kind is used to describe the interaction of a nucleon with a core nucleus. It is therefore not surprising that the general nature of the nuclear spectra found in such an approach (for typical three-particle nuclei such as ^{6}Li, ^{9}Be, ^{12}C, etc.) is similar to what is found in variational calculations with local interactions containing a local repulsive core.[71,74]

Figure 7 shows the spectrum of the levels with $T=0$ of the best studied nucleus ^{12}C, calculated on the basis of the Faddeev equations in the 3α model for $\alpha\alpha$ potentials with and without a repulsive core but with the introduction of an orthogonality condition on the $\alpha\alpha$ scattering wave function (for a more detailed discussion of the applicability of the 3α model to the ^{12}C nucleus, see the following section). It can be seen clearly that the standard (i.e., NN-like) approach to this problem leads to a spectrum that is "contracted" compared with the experimental spectrum. The rms radius of the nucleus is also overestimated. This means essentially that the repulsive core incorrectly simulates the effect of the Pauli principle in such systems, and that a more adequate approach is needed, which, for example, should take into account the conditions of orthogonality to the two-particle forbidden states in the formalism of the Faddeev equations. However, Feshbach's well-known technique of orthogonal projection (used by Lovas[71]) does not lead to a simple scheme of rearrangement of the equations. The difficulties here can be best understood by attempting to write down the Faddeev equations in which the two-body interaction is described by the orthogonality-condition model (26) and (27).

In an attempt to avoid these difficulties, it was suggested that one should use oscillating separable potentials based on the shell wave functions and describing not only the experimental phase shifts but also the shell structure of the radial scattering wave functions in the inner region. In other words, the oscillating separable potentials give scattering wave functions that are approximately orthogonal to the wave functions of the occupied states of the system. Such potentials were constructed in Ref. 72 for all pairs of light clusters of the type α^3He, td, etc., and it was shown[72] that such potentials have numerous attractive features which distinguish them from the purely phenomenological constructions frequently used for the same purposes. In particular, these potentials include few free parameters, while the remaining parameters are taken directly from the shell model.[72] This, in its turn, makes it possible to relate the potentials for different partial waves, different spin–isospin states, and even for different particles; in addition, without any calculations one can predict the general nature of the phase shifts and, in particular, the values of the energy at which the phase shifts are equal to zero or $n\pi, n = 1, 2, \ldots$.

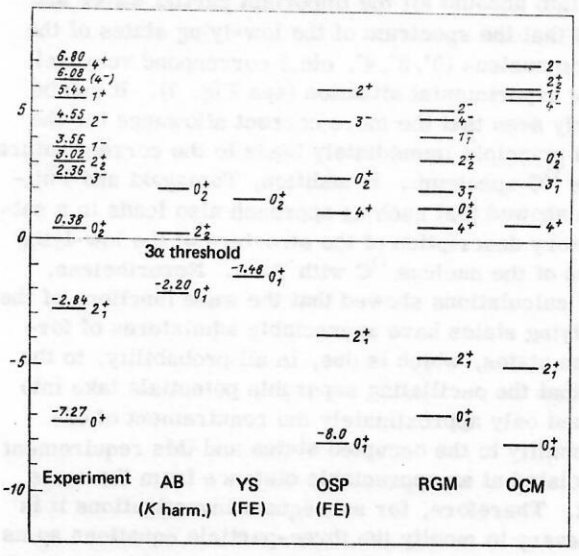

FIG. 7. Comparison of the spectra of the ^{12}C nucleus in the 3α model found in different approaches. First on the left is the experimental spectrum of the $T=0$ levels of the nucleus ^{12}C; second on the left, the standard variational calculation with local Ali–Bodmer $\alpha\alpha$ potential, which contains a repulsive core with large radius (the calculation was made by the method of K harmonics); third from the left, the standard approach with Faddeev equations with separable Yamaguchi potentials[101]; third from the right, Faddeev equations with oscillating separable $\alpha\alpha$ potentials leading to approximate orthogonality of the continuum functions to the forbidden $\alpha\alpha$ states; second from the right, completely microscopic calculation in the generator-coordinate method; extreme right, semiempirical orthogonality-condition approach.

In the following years, these oscillating separable potentials were used in the solution of the Faddeev equations for the 3α system,[3,73] in which it was shown that the energies of the two 0^+ states of ^{12}C correspond very well to the experimental values. The structure of the ^{12}C states was investigated in such an approach in particular detail by Tamagaki and Fujiwara.[3] They

took into account all the important partial waves and found that the spectrum of the low-lying states of the carbon nucleus ($0^+, 2^+, 4^+$, etc.) correspond very well to the experimental situation (see Fig. 7). It can be clearly seen that the more correct allowance for the Pauli principle immediately leads to the correct nature of the ^{12}C spectrum. In addition, Tamagaki and Fujiwara showed that such an approach also leads to a satisfactory description of the structure of the low-lying states of the nucleus ^{12}C with $T=0$. Nevertheless, their calculations showed that the wave functions of the low-lying states have appreciable admixtures of forbidden states, which is due, in all probability, to the fact that the oscillating separable potentials take into account only approximately the requirement of orthogonality to the occupied states and this requirement is violated at an appreciable distance from the mass shell. Therefore, for subsequent investigations it is necessary to modify the three-particle equations so as to make their solutions strictly orthogonal to the wave functions of the occupied states in each two-particle system and, in addition, to eliminate the corresponding forbidden virtual transitions in all intermediate states.

Faddeev Equations with Orthogonalization to the Two-Particle State. Thus we can consider a system of three composite particles with two-body interactions described by potentials V_i with the orthogonality condition $\Gamma_i\varphi=0$. The projection operators Γ_i are now infinite-dimensional and can be expressed in, for example, the coordinate representation in the form

$$\Gamma_i=\sum_n \varphi^n(\mathbf{r}_i)\varphi^{n*}(\mathbf{r}_i')\,\delta(\boldsymbol{\rho}_i-\boldsymbol{\rho}_i'),$$

where $\mathbf{r}_i=\mathbf{r}_{jk}$ and $\boldsymbol{\rho}_i$ are Jacobi coordinates, and the sum over n is over all forbidden states. Further, we introduce the orthogonalizing pseudopotentials $V=\tilde{V}_i+\lambda_i\Gamma_i$, the pseudo-Hamiltonian $\tilde{H}=H_0+\tilde{V}_1+\tilde{V}_2+\tilde{V}_3$, and the corresponding Green's functions:

$$\tilde{G}=(E-\tilde{H})^{-1};\quad \tilde{G}_i=(E-H_0-\tilde{V}_i)^{-1},\quad i=1,\ 2,\ 3.$$

Using the standard identities

$$\tilde{G}=G_0+G_0\tilde{V}\tilde{G};\quad \tilde{V}=\tilde{V}_1+\tilde{V}_2+\tilde{V}_3;\quad \tilde{G}_i=G_0+G_0\tilde{V}_i\tilde{G}_i$$

and the Faddeev reduction,[75] we obtain a modified system of Faddeev equations for the Green's functions[28]:

$$\left.\begin{aligned}&\tilde{G}=G_0+\tilde{G}^{(1)}+\tilde{G}^{(2)}+\tilde{G}^{(3)};\\&\tilde{G}^{(i)}=\tilde{G}_i\tilde{V}_i(G_0+\tilde{G}^{(j)}+\tilde{G}^{(k)}),\end{aligned}\right\}\tag{80}$$

where the components $G^{(i)}$ are determined by the equation

$$\tilde{G}^{(i)}=G_0\tilde{V}_i\tilde{G}.$$

In the system (80), we now go to the limit $\lambda_i\to\infty$, using the relation

$$\lim_{\lambda_i\to\infty}\tilde{G}_i(\lambda)\tilde{V}_i(\lambda)=\tilde{G}_iV_i-G_i\Gamma(\Gamma G_i\Gamma)^{-1}\Gamma_i,\tag{81}$$

[$\tilde{G}_i$ is defined by the expression (37)]. If we now apply the projection operator Γ_i to equation i of system (80), we obtain

$$\Gamma_i\tilde{G}^{(i)}=-\Gamma_i(G_0+\tilde{G}^{(j)}+\tilde{G}^{(k)})$$

or

$$\Gamma_i\tilde{G}=0\quad\text{as}\quad\lambda_i\to\infty,\quad i=1,\ 2,\ 3.$$

Similarly, we can show that $\tilde{G}\Gamma_i=0$ as $\lambda_i\to\infty$.

Thus, the derived system of Faddeev equations has solutions strictly orthogonal to the forbidden states included in the projection operators Γ_i. Note that if there are no forbidden states in pair i (for example, when the two particles j and k are nucleons), one must take $\lambda_i=0$. Thus, the system (80) includes the most general case of three composite particles.

It is also important to add that if all $\lambda_i\to\infty$, then $\Gamma\tilde{G}=\tilde{G}\Gamma=0$, where Γ is the *total* projection operator defined by the conditions

$$\Gamma_i\Gamma=\Gamma\Gamma_i=\Gamma_i;\quad\Gamma^2=\Gamma.$$

And since the different Γ_i *do not commute with one another*, the total projection operator Γ is an infinite series of products of the projection operators Γ_i, Γ_j, and Γ_k, with which it is very inconvenient to operate. The method described here enables one, as follows from the above relations, to obtain orthogonalization *without using the total projection operator*.

Using the system of Faddeev equations (80) for the Green's functions, we can now readily derive the Faddeev equations for the wave functions by means of the well-known relation for the total projected wave function

$$\tilde{\Psi}=\lim_{\varepsilon\to0}i\varepsilon\tilde{G}(E+i\varepsilon)\Phi,$$

which, like the total Green's function, is orthogonal to all the forbidden states included in Γ_i. For example, for scattering of particle 1 on the bound state (23), we find

$$\left.\begin{aligned}&\tilde{\Psi}_1=\tilde{\psi}_1^{(1)}+\tilde{\psi}_1^{(2)}+\tilde{\psi}_1^{(3)};\\&\tilde{\psi}_1^{(i)}=\tilde{\Phi}_1\delta_{i1}+\tilde{G}_iV_i(\tilde{\psi}_1^{(j)}+\tilde{\psi}_1^{(k)}),\end{aligned}\right\}\tag{82}$$

where the function of the initial state $\tilde{\Phi}_1=\tilde{\Phi}_1(\mathbf{k}_1)\delta(\mathbf{p}_1-\mathbf{p}_1^0)$ must be an eigenfunction of the channel pseudo-Hamiltonian $\tilde{H}_1$ (i.e., with allowance for the orthogonality condition) as $\lambda\to\infty$.

These three-particle equations are suitable not only when the two-particle interaction is represented by oscillating separable potentials, but also for optical potentials with forbidden states. In this last case,

$$\tilde{G}_i=G_i-\sum_n\frac{|\varphi_i^n\rangle\langle\varphi_i^n|}{E-E_i^n},$$

i.e., the orthogonalized Green's function $\tilde{G}_i$ is equal to the original Green's function G_i with subtraction of the spectral terms that correspond to the forbidden states with energy E_i^n. At the same time, it is easy to show that the correction due to the orthogonalization to the kernel of the Faddeev equations is

$$\Delta K_i=\tilde{G}_i\tilde{V}_i-G_iV_i=\sum_n|\varphi_i^n\rangle\langle\varphi_i^n|\times\left(\frac{V_i}{E-E_i-p_i^2/2\mu_i}+1\right)\delta(p_i-p_i').$$

The Faddeev equations (80) and (82) written above for the scattering of three composite particles were proposed in Ref. 7 for eigenstate projection, i.e., when the forbidden states are eigenstates of the optical

Hamiltonian, and in Ref. 28 in the more general case of noneigenstate projection, including oscillating separable potentials (see also Ref. 27).

Equations for deuteron reactions. When one of the particles is infinitely heavy, for example, $m_3=\infty$, it is convenient to use a different scheme of Faddeev reduction proposed by Baz, and also by Dodd and Greider.[76] A three-particle model of this kind can be conveniently used for integral description of direct nuclear reactions involving deuterons. Forbidden states are present only in the pairs 13 and 23, and the projection operators Γ_{13} and Γ_{23} commute. We now use a decomposition of the form

$$G=G_0+G^{(12)}+G^{(3)},$$

corresponding to the Hamiltonian

$$H=H_0+V_{12}+V_3, \quad V_3=V_{13}+V_{23}. \tag{83}$$

We introduce a pseudo-Hamiltonian with $\tilde{V}_{13}=\tilde{V}_{13}+\tilde{V}_{23}$ and after the Faddeev reduction corresponding to the decomposition (83) we obtain the modified system of Faddeev equations

$$\left.\begin{aligned}&\tilde{G}=G_0+\tilde{G}^{(12)}+\tilde{G}^{(3)};\\&\tilde{G}^{(12)}=G_{12}V_{12}(G_0+\tilde{G}^{(3)});\\&\tilde{G}^{(3)}=\tilde{G}_3\tilde{V}_3(G_0+\tilde{G}^{(12)}),\end{aligned}\right\} \tag{84}$$

where

$$\tilde{G}^{(12)}=G_0V_{12}\tilde{G}, \quad \tilde{G}^{(3)}=G_0\tilde{V}_3\tilde{G}.$$

As in the case of (81), one can show that

$$\lim_{\lambda\to\infty}\tilde{G}_3(\lambda)\,\tilde{V}_3(\lambda)=\tilde{G}_3V_3-G_3\Gamma(\Gamma G_3\Gamma)^{-1}\Gamma, \tag{85}$$

where $\Gamma=\Gamma_{13}+\Gamma_{23}-\Gamma_{13}\Gamma_{23}$ is the total projection operator. Applying the operator Γ to the second equation of (84), we obtain

$$\lim_{\lambda\to\infty}\Gamma\tilde{G}=\lim_{\lambda\to\infty}\tilde{G}\Gamma=0$$

and

$$\Gamma_{13}\tilde{G}=0, \quad \Gamma_{23}\tilde{G}=0 \quad \text{as} \quad \lambda\to\infty,$$

i.e., we again have the required orthogonality of a total Green's function to the forbidden states in the nucleon–nucleus subsystems. One can now show[77] that

$$G_3(E)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}g_{13}(\varepsilon)\,g_{23}(E-\varepsilon)\,d\varepsilon,$$

i.e., the Green's function of two noninteracting particles in the field of the core is given by the convolution of the two single-particle Green's functions (a detailed discussion of the ways of calculating this convolution is given in Ref. 78). Similarly, we can readily find

$$\tilde{G}_3(E)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\tilde{g}_{13}(\varepsilon)\,\tilde{g}_{23}(E-\varepsilon)\,d\varepsilon$$

and, projecting onto the eigenstates of the subsystems 13 and 23, i.e., using an optical potential with forbidden states, we obtain

$$\tilde{G}_3=(1-\Gamma_{13})(1-\Gamma_{13})G_3=(1-\Gamma)G_3.$$

In this case,

$$\lim_{\lambda\to\infty}\tilde{G}_3(\lambda)\,\tilde{V}_3(\lambda)=\tilde{G}_3V_3-\Gamma.$$

Further, in the standard manner one can readily derive the projected equations for the wave functions (for details of the derivation, see Refs. 7, 28, and 79) and find the correction terms in the kernel that are entirely due to the effect of the Pauli principle. The correction is $\Delta K=T_{12}(\tilde{G}_3-G_3)$, where T_{12} is the scattering matrix of particles 1 and 2. For eigenstate projection, we find

$$\Delta K=-T_{12}\Big[\sum_n|\varphi^n_{13}\rangle\langle\varphi^n_{13}|\,g_{23}(E-E^n_{13})+(1\rightleftarrows 2)-\sum_{n,m}\frac{|\varphi^n_{13}\rangle\langle\varphi^n_{13}|\varphi^m_{23}\rangle\langle\varphi^m_{23}|}{E-E^n_{13}-E^m_{23}}\Big].$$

Equations for scattering of a nucleon by a bound state of a nucleon and a nucleus can be derived similarly.

5. THE ^{12}C NUCLEUS AS A 3α SYSTEM WITH FORBIDDEN STATES

Oscillator Basis for Three-Boson System "Purified" of Forbidden States. It is well known that there are two different approaches to the three-body problem; these are through the Faddeev equations and the variational method. In the preceding section, we have discussed the modification of the Faddeev equations for three composite particles; in this section, taking the example of the ^{12}C nucleus, we discuss the second approach, regarding ^{12}C as a 3α system. As variational basis, we use the oscillator basis of the translationally invariant shell model, and we choose the two-body αα interaction in the form of an optical potential with forbidden states.

Attempts to treat the ^{12}C nucleus (in the ground state and low-lying states with $T=0$) as a 3α system were frequently made quite some time ago (see the review of Ref. 80), but in the overwhelming majority of investigations the Pauli principle in the αα interaction was taken into account too crudely by the introduction into the potential of an L-dependent local repulsive core. Naturally, none of these potentials leads to a correct, from the microscopic point of view, wave function of the relative motion in the αα subsystem.

Although the 3α model of the ^{12}C nucleus does not take into account a number of factors (triple exchange forces, spin–orbit interaction in the system of 12 nucleons, etc.) it is still of interest to use optical potentials with forbidden states in the 3α system and consider how they reproduce the true interaction off the mass shell, whether they give a reasonable value for the binding energy, and so forth.

A specific feature of the use of a complete basis of the translationally invariant shell model in our case is that it must be "purified" of forbidden states with respect to each pair of particles. This not entirely elementary requirement can be readily taken into account with precisely the oscillator basis, in view of the facility of recoupling of the particles that it admits. Here, we consider the simplest case of the construction of a projected basis of the translationally invariant shell model corresponding to the assumption that the forbidden states of the two-body αα Hamiltonian are approximated by oscillator wave functions.

The best approximation of the wave functions of the forbidden states is attained at the value $\hbar\omega = 22.5$ MeV of the oscillator parameters, which was used.

In accordance with Refs. 81–84, we shall label the states of the basis of the translationally invariant shell model for three composite bosons by the quantum numbers $N, [f], (\lambda\mu), K, \Omega, L, M$. Since the ^{12}C nucleus in the shell model has lowest configuration s^4p^8, we restrict ourselves to the set of states with total number $N \geq 8$ of oscillator quanta. The permutational symmetry $[f] = [3]$ of the α particles imposes the following restrictions[83] on the number $K = \lambda, \lambda-2, \lambda-4, \ldots,$ 1 or 0: $K = 0\{\text{mod } 3\}$; if $K = 0$, then μ must be even. A complete list of the basis vectors of the translationally invariant shell model for $N \leq 12$ is given in Table I. However, not all states with $N \geq 8$ are free of forbidden components, which can be constructed as follows. We multiply the oscillator function $|nlm\ (\mathbf{r})\rangle$ of the forbidden state $(nl = 00, 20, 22)$ of the $\alpha\alpha$ subsystem with coordinate $\mathbf{r} = \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ of the relative motion of the two α clusters by some oscillator function $|N-n, \Lambda M_\Lambda(\rho)\rangle$, which depends on the second Jacobi coordinate $\boldsymbol{\rho} = \boldsymbol{\rho}_3 = (1/2)(\mathbf{r}_1 + \mathbf{r}_2) - \mathbf{r}_3$. Using the Clebsch–Gordan coefficients for SU(3), we construct from these products states with definite SU(3) symmetry $(\lambda\mu)$:

$$|n,\ N-n\,(\lambda\mu)\,\Omega LM\rangle = \sum \langle (n0)\, l\,(N-n,\ 0)\,\Lambda\,|(\lambda\mu)\,\Omega\Lambda\rangle\ |nl\,(\mathbf{r}_{12}),\ N-n\Lambda\,(\boldsymbol{\rho}_3) : LM\rangle. \quad (86)$$

If $n = 0$, then one can have only $(\lambda\mu) = (NO)$. If $n = 2$, one can have $(\lambda\mu) = (NO)$, $(N-2, 1)$, and $(N-4, 2)$. We now symmetrize the vector (86) with respect to permutation of the α particles. Since the vector (86) is symmetric under the permutation P_{12}, the symmetrization operator S takes the form

$$S = 1 + P_{13} + P_{23}$$

and for the function of the forbidden state we obtain the expression

$$|A = 3N\,[3]\,(\lambda\mu)\,\Omega LM\rangle_{\text{forb}} = (1/W)\,S\,|n,\ N-n\,(\lambda\mu)\,\Omega LM\rangle, \quad (87)$$

where the normalization factor can be expressed by means of the results of Ref. 83 in the form

$$W^2 = 3\,[1 + 2\,\langle n,\ N-n\,(\lambda\mu)\,\Omega LM\,|P_{23}|n,\ N-n\,(\lambda\mu)\,\Omega LM\rangle = 3\,[1 + 2\,(-1)^{N-n}\,D^{\lambda/2}_{n-N/2,\ n-N/2}\,(2\pi/3)]. \quad (88)$$

The condition of orthogonality of a symmetric function $\bar{\psi}_{LM}$ to the function (87) has the form

$$\langle \bar{\psi}_{LM}|A = 3,\ N\ [3]\ (\lambda\mu)\,\Omega LM\rangle = (3/W)\,\langle \psi_{LM}|n,\ N-n\,(\lambda\mu)\,\Omega LM\rangle = 0, \quad (89)$$

TABLE I.

Number of quanta N	Total set of states	Allowed states
0	(00)	—
2	(20)	—
3	(30)	—
4	(40)(02)	—
5	(50)(31)	—
6	$(60)^2(22)$	—
7	(70)(51)(32)	—
8	$(80)^2(61)(42)(04)$	(04)
9	$(90)^2(71)(52)(33)$	(33)
10	$(10.0)^2(81)(62)^2(24)$	(62), (24)
11	$(11.0)^2(91)^2(72)(53)(34)$	(91), (53), (34)
12	$(12.0)^3(10.1)(82)^2(63)$ (44)(06)	(12.0)(82)(63) (44)(06)

where $n \leq 2$, and the quantum numbers $N(\lambda\mu)\Omega$ take all possible values. Since the transformation (86) is unitary, we can write

$$\langle \bar{\psi}_{LM}|nl\,(\mathbf{r}_{12}),\ N-n\Lambda\,(\boldsymbol{\rho}_3) : LM\rangle = 0, \quad nl = 00,\ 20,\ 22. \quad (90)$$

Here, the values of $N-n$ and Λ are arbitrary, and we therefore obtain the condition

$$\langle \bar{\psi}_{LM}|nlm\,(\mathbf{r})\rangle = 0, \quad nl = 00,\ 20,\ 22. \quad (91)$$

By the symmetry of the function $\bar{\psi}_{LM}$ under permutations of the α particles, the condition of orthogonality to the bound states of the three-particle system (89) reduces to the condition (91), in which there is only the single degree of freedom $\mathbf{r} = \mathbf{r}_{12}$ with fixed numbers of the α particles.

Direct calculation shows that for $N \geq 8$ all states (87) with $n = 0$, $(\lambda\mu) = (NO)$ or $n = 2$, $(\lambda\mu) = (NO)$, $(N-2, 1)$, and $(N-4, 2)$ are linearly independent nonzero vectors. From this we obtain the following procedure for constructing the projected basis of the translationally invariant shell model "purified" of the forbidden states. For each N, we must construct the total basis $\bar{\psi}_{NLM}$ of the model, construct the complete set of forbidden states (87), and, finally, orthogonalize the basis state $\bar{\psi}_{NLM}$ with respect to the forbidden states by, for example, the Gram–Schmidt procedure. The overlap integrals of the original basis vectors $\bar{\psi}_{NLM}$ with forbidden states are given by Eqs. (89) and (90). Concretely, for the nucleus ^{12}C the procedure we have described leads to the following results. In the ground state, this nucleus has spin 0^+, and therefore its wave function can contain only vectors of the translationally invariant shell model with even N and μ. Therefore, for fixed N, there are three types of linearly independent vectors of forbidden states, namely,

$$\left.\begin{array}{l}\text{two sets of vectors with } \mu = 0,\\ \text{one set of vectors with } \mu = 2.\end{array}\right\} \quad (92)$$

All vectors with $\mu > 2$ are allowed, and therefore in practice the procedure of orthogonalization to the forbidden states described above need be carried out only for the vectors of the basis of the model with $\mu = 0$ and 2 (see Table I).

From the condition (91) there follows a further possibility for projecting the forbidden states in the three-particle system. It reduces to diagonalization on the total basis of the translationally invariant shell of the operator $P = P_1 + P_2 + P_3$, where P_1, P_2, P_3 are the projection operators on the forbidden states for the degrees of freedom $\mathbf{r}_{12}, \mathbf{r}_{13}, \mathbf{r}_{23}$. Because of the symmetry of the three-boson states under permutations of the particles, it is sufficient to diagonalize part of the operator P, for example,

$$P_1 = |00\rangle\langle 00| + |20\rangle\langle 20| + |22\rangle\langle 22|. \quad (93)$$

The allowed states correspond to the zero eigenvalues of this operator. It is clear that this last approach can also be applied to systems of four or more α clusters. It also makes it possible to generalize the projection procedure to the case when one uses, not oscillator wave functions, but functions of a more general form.

There are other methods for separating allowed and

forbidden states in a system of three (Ref. 2) and four (Ref. 85) α clusters, and also for other many-cluster systems based on study of the properties of the eigenvalues and eigenfunctions of the three-cluster (and more complicated) overlap integrals similar to those considered for two-cluster systems. For the 3α system, they lead to the same results as were described above.

We now turn to the results of actual calculations.

Levels of the ^{12}C Nucleus in the 3α Model with Forbidden States. In the variational calculation of Ref. 5, the trial function was a linear combination of allowed basis vectors of the translationally invariant shell model:

$$\psi_{\text{trial}} = \sum_{i=1}^{i_{\max}} C_i |A = 3N\,[3]\,(\lambda\mu)\,\omega LM\rangle_{\text{allow}}\,. \qquad (94)$$

Here, the subscript i labels the complete set of quantum numbers of the translationally invariant shell model: $\{N, (\lambda\mu), \omega\}$; $i_{\max}$ is the number of the vector at which the basis is "truncated." The unknown coefficients C_i and the energies E of the levels are obtained by solving the system of linear equations

$$(\partial/\partial C_i^*)\,(\psi_{\text{trial}}\,|H-E|\,\psi_{\text{trial}}) = 0, \quad i = 1, 2, \ldots, i_{\max} \qquad (95)$$

and the corresponding secular equations.

The two-body $\alpha\alpha$ interaction in the Hamiltonian H has the form (see Sec. 3)

$$V_{\alpha\alpha}(r) = V_0\{1+\exp[(r-r_0)/a]\}^{-1} + V_{\text{Coul}}(r), \qquad (96)$$

where $V_0 = -125$ MeV, $r_0 = 1.78$ F, and $a = 0.66$ F. Note that in this calculation it was not possible, in contrast to the usual case, to vary the parameter, $\hbar\omega$, since it was fixed in advance ($\hbar\omega = 22.5$ MeV) by the condition of best approximation of the forbidden states. Therefore, the class of trial functions (94) in such a calculation is less flexible than in the usual variational calculations on an oscillator basis. As a result, to obtain good convergence it is necessary to use a basis of sufficiently large dimension. The calculation was made up to $N_{\max} = 24$ (a 68×68 matrix was diagonalized). The energy of the 0^+ ground state and the positions of the first two excited 0_2^+ and 0_3^+ states were determined:

$$E_{0_1^+} = -15.06 \text{ MeV}; \quad E_{0_2^+} = +9.12 \text{ MeV}; \quad E_{0_3^+} = 11.75 \text{ MeV}. \qquad (97)$$

For comparison, we made a calculation of the 3α system with the interaction (96) on the complete basis of the translationally invariant shell model (i.e., without orthogonalization to the forbidden states) and obtained

$$E'_{0_1^+} = -217.3 \text{ MeV}; \quad E'_{0_2^+} = -164.9 \text{ MeV}; \quad E'_{0_3^+} = -116.9 \text{ MeV}. \qquad (98)$$

Thus, orthogonalization to the forbidden states in the absence of repulsion in the $\alpha\alpha$ potential does indeed keep the 3α system from collapse. This fact once more confirms our basic assumption that there is no need to introduce a repulsive core in the $\alpha\alpha$ interaction.

It can also be seen that the scales of the kinetic and potential energy in the 3α system are large. In comparison with these scales, the obtained overestimation of the ^{12}C binding energy by 7.8 MeV[7)] can be regarded as a relatively small deviation if one bears in mind that the model is only a "first approximation," since it does not take into account the following aspects.

1. The ^{12}C nucleus in the ground state evidently has a structure intermediate between shell and 3α-cluster structure. Orthogonalization to the two-body forbidden states takes into account only the contribution from the two-body exchanges of identical nucleons from different α particles, but triple exchanges must also make a contribution in the 3α system. This leads to a renormalization of the $\alpha\alpha$ interaction in the 3α system.

2. As calculations in the resonating-group method show,[1] the interaction between the α clusters associated with the two-body exchanges is nonlocal and energy dependent. The potential (96) is equivalent to such an interaction in the sense of describing the phase shifts and the fact that certain states are forbidden. However, we do not take into account the energy dependence of the potential. Therefore, the t matrix for the potential (96) may still differ from the t matrix for the "true" nonlocal interaction.

3. If we are guided by the nuclear shell model (actually, this corresponds to the central region, where the eensity of nucleons is high), then with high probability the ^{12}C nucleus contains, as virtual, α particles in excited states,[88] which can, for example, be in the $2S$ state of relative motion, etc., i.e., they must be treated in a special manner. However, the calculations of Jackson *et al.*[89] show that their contribution to the binding energy of the ^{12}C nucleus is small.

Thus, the "second approximation" must take into account the effects listed under 1)–3).

With regard to the excited 0_2^+ and 0_3^+ states, they probably have an α-cluster nature. This conclusion is in agreement with the results of microscopic calculations,[90] which clearly indicate that the ^{12}C nucleus in the 0_2^+ state is a vibrating chain of α clusters.

We have considered here only the 0^+ levels of the ^{12}C nucleus. A similar scheme (on the basis of the orthogonality-condition model described in Sec. 2) can also be applied to the states with different angular momenta[2,91] and gives a good description of all the levels of the ^{12}C nucleus with excitation energy below 15 MeV, at which breakup of the α clusters commences (see Fig. 7). The results of these calculations are also in good agreement with the exact calculation in the resonating-group method.[92]

CONCLUSIONS

We mention here possible uses of the theoretical schemes described in the review. First, they can be

[7)] Note that calculations with an $\alpha\alpha$ potential containing a repulsive core usually lead to a strongly underbound ^{12}C nucleus.[87]

used for different nuclear reactions at comparatively low energies in three-cluster systems, e.g., ^{6}Li$(\alpha d)^8$Be, ^{6}Li$(t,d)^7$Li, ^{16}O$(^6$Li$,d)^{20}$Ne, which are not accompanied by rearrangement of the clusters themselves but are characterized in the diagram description by a complex play of different mechanisms.[93] In our scheme, they must be described by modified Faddeev equations. There is a possible simplification[94] associated with the use of a sum of oscillating separable potentials[72] for each pair of clusters. For example, for the pair αt bound states and resonances are present in the channels $^2P_j(j=3/2$ and $1/2)$ and $^2F_j(J=7/2$ and $5/2)$. Here, we can also include the problem of investigating resonance states in the 3α system, for the solution of which the first useful steps have been taken.[3] True, a certain admixture of forbidden states remains.[3]

Further, we can mention the stripping reaction (d,p) on light nuclei in the region of comparatively low energies 3–10 MeV with capture of a neutron in single-particle levels [for example, ^{12}C$(d,p)^{13}$C*, $E^*=3.09$ MeV, $2s$ is the level of the nucleon]. Here, there is every reason to expect a non-Bohr mechanism of a direct nuclear reaction (significant contribution of many ladder diagrams), i.e., a three-body approach is necessary.[95] Similarly, one must consider at relatively low energies the inelastic processes (p,p') or (n,n') on the nuclei ^{9}Be, ^{13}C, and ^{17}O with excitation of single-particle levels.

It is of interest to consider the structure of light nuclei such as ^{6}Li–^{6}Be–^{6}He, ^{9}Be–^{9}B, etc., as systems of three bodies with known $\alpha\alpha$ and αn interactions for which one can use either the modified Faddeev equations or the projected variational basis of the type described in Sec. 5, but for particles with different masses. Certain steps in this direction have already been taken.[96] As we see, there are quite a number of nice problems of nuclear physics in this field.

Finally, interesting possibilities are opened up by the application of these ideas to the *NN* problem. Namely, it is entirely possible that in the *NN* interaction there is no repulsive core, but instead a node of the wave function.[97] One can imagine what kind of interaction between quarks leads to such a result,[98] predict qualitatively the spectrum of excitations in the *NN* system, calculate the $\Delta\Delta$ admixture in the deuteron,[99] the form factors of electron scattering by the deuteron,[98] and so forth.

[1]K. Wildermuth and Y. C. Tang, A Unified Theory of the Nucleus, Vieweg Verlag, Braunschweig (1977).
[2]H. Horiuchi, Prog. Theor. Phys. **51**, 1266 (1974); **53**, 447 (1975); in: Proc. Intern. Conf. on Nuclear Structure, Tokyo (1977); J. Phys. Soc. Jpn. Suppl. **44**, 144 (1978).
[3]Y. Fujiwara and R. Tamagaki, Prog. Theor. Phys. **56**, 1503 (1976).
[4]V. G. Neudatchin and Yu. F. Smirnov, in: Sovremennye problemy optiki i yadernoĭ fiziki (Modern Problems of Optics and Nuclear Physics), Naukova Dumka, Kiev (1974), p. 225; V. G. Neudatchin, in: Proc. Second Intern. Conf. on Clustering Phenomena in Nuclei, Park College, Maryland (1975).
[5]Yu. F. Smirnov *et al.*, Nucl. Phys. **A235**, 289 (1974).
[6]V. I. Kukulin, V. G. Neudatchin, and Yu. F. Smirnov, Nucl. Phys. **A245**, 429 (1975).
[7]V. I. Kukulin, V. G. Neudatchin, and V. N. Pomerantsev, Yad. Fiz. **24**, 298 (1976) [Sov. J. Nucl. Phys. **24**, 155 (1976)].
[8]V. G. Neudachin and Yu. F. Smirnov, Nuklonnye assotsiatsii v legkikh yadrakh (Nucleon Associations in Light Nuclei), Nauka, Moscow (1969).
[9]V. G. Neudatchin, Yu. F. Smirnov, and I. P. Yudin, Zh. Eksp. Teor. Fiz. **37**, 1782 (1959) [Sov. Phys. JETP **10**, 1256 (1960)].
[10]Th. Kannelopoulos and K. Wildermuth, Nucl. Phys. **20**, 10 (1960).
[11]J. P. Elliott and T. H. R. Skyrme, Proc. R. Soc. **A232**, 561 (1955).
[12]G. Reidemeister, Nucl. Phys. **A197**, 631 (1972).
[13]H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962); Ann. Rev. Nucl. Sci. **8**, 49 (1958); in: Topics in the Theory of Nuclear Reactions, Part II. Reaction Dynamics, Gordon and Breach, New York (1973).
[14]N. Auerbach *et al.*, Rev. Mod. Phys. **44**, 48 (1972).
[15]D. Clement and F. Schmid, in: Proc. Second Intern. Conf. on Clustering Phenomena in Nuclei, Maryland (1975).
[16]S. Saito *et al.*, Preprint DPNU-15, Nagoya Univ. (1973).
[17]M. Kamimura, T. Matsuse, and K. Tanoda, Prog. Theor. Phys. **47**, 1537 (1972).
[18]D. Clement, E. W. Schmid, and A. G. Teufel, Phys. Lett. **B49**, 308 (1974).
[19]V. P. Zhigunov and B. N. Zakhar'ev, Metody silnoĭ svyazi kanalov v kvantovoĭ teorii rasseyaniya (Coupled-Channel Methods in the Quantum Theory of Scattering), Atomizdat, Moscow (1974).
[20]V. I. Kukulin and V. N. Pomerantsev, Yad. Fiz. **27**, 1668 (1978) [Sov. J. Nucl. Phys. **27**, 675 (1978)].
[21]V. I. Kukulin, Fiz. **9** (Suppl. 4), 395 (1977).
[22]S. Saito, Prog. Theor. Phys. **41**, 705 (1969).
[23]Y. Fujiwara, H. Horiuchi, and R. Tamagaki, in: Intern. Symposium on Clustering Phenomena in Nuclei, Tokyo (1977).
[24]V. M. Krasnopol'skiĭ and V. I. Kukulin, Yad. Fiz. **20**, 883 (1974) [Sov. J. Nucl. Phys. **20**, 470 (1974)]; Teor. Mat. Fiz. **27**, 373 (1976).
[25]H. Horiuchi, Fiz. **9** (Suppl. 3), 251 (1977).
[26]S. Saito *et al.*, Prog. Theor. Phys. **50**, 156 (1973).
[27]V. N. Pomerantsev, Dis. na soisk. uchen. stepeni kand. fiz.-matem. nauk (Candidate's Dissertation), Moscow State University (1978).
[28]V. I. Kukulin, V. G. Neudatchin, and V. N. Pomerantsev, J. Phys. G **4**, 1409 (1978).
[29]B. A. Lippmann and H. M. Schey, Phys. Rev. **121**, 1112 (1961).
[30]P. G. Burke and N. Chandra, J. Phys. B **5**, 1696 (1972).
[31]C. M. Shakin and M. S. Weiss, Phys. Rev. **C11**, 756 (1975).
[32]P. G. Burke and A. L. SinFailam, J. Phys. B **3**, 641 (1970).
[33]N. Chandra and A. Temkin, Phys. Rev. **A13**, 188 (1976); B. D. Buckley and P. G. Burke, J. Phys. B **10**, 725 (1977).
[34]M. Coz, L. G. Arnold, and A. D. McKellar, Ann. Phys. (N.Y.) **58**, 504 (1970); **59**, 219 (1970).
[35]S. A. Afzal, A. A. Ahmad, and S. Ali, Rev. Mod. Phys. **41**, 247 (1969).
[36]S. Okai and S. C. Park, Phys. Rev. **145**, 787 (1966).
[37]V. G. Neudatchin *et al.*, Phys. Lett. **B34**, 58 (1971).
[38]V. G. Neudatchin *et al.*, Lett. Nuovo Cimento **5**, 834 (1972).
[39]V. I. Kukulin *et al.*, in: Voprosy atomnoĭ nauki i tekhniki. Ser. Fizika vysokikh énergiĭ i atomnogo yadra (Problems of Atomic Science and Technology. In the Series: Physics of High Energies and the Nucleus), No. 2(4), Khar'kov (1973).
[40]V. P. Korennoĭ, Dis. na soisk. uchen. stepeni kand. fiz.-matem. nauk (Candidate's Dissertation), Moscow State University (1973).
[41]R. M. Él'Khovari, Dis. na soisk. uchen. stepeni kand. fiz.-matem. nauk (Candidate's Dissertation), Moscow State University (1977).
[42]Prog. Theor. Phys. Suppl. **52** (in particles, see the paper of

J. Hiura and R. Tamagaki in Ch. II).
[43]J. M. Ziman, Solid State Phys. **26**, 1 (1971) (Russian translation published by Mir, Moscow (1973)).
[44]P. Swan, Proc. R. Soc. London **228**, 10 (1955); Ann. Phys. (N.Y.) **48**, 455 (1968).
[45]W. Glockle and J. Le Turneux, Nucl. Phys. **A269**, 16 (1976).
[46]A. G. Sitenko, Lektsii po teorii rasseyaniya (Lectures on Scattering Theory), Vishcha Shkola, Kiev (1971).
[47]J. M. Jauch, Helv. Phys. Acta **30**, 143 (1957).
[48]R. G. Newton, Scattering Theory of Waves and Particles, McGraw-Hill, New York (1966) (Russian translation published by Mir, Moscow (1966)).
[49]J. C. Fong, G. Igo, and V. Perez-Mendez, Nucl. Phys. **A262**, 365 (1976).
[50]Yu. F. Smirnov and R. M. Él' Khavari, Izv. Akad. Nauk, Ser. Fiz. **39**, 2084 (1975).
[51]A. S. Davydov, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, Moscow (1963).
[52]D. Clement, E. F. Kannelopoulos, and K. Wildermuth, Phys. Lett. **B55**, 19 (1972).
[53]J. V. Park, W. Sheid, and W. Greiner, Phys. Rev. **C6**, 1565 (1972).
[54]K. A. Brueckner, Phys. Rev. **173**, 944 (1968).
[55]W. Scheid and W. Greiner, Z. Phys. **266**, 364 (1969).
[56]T. Yukawa, Nucl. Phys. **A186**, 127 (1972).
[57]A. I. Baz', Pis'ma Zh. Eksp. Teor. Fiz. **14**, 607 (1971) [JETP Lett. **14**, 423 (1971)].
[58]W. Von Oertzen *et al.*, Nucl. Phys. **A148**, 529 (1970).
[59]S. Saito *et al.*, Prog. Theor. Phys. **50**, 1561 (1973).
[60]W. Meier and W. Glöckle, Nucl. Phys. **A255**, 211 (1975).
[61]A. Böinghoff, H. Hüsken, and A. Weiguny, Phys. Lett. **B61**, 9 (1976).
[62]Y. C. Tang, in: Intern. Conf. on Clustering Phenomena in Nuclei, Bochum, 1969, IAEA, Vienna (1969), p. 109.
[63]R. Tamagaki, Prog. Theor. Phys. Suppl. Extra Number 42 (1969).
[64]F. Perey and B. Buck, Nucl. Phys. **32**, 353 (1962).
[65]F. Perey, in: Direct Interaction and Nuclear Reactions Mechanisms, Gordon and Breach, New York (1963).
[66]M. Coz, Prog. Theor. Phys. **50**, 111 (1973); H. Fiedeldey, Nucl. Phys. **77**, 149 (1966).
[67]J. B. Furness and I. E. McCarthy, J. Phys. B **6**, 2280 (1973).
[68]N. De Takaszy, Phys. Rev. C **5**, 1883 (1972).
[69]B. Giraud, F. C. Hocquenghem, and A. Lumbroso, Phys. Rev. **C7**, 2274 (1973).
[70]H. Fiedeldey, Nucl. Phys. **A96**, 463 (1967).
[71]R. E. Kreps and P. Nath, Phys. Rev. **152**, 1475 (1966); B. Charnomordic, C. Fayard, and G. H. Lamot, Phys. Rev. **C15**, 864 (1977); D. S. Chum, C. S. Han, and D. L. Lin, Phys. Rev. **C9**, 2086 (1974); A. Ghovanlou and D. R. Lehman, Phys. Rev. **C9**, 1730 (1974); Y. Kawazoe *et al.*, Prog. Theor. Phys. **51**, 428 (1974); I. Lovas, Ann. Phys. (N.Y.) **89**, 96 (1975); P. Beregi, I. Lovas, and J. Revai, Ann. Phys. (N.Y.) **61**, 57 (1970); A. S. Reiner and A. I. Jaff, Phys. Rev. **161**, 935 (1967); J. R. Bunati and G. W. Bund, Nucl. Phys. **A306**, 139 (1978).
[72]V. I. Kukulin and V. G. Neudatchin, Nucl. Phys. **157**, 609 (1970); L. M. Kuznetsova, V. I. Kukulin, and V. G. Neudatchin, Yad. Fiz. **13**, 694 (1971) Sov. J. Nucl. Phys. **13**, 394 (1971)].
[73]V. I. Kukulin, Czech. J. Phys. **B21**, 923 (1971).
[74]H. Horiuchi, in: Proc. Third Intern. Conf. on Clustering Aspects of Nuclear Structure, Manitoba (1978).
[75]L. D. Faddeev, Zh. Eksp. Teor. Fiz. **39**, 1459 (1960) [Sov. Phys. JETP **12**, 1014 (1961)].
[76]A. I. Baz', V. F. Lemin, and I. I. Kuz'min, Yad. Fiz. **4**, 737 (1966) [Sov. J. Nucl. Phys. **4**, 525 (1966)]; R. R. Greider and L. R. Dodd, Phys. Rev. **146**, 671 (1966); **146**, 675 (1966).
[77]A. I. Baz', Ya. B. Zel'dovich, and A. M. Perelomov, Rasseyanie, Reaktsii i raspady v nerelyativistskoĭ kvantovoĭ mekhanike, Nauka, Moscow (1971); English translation: Scattering, Reactions and Decay in Nonrelativistic Quantum Mechanics, Jerusalem (1969).
[78]R. C. Fuller, Phys. Rev. **C3**, 1042 (1971).
[79]V. I. Kukulin, V. G. Neudatchin, and V. N. Pomerantsev, Yad. Fiz. **24**, 298 (1976) [Sov. J. Nucl. Phys. **24**, 155 (1976)]; Preprint, Prague Inst. of Nuclear Physics, Řež (1976).
[80]H. Horiuchi, Fiz. **9** (Suppl. 4), 251 (1977).
[81]Yu. F. Smirnov and K. V. Shitikova, Izv. Akad. Nauk SSSR, Ser. Fiz. **27**, 1442 (1963).
[82]L. V. Kurdyumov *et al.*, Nucl. Phys. **A145**, 593 (1970).
[83]P. Kramer and M. Moshinsky, Nucl. Phys. **A125**, 321 (1969); M. Moshinsky, Harmonic Oscillator in Modern Physics: From Atoms to Quark, Gordon and Breach, New York (1969) (Russian translation published by Mir, Moscow (1972)).
[84]V. V. Vanagas, Algebraicheskie metody v teorii yadra (Algebraic Methods in Nuclear Theory), Mintis, Vil'nyus (1971).
[85]H. Horiuchi, Prog. Theor. Phys. **55**, 1448 (1974); Y. Suzuki, in: Proc. Intern. Conf. on Nuclear Structure, Tokyo (1977).
[86]H. Horiuchi, Prog. Theor. Phys. **38**, 204 (1977).
[87]V. C. Aguilira-Navarro and O. Portilho, Ann. Phys. (N.Y.) **107**, 126 (1977).
[88]N. F. Golovanova *et al.*, Yad. Fiz. **23**, 63 (1976) [Sov. J. Nucl. Phys. **23**, 31 (1976)].
[89]A. D. Jackson, A. Lande, and P. U. Sauer, Nucl. Phys. **A156**, 1 (1970).
[90]N. De Takaszy, Nucl. Phys. **A178**, 469 (1972).
[91]M. Kamimura, Y. Fukushima, and A. Tohsaki Suzuki, Fiz. **9** (Suppl. 2), 33 (1977).
[92]Y. Fukushima and M. Kamimura, Fiz. **9** (Suppl. 2), 35 (1977).
[93]M. F. Werby *et al.*, Phys. Rev. **C8**, 106 (1973); **10**, 564 (1974).
[94]J. S. Levinger, Springer Tracts in Modern Physics, Berlin **71**, 88 (1974); B. Charnomordic, C. Fayard, and G. H. Lamot, Phys. Rev. **C15**, 864 (1977).
[95]V. G. Neudatchin *et al.*, Yad. Fiz. **29**, 343 (1979) [Sov. J. Nucl. Phys. **29**, 170 (1979)].
[96]B. Barsella, L. Lovitch, and S. Rosati, Nucl. Phys. **A117**, 638 (1968).
[97]V. G. Neudatchin *et al.*, Phys. Rev. **C11**, 128 (1975).
[98]V. G. Neudatchin, Yu. F. Smirnov, and R. Tamagaki, Prog. Theor. Phys. **58**, 1072 (1977).
[99]Yu. F. Smirnov and Yu. M. Tchuvilsky, J. Phys. G **4**, 1 (1978).

Translated by Julian B. Barbour