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N-cluster dynamics and effective interaction of composite particles. I. The dynamical equation

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A nonrelativistic wave equation for the relative motion of composite particles is derived from a given, microscopic Schrödinger equation. For two composite particles, the theory is identical to resonating group theory. For three and more composite particles it differs by the use of distortion functions with a continuous degree of freedom which allows a correct asymptotic description of the system. The dynamical equation, formally, is a multichannel Schrödinger equation with a matrix of nonlocal and energy-dependent interactions. The internal degrees of freedom of the composite particles and the Pauli principle are incorporated into the interaction. The relative motion wave function of the composite particles is a probability density amplitude in the asymptotic region only. In regions where the composite particles interact, the relative motion function is not a probability density amplitude and may even have a certain degree of off-shell ambiguity. In all regions of configuration space, however, the probability density of particles is defined by the microscopic wave function. The theory is formulated for nuclear fragments but is valid also for atoms and particles consisting of quarks.

[NUCLEAR REACTIONS Scattering theory, nuclear fragments, atoms, bags of quarks. N-cluster theory. Composite particle interaction.]

I. INTRODUCTION

The central problem of theoretical atomic and nuclear physics is the derivation of the dynamical behavior of A particles from an A-particle Schrödinger equation with phenomenologically given interactions. As is well known, an A-particle system has so many degrees of freedom that there is no hope for a general solution of the problem, when A is larger than, say, three or four. In many practical cases, however, not all degrees of freedom come into play. In scattering experiments, energy is a chosen parameter. Sometimes its value is not large enough to allow the system to disintegrate into A free particles. When this is so, then not all parts of the $3A$-dimensional space are accessible, and some degrees of freedom are not needed. A quantum dynamical theory should be able to take advantage of that. In the following, we are presenting such a theory. It will be valid in a limited energy range. Degrees of freedom which are only needed when energy is higher than the limit will not appear.

The idea we use is essentially the resonating group idea which has been introduced by Wheeler[1] in 1937. It has been reintroduced and worked out in the two-cluster case by Wildermuth and collaborators.[2,3] The concept of treating clusters as point particles while putting the Pauli principle and internal degrees of freedom into the interaction has been discussed for three clusters.[4] The present paper deals with the general N-cluster, multichannel formalism. The dynamical equation will be a set of coupled second order differential equations with nonlocal, energy-dependent interactions. Despite its complicated mathematical structure, the theory will allow one to study general features of composite particle dynamics and will lead the way to new approximation schemes.

It has been emphasized earlier[5] that there is a striking similarity between the interaction of hadrons and the interaction of typical composite particles such as α particles. The present theory is formulated in terms of nuclear clusters. We should bear in mind, however, that it is valid also for atoms and for bags of quarks, provided that quark motion obeys the nonrelativistic Schrödinger equation.

In Sec. II of this paper the microscopic A-particle wave function is expressed in terms of internal and relative motion wave functions of clusters, together with cluster distortion functions. In Sec. III the dynamical equation is derived. In Sec. IV it is shown that unitarity is conserved and in Sec. V the asymptotic behavior of the solution is investigated. Some general features of the relative motion wave function of composite particles are discussed in Sec. VI.

In part II of this series of papers, the interaction of composite particles, as it is present in the dynamical equation, will be studied. It will be shown that, despite its complicated mathematical form,

the interaction is readily understood in terms of physics and can be approximated by separable potentials.

II. THE N-CLUSTER WAVE FUNCTION

An A-particle system can be decomposed into asymptotically stable clusters in various ways. For each decomposition we assume the eigenenergies and eigenstates of the clusters to be known (approximate description of clusters will be discussed later). The sum of cluster eigenenergies is the minimum energy needed to disintegrate the system into free clusters. At zero energy, by definition, the system can disintegrate into A free particles.

As has been said in the introduction, we want to take advantage of a limitation of energy. Let us pick a particular threshold energy and define this energy as upper limit of an allowed energy range. A lower limit will not be needed. The maximum number of clusters, into which the system can decay within the allowed energy range, is called N.

Let us try to find an ansatz for the scattering function which has all the needed degrees of freedom, but which has as little unnecessary degrees of freedom as possible. When all clusters of a certain decomposition i are separated from each other by very large distances, the scattering function rigorously goes over into an antisymmetrized product of cluster eigenstates $\varphi_{i,1}\varphi_{i,2}\cdots$ times a function $\chi_i(\xi_{i,1},\xi_{i,2},\dots)$ which describes the center of mass motion of the clusters[6]:

$$\psi \to \mathbf{A}\{\varphi_{i,1}\varphi_{i,2}\cdots\chi_i(\xi_{i,1},\xi_{i,2},\dots)\}. \tag{1}$$

The eigenstates of the clusters include spin and isospin, while the function χ_i depends on the Jacobi coordinates $\xi_{i,1},\xi_{i,2},\dots$ only. $\mathbf{A}$ denotes antisymmetrization. Asymptotic scattering states, which are eigenstates of total angular momentum and, if desired, of total isospin, are obtained by taking appropriate superpositions.

When two or more clusters interact with each other, an expression like Eq. (1) can no longer describe the true scattering wave function. It has to be supplemented in two ways: (1) Asymptotic channels with different fragmentation are coupled and we have to add the relevant functions. (2) The clusters become distorted while they interact. This means that their internal motion is no longer described by the bound state wave function of free clusters. We have to add correction functions which we will sometimes call distortion functions and sometimes compound state corrections. A typical correction function consists of a chosen wave function $\tilde{\varphi}_{j,1}$, which is a square integrable compound state of two or more clusters, multiplied by the ground state functions $\varphi_{j,2}\varphi_{j,3}\cdots$ of the remaining clusters (the "spectators"). This product of internal motion states is multiplied by a function $\tilde{\chi}_j(\xi_{j,1},\xi_{j,2},\dots)$ which describes the center-of-mass motion of the state $\tilde{\varphi}_{j,1}$ and of the clusters $\varphi_{j,2}\varphi_{j,3},\dots$ in terms of Jacobi coordinates $\xi_{j,1},\xi_{j,2},\dots$. The full product is antisymmetrized:

$$\mathbf{A}\{\tilde{\varphi}_{j,1}\varphi_{j,2}\varphi_{j,3}\cdots\tilde{\chi}(\xi_{j,1},\xi_{j,2},\dots)\}. \tag{2}$$

It is easy to write down more correction functions. We can either replace $\tilde{\varphi}_{j,1}$ by other compound states of the same particles, or we can introduce compound states of pairs or groups of other clusters. To simplify notation we put the tilde on all functions and Jacobi coordinates which appear in a correction term, knowing that some of the $\tilde{\varphi}_{j,k}$'s may be ground states.

Putting it all together we get the following ansatz[7] for the microscopic A-particle wave function:

$$\begin{aligned}
\psi = &\sum_{i=1}^{n_N} \mathbf{A}\{\varphi_{i,1}\varphi_{i,2}\cdots\varphi_{i,N}\chi_i(\xi_{i,1},\xi_{i,2},\dots,\xi_{i,N})\} + \sum_{i=n_N+1}^{n_N+n_{N-1}} \mathbf{A}\{\varphi_{i,1}\varphi_{i,2}\cdots\varphi_{i,N-1}\chi_i(\xi_{i,1},\xi_{i,2},\dots,\xi_{i,N-1})\} + \cdots \\
&+ \sum_{i=n_N+n_{N-1}+\cdots+n_3+1}^{n} \mathbf{A}\{\varphi_{i,1}\varphi_{i,2}\chi_i(\xi_{i,1},\xi_{i,2})\} + \sum_{i=1}^{\tilde{n}_{N-1}} \mathbf{A}\{\tilde{\varphi}_{i,1}\tilde{\varphi}_{i,2}\cdots\tilde{\varphi}_{i,N-1}\tilde{\chi}_i(\tilde{\xi}_{i,1}\tilde{\xi}_{i,2},\dots,\tilde{\xi}_{i,N-1})\} \\
&+ \sum_{i=\tilde{n}_{N-1}+1}^{\tilde{n}_{N-1}+\tilde{n}_{N-2}} \mathbf{A}\{\tilde{\varphi}_{i,1}\tilde{\varphi}_{i,2}\cdots\tilde{\varphi}_{i,N-2}\tilde{\chi}_i(\tilde{\xi}_{i,1},\tilde{\xi}_{i,2},\dots,\tilde{\xi}_{i,N-2})\} \\
&+ \cdots \\
&+ \cdots \\
&+ \cdots \\
&+ \sum_{i=\tilde{n}_{N-1}+\tilde{n}_{N-2}+\cdots+\tilde{n}_2+1}^{\tilde{n}} \mathbf{A}\{\tilde{\varphi}_i\tilde{\chi}_i(\tilde{\xi}_i)\}.
\end{aligned} \tag{3}$$

The first sum includes all decompositions into N clusters, the second into $(N-1)$ clusters, and so on. Some of the $\varphi_{i,j}$'s may stand for particles, instead of clusters. In that case, $\varphi_{i,j}$ is simply the spin-isospin state of the particle. The antisymmetrization operator $\mathbf{A}$ operates on the expressions in curly brackets. Within the curly brackets, natural ordering of particle numbers is assumed. The no-distortion part ends with a sum over two-cluster decompositions.

The distortion part starts with a sum over $(N-1)$ cluster corrections, and ends with a sum over one-cluster corrections. In the general case, the distortion part has very many terms.

In ansatz (3) for the scattering function, all φ's and $\tilde{\varphi}$'s are kept fixed, while all χ's and $\tilde{\chi}$'s have to be determined by a dynamical equation. Currently, we assume that the internal cluster states $\varphi_{i,j}$ are rigorous bound states of the respective parts of the full A-particle Hamiltonian. We keep in mind, however, that in practical applications we have to allow approximate cluster eigenstates. The states $\tilde{\varphi}_{i,j}$ are either bound eigenstates, when the cluster is a spectator, or they are chosen functions. The question arises as how to choose them. In principle, any square integrable function of the respective space-, spin-, and isospin coordinates may be chosen. There is no condition of orthogonality. Only linear dependency is an undesirable feature. Just to have something on hand, we give one of the many possible prescriptions for choosing correction states $\tilde{\varphi}_{i,j}$: Generate states by an oscillator shell model. Take all those particle-hole excitations, two particle-two hole excitations and so on, which are believed to play a role in the scattering process. Delete the rest. Now try to reduce overlap with the no-distortion part of the ansatz. Take those no-distortion functions which can have nonzero overlap with the shell model states. Replace the relative motion part by one or more square integrable functions which, at short distances, oscillate with a wave length which is typical for scattering states. Take the so-obtained square integrable no-distortion states out of the shell model basis by a (numerical) subtraction procedure. What will be left from the shell model states can be used as correction states $\tilde{\varphi}_{i,j}$.

Another kind of linear dependency is easily removed from Eq. (3). Consider an example where, in the N-cluster decomposition, a proton appears as one cluster and a neutron as another cluster. In this case, the N-cluster sum can rigorously describe an $(N-1)$ cluster state in which these two particles form a deuteron. Therefore, this $(N-1)$ cluster part is left out from the second sum, because it is already present in the first sum. We also leave out such $(N-1)$ cluster decompositions which are approximately contained in the N-cluster sum. As an example, think of a deuteron and a neutron at the N-cluster level which can form something with the quantum numbers of a triton. Of course, a deuteron and a neutron in relative motion will not correctly describe the eigenstate of a triton. But we are introducing corrections, anyway: therefore we leave out the respective cluster decomposition in the second sum.

It is clear how to proceed. In the third sum we leave out everything which is contained, rigorously or approximately, in the first two sums, and so on. In this way, certain sources of linear dependency are removed from the ansatz (3) without use of projection operators. In complicated systems, there still remain sources of linear dependency, which will be discussed later.

The reader may feel that there is much room for ambiguity in Eq. (3). Indeed, there is. But we shall see that this is not a fault of the theory. It reflects a general property of composite particle dynamics and is related to the off-shell and multi-body-force ambiguity which, in case of the hadronic interaction (as an interaction of particles with internal degrees of freedom) has been a focus of interest for a long time.[8]

In Sec. III, a more compact form of Eq. (3) will be needed. We denote the products of internal motion states $\varphi_{i,1}\varphi_{i,2}\cdots$ by ϕ_i, and write

$$\psi=\sum_{i=1}^{n}\mathbf{A}\{\phi_i\chi_i\}+\sum_{i=1}^{\tilde{n}}\mathbf{A}\{\tilde{\phi}_i\tilde{\chi}_i\}\equiv\sum_{i=1}^{n+\tilde{n}}\mathbf{A}\{\hat{\phi}_i\hat{\chi}_i\}. \quad (4)$$

In this paper, the tilde will always refer to distortion states and the hat will be used when an index runs over no-distortion and distortion states as well. It has already been said that the φ's and $\tilde{\varphi}$'s are chosen and kept fixed, while the χ's and $\tilde{\chi}$'s are freely adjustable. With the new shorthand notation we can express this more precisely by saying that all variations of the χ's and $\tilde{\chi}$'s in Eq. (3) define the test function space $\delta\psi$:

$$\delta_\psi=\sum_{i=1}^{n}\mathbf{A}\{\phi_i\delta\chi_i\}+\sum_{i=1}^{\tilde{n}}\mathbf{A}\{\tilde{\phi}_i\tilde{\delta}\tilde{\chi}_i\}$$

$$\equiv\sum_{i=1}^{n+\tilde{n}}\mathbf{A}\{\hat{\phi}_i\hat{\delta}\hat{\chi}_i\}. \quad (5)$$

A general N-cluster ansatz has also been presented by other authors.[9-11] Their ansatz differs from the present one in two respects: (i) all distortion functions are of the one-cluster type, (ii) all open channels are carried along, including those which are, rigorously or approximately, contained in a higher cluster decomposition.

Example 1. Consider the ^{7}Li scattering system. From the energy eigenvalues of the fragments one

gets the following thresholds[12]: α-t (−36.777 MeV), ^{6}Li-n (−31.990 MeV), α-d-n (−30.520 MeV), ^{6}He-p (−29.259 MeV), α-n-n-p (−28.295 MeV), t-t-p (−16.964 MeV), ^{3}He-t-n (−16.199 MeV), t-d-d (−12.92 MeV),.... As upper limit of the energy range we choose the t-t-p threshold, which means $N=4$.

The first sum of Eq. (3), in the present example, describes the motion of an undistorted α particle, of two neutrons, and of a proton. As internal motion states we have the eigenstate of an α particle and the spin-isospin states of the neutrons and of the proton. In order to construct a ^{7}Li scattering state with good quantum numbers, several spin orientations of the nucleons are needed. Therefore we have a sum over four-cluster states. We call it a natural order when nucleons 1–4 occupy the α-particle state and nucleons 5–7 occupy, in sequence, the states of the two neutrons and of the proton.

The channels with lower threshold energies are already included in the α-n-n-p channel. All degrees of freedom needed to form either a triton or a deuteron out of three nucleons are already present. Also present are the degrees of freedom needed to form, in no-distortion approximation, a ^{6}Li or a ^{6}He from the α cluster and the relevant nucleons.

In correction space, we have a three-cluster, a two-cluster, and a one-cluster sum. The three-cluster sum contains square integrable compound states formed by the nucleons of the α cluster together with one of the nucleons 5, 6, or 7. The remaining two spectator nucleons are described by their spin-isospin states and by the functions $\tilde{\chi}_i$. The number of different spin-isospin states of the nucleons 5, 6, 7 and the number of chosen compound states determine the number $\tilde{n}_3$ of terms in this sum. The α-nucleon compound states should have little or no overlap with states formed by an undistorted α particle in relative motion with a nucleon.

In the sum over two-cluster correction states, the compound states are formed by the nucleons of the α cluster together with two single nucleons. The spectator nucleon is described by its spin-isospin state and by $\tilde{\chi}_i$. Again, the overlap with all states mentioned so far should be kept small.

The one-cluster sum is identical to the distortion part of a conventional resonating group ansatz.[9-11] Even though we are trying, from the beginning, to reduce overlap of states as much as possible, linear dependency will become unavoidable when the number of particles, clusters, and channels becomes large. A second example will show a typical linear dependency.

Example 2. Consider a system of two protons and two neutrons and assume a fictitious interaction which causes the triplet deuteron as well as the singlet deuteron to be bound. Exclude four-particle breakup by taking its threshold as upper limit of allowed energies. Then $N=3$, and the three-cluster sum will consist of two types of functions: (1) a triplet deuteron in relative motion with a neutron and a proton, (2) a singlet deuteron in relative motion with a neutron and a proton. In no-distortion approximation, each one of the two types of functions is fully capable of describing a singlet deuteron in relative motion with a triplet deuteron. The ansatz is overcomplete in the sense that a no-distortion two-body channel can be formed in two ways. Which consequences do we expect?

Overcompleteness of the function basis will certainly be an unpleasant mathematical feature. We believe, however, that it will not be prohibitive. A simple example of similar structure is the following. Consider an operator eigenvalue equation which generates a discrete set of eigenvalues and eigenstates. If a complete and orthogonal representation space for this equation is extended and made overcomplete by the addition of linear combinations of basis states, then the eigenvalues and eigenvectors are still uniquely defined. Numerical methods, also, are available to solve the problem.[13] Only the representation of eigenvectors in the linearly dependent basis will be nonunique.

Similarly, in the present four nucleon example, there is more than one way to express a given microscopic wave function ψ by relative motion functions $\hat{\chi}_i$. The final equation to be solved will be a coupled set of three-body equations. We cannot quote an existing numerical method to solve this problem, but we believe that it can be constructed and that an extra boundary condition will play the essential role in handling the redundant degree of freedom.

The dynamical equation, which is derived in Sec. III, will be very complicated. It has many channels coupled by an interaction matrix. The elements of this matrix contain complicated nonlocal, multibody interactions of infinite range. In order to break down this mathematical monster to its physical contents, a powerful tool will be needed. This tool is the asymptotic serparation property of the dynamical equation. It will be shown that the asymptotic solutions of the full equation satisfy subsystem equations which are similar, in structure, to the full equation.

We want to choose from the function space spanned by Eq. (3) all functions which describe a situation where one part of the A-particle system is confined to one remote area of configuration space, while the remaining part is confined to

another remote area; within both areas the subsystems may undergo scattering and reactions. We call this situation an asymptotic separation of the system. In a multichannel system of identical particles it is not trivial to describe an asymptotic separation. Therefore we give a prescription of how to choose the relevant functions from Eq. (3). Choose one term of the no-distortion part of Eq. (3) and divide the clusters, as defined by their internal motion functions $\varphi_{i,j}$, into two groups. One group of clusters forms subsystem A, the other group forms subsystem B. Introduce a transformation of the Jacobi coordinates $\xi_{i,j}$ in such a way that each one of the two groups of clusters has its own system of Jacobi coordinates. Now, let the center of mass motion of the two groups of clusters be described by two nonoverlapping asymptotic wave packets and use this antisymmetrized cluster state as a probe ψ_i^P. Discard all states ψ_i^C which, because of the separation, are not coupled to the probe by the Hamiltonian

$$\langle\psi_i^P|H|\hat{\psi}_j^C\rangle = \langle\psi_i^P|\hat{\psi}_j^C\rangle = 0\,. \tag{6}$$

The states which do not necessarily have zero coupling can be written in a form similar to the probe. They factorize into an antisymmetrized product of two functions:

$$\psi_k^{A,B} = \mathbf{A}\{\hat{\phi}_k\hat{\chi}_k(\hat{\xi}_k)\}$$
$$= \mathbf{A}\{\hat{\phi}_k^A\hat{\chi}_k^A(\hat{\xi}_k^A)\hat{\phi}_k^B\hat{\chi}_k^B(\hat{\xi}_k^B)\}\,, \tag{7a}$$

$$\langle\psi_i^P|H|\hat{\psi}_k^{A,B}\rangle \neq 0. \tag{7b}$$

The symbol $\hat{\xi}_k$ represents the Jacobi coordinates $\hat{\xi}_{k,1}, \hat{\xi}_{k,2}, \ldots$ of the kth cluster configuration, $\hat{\xi}_k^A$ and $\hat{\xi}_k^B$ represent the relevant subsystem Jacobi coordinates. Adding up the relevant factors $\hat{\phi}_k^A\hat{\chi}_k^A$ and $\hat{\phi}_k^B\hat{\chi}_k^B$, respectively, one gets two expressions which are similar to expression (3) or (5),

$$\psi^A = \sum_k{}' \mathbf{A}\{\hat{\phi}_k^A\hat{\chi}_k^A\}, \quad \psi^B = \sum_k{}' \mathbf{A}\{\hat{\phi}_k^B\hat{\chi}_k^B\}\,. \tag{8}$$

They describe the two subsystems as if they were isolated scattering systems. In Eq. (8), the prime at the sum symbols indicates that not all of the $(n+\bar{n})$ values of k are present in the sum; the states of the probe, of course, are included.

The upper limit of allowed energies, for each subsystem, is obtained by subtraction of the lowest possible physical energy (bound state energy or lowest threshold energy) of the other subsystem from the upper energy limit of the full system.

Our example 1 may again serve as an illustration. Let subsystem A consist of an α-particle and a neutron. The remaining two nucleons form subsystem B, which is assumed to be so far away that the two subsystems do not interact. At the four-cluster level we then have

$$\mathbf{A}\{\phi_i\chi_i(\xi_{i,1},\ldots,\xi_{i,4})\} \to \mathbf{A}\{\phi_i^A\chi_i^A(\xi_{i,1}^A,\xi_{i,2}^A)\phi_i^B\chi_i^B \times (\xi_{i,1}^B,\xi_{i,2}^B)\}\,, \tag{9}$$

where $\xi_{i,1}^A$ and $\xi_{i,1}^B$ are the α-neutron (1) distance and the proton-neutron (2) distance, respectively, while $\xi_{i,2}^A$ and $\xi_{i,2}^B$ are the center of mass coordinates of the two subsystems. The range of indices $_i$ is such that a triplet deuteron with three spin orientations and a singlet deuteron can be formed in subsystem B while the neutron in subsystem A can have spin up or down.

Now we pick a special value of i, say $i=1$, and identify

$$\psi_1^P = \mathbf{A}\{\phi_1^A\chi_1^A\phi_1^B\chi_1^B\} \tag{10}$$

as a probe. Obviously, $\langle\hat{\psi}_j|H|\psi_i^P\rangle$ is equal to zero whenever j refers to a one-cluster state, because the seven-nucleon compound states are square integrable, except for total center of mass motion. We also get zero when j refers to the two-cluster level, because the ^{6}Li and ^{6}He compound states have a finite extension. At the three-cluster level the coupling is not necessarily zero. The correction states, which correct the α-n motion, are coupled to the probe unless some good quantum numbers are different in either subsystem A or B. At the four-cluster level, all those states are coupled to the probe which are needed to construct states with good quantum numbers in both subsystems or, in other words, to construct an irreducible representation of H in cluster space. The asymptotic wave function can be written as

$$\psi^{A,B} = \sum_{i=1}^{n_4}{}' \mathbf{A}[\mathbf{A}\{\varphi_{i,1}\varphi_{i,2}\chi_i^A(\xi_{i,1}^A,\xi_{i,2}^A)\} \times \mathbf{A}\{\varphi_{i,3}\varphi_{i,4}\chi_i^B(\xi_{i,3}^B,\xi_{i,2}^B)\}]$$
$$+ \sum_{i=1}^{n_3} \mathbf{A}[\mathbf{A}\{\tilde{\varphi}_{i,1}\tilde{\chi}_i^A(\tilde{\xi}_{i,1}^A)\} \times \mathbf{A}\{\tilde{\varphi}_{i,2}\tilde{\varphi}_{i,3}\tilde{\chi}_i^B(\tilde{\xi}_{i,1}^B,\tilde{\xi}_{i,2}^B)\}]\,, \tag{11}$$

where the prime at the sum symbol again indicates that some i values are left out in the sum. The antisymmetrizer in front of the square bracket is needed, otherwise Eq. (11) would not be compatible with Eq. (3).

One more word about compatibility of a separation with the full ansatz. Equation (3) spans a space from which one will later construct an irreducible representation space for the dynamical equation. By choosing a probe and using Eq. (6) one will, in general, exclude certain parts of an irreducible subsystem space. Without a tensor force, the triplet deuteron with spin down would be excluded in the present example if the relevant nucleon spin states of the probe have spin up. In

practice, this reduction of the space is a desired feature. If, for an analytic investigation, the reduction is not wanted, one has to use several probes and add all functions which are coupled to at least one of the probes.

From Eq. (11) one sees that the asymptotic separation leads to an ansatz $\psi^{A,B}$ which is, save for an antisymmetrizer in front, a direct product of a subsystem A space and a subsystem B space.

III. THE N-CLUSTER DYNAMICAL EQUATION

The dynamical equation of resonating group theory is obtained by solving the A-particle Schrödinger equation in a space of cluster functions. In the present case, the wave function is given by Eq. (4) and we demand that, with this wave function, the Schrödinger equation is satisfied in the function space given by Eq. (5). In short notation, the dynamical equation reads

$$\langle \delta\psi | (H-E) | \psi \rangle = 0 , \tag{12}$$

where H is the given A-particle Hamiltonian. Inserting Eqs. (4) and (5) we get

$$\sum_{j=1}^{n+\tilde{n}} \langle \mathbf{A}\{\hat{\phi}_i \delta\hat{\chi}_i\} | (H-E) | \mathbf{A}\{\hat{\phi}_j \hat{\chi}_j\} \rangle = 0 . \tag{13}$$

We want to bring this equation into the form: operator × wave function = zero. The states appearing in the matrix elements can be written as

$$\mathbf{A}\{\hat{\phi}_j \hat{\chi}_j(\hat{\xi}_j)\} = \int d\hat{\xi}_j' [\mathbf{A}\{\hat{\phi}_j \delta(\hat{\xi}_j - \hat{\xi}_j')\}] \hat{\chi}_j(\hat{\xi}_j') . \tag{14}$$

The symbol $\hat{\xi}_j$ represents all coordinates $\xi_{j,1}$, $\xi_{j,2}, \ldots$. The integral is a multidimensional one and $\delta(\hat{\xi}_j - \hat{\xi}_j')$ is a product of Dirac δ functions. Note that the antisymmetrizer $\mathbf{A}$ does not operate on primed coordinates. In Dirac notation, we can write

$$|\mathbf{A}\{\hat{\phi}_j \hat{\chi}_j\}\rangle = \int d\hat{\xi}_j' |\mathbf{A}\{\hat{\phi}_j \hat{\xi}_j'\}\rangle \langle \hat{\xi}_j' | \hat{\chi}_j \rangle . \tag{15}$$

The function space $|\mathbf{A}\{\hat{\phi}_i \delta\chi_i\}\rangle$ is written similarly:

$$|\mathbf{A}\{\hat{\phi}_i \delta\hat{\chi}_i\}\rangle = \int d\hat{\xi}_i' |\mathbf{A}\{\hat{\phi}_i \hat{\xi}_i'\}\rangle \langle \hat{\xi}_i' | \delta\hat{\chi}_i \rangle . \tag{16}$$

The states $|\mathbf{A}\{\hat{\phi}_i \hat{\xi}_i'\}\rangle$, for all i and all $\hat{\xi}_i'$, span the same function space as $|\mathbf{A}\{\hat{\phi}_i \delta\hat{\chi}_i\}\rangle$. Therefore Eq. (13) can be written as

$$\sum_{j=1}^{n+\tilde{n}} \int d\xi_j'' \langle \mathbf{A}\{\hat{\phi}_i \hat{\xi}_i'\} | (H-E) | \mathbf{A}\{\hat{\phi}_j \hat{\xi}_j''\} \rangle \langle \hat{\xi}_j'' | \hat{\chi}_j \rangle = 0 , \tag{17}$$

which is the operator form we are looking for. It is a matrix-integro-differential equation. Together with boundary conditions it defines the relative motion functions $\hat{\chi}_j(\hat{\xi}_j)$, from which the microscopic A-particle wave function is obtained by Eq. (4).

The evaluation of the operators

$$\langle \mathbf{A}\{\hat{\phi}_i \hat{\xi}_i'\} | (H-E) | \mathbf{A}\{\hat{\phi}_j \hat{\xi}_j''\} \rangle$$

is straightforward, in principle, provided that the internal states $\hat{\phi}_i$ are given. A classical example is $\alpha - \alpha$ scattering in no-distortion approximation with oscillator shell model ground states as approximate α-particle internal states.[14] Many other two-cluster examples are discussed in Ref. 3. For larger particle numbers, or when distortion corrections are taken into account, Eq. (17) becomes very complicated. Group theoretical methods are very helpful, then, to reduce the number of exchange terms arising from antisymmetrization. We refer to the method of double coset decomposition[15] and to the generator coordinate method.[17] An SU_3 approach[16] to multicluster systems seems to be very promising.

Equation (17) is not yet the final dynamical equation. We want to treat clusters like elementary particles, namely as point particles which are coupled by an interaction. The internal degrees of freedom of the clusters as well as the Pauli principle should enter by the interaction, only. Equation (17) still includes the distortion amplitudes $\tilde{\chi}_i$ as unknown functions, while we want to have a theory in terms of the functions χ_i alone. Therefore we eliminate the functions $\tilde{\chi}_i$. In the more explicit notation of Eq. (4), Eq. (17) reads

$$\sum_{j=1}^{n} \int d\xi_j'' \langle \mathbf{A}\{\phi_i \xi_i'\} | (H-E) | \mathbf{A}\{\phi_j \xi_j''\} \rangle \langle \xi_j'' | \chi_j \rangle + \sum_{j=1}^{\tilde{n}} \int d\tilde{\xi}_j'' \langle \mathbf{A}\{\phi_i \xi_i'\} | (H-E) | \mathbf{A}\{\tilde{\phi}_j \tilde{\xi}_j''\} \rangle \langle \tilde{\xi}_j'' | \tilde{\chi}_j \rangle = 0 \quad i = 1, \ldots, n , \tag{18a}$$

$$\sum_{j=1}^{n} \int d\xi_j'' \langle \mathbf{A}\{\tilde{\phi}_i \tilde{\xi}_i'\} | (H-E) | \mathbf{A}\{\phi_j \xi_j''\} \rangle \langle \xi_j'' | \chi_j \rangle + \sum_{j=1}^{\tilde{n}} \int d\tilde{\xi}_j'' \langle \mathbf{A}\{\tilde{\phi}_i \tilde{\xi}_i'\} | (H-E) | \mathbf{A}\{\tilde{\phi}_j \tilde{\xi}_j''\} \rangle \langle \tilde{\xi}_j'' | \tilde{\chi}_j \rangle = 0 \quad i = 1, \ldots, \tilde{n} . \tag{18b}$$

The elimination is achieved by solving the second equation for $\langle \tilde{\xi}_j | \tilde{\chi}_j \rangle$ and inserting the formal solution into the first equation. The solutions of

$$\sum_{j=1}^{\tilde{n}} \int d\tilde{\xi}_j'' \langle \mathbf{A}\{\tilde{\phi}_i \tilde{\xi}_i'\} | (H-E) | \mathbf{A}\{\tilde{\phi}_j \tilde{\xi}_j''\} \rangle \langle \tilde{\xi}_j'' | \tilde{\chi}_j \rangle = 0 , \tag{19}$$

for a full set of boundary conditions and all energies, allow the construction of a matrix Green's function

$$G_{ik}(E,\tilde{\xi}_i'',\tilde{\xi}_k') = \sum_e \langle\tilde{\xi}_i''|\tilde{\chi}_i(e)\rangle \frac{1}{E-E(e)} \langle\tilde{\chi}_k(e)|\tilde{\xi}_k'\rangle . \tag{20}$$

The symbol e labels the spectrum of solutions. It characterizes the boundary condition and the energy $E(e)$, for which $\langle\tilde{\xi}_j|\tilde{\chi}_j(e)\rangle$ is a solution of Eq. (19). Since we do not yet want to introduce a special boundary condition, such as a boundary condition which specifies the incoming wave, no $i\epsilon$ appears in the denominator. The singularity is just left as it is. We will come back to this point in Sec. VI. With this Green's function we can formally solve Eq. (18):

$$\langle\tilde{\xi}_j''|\tilde{\chi}_j\rangle = \sum_e \langle\tilde{\xi}_j''|\tilde{\chi}_j(e)\rangle \frac{1}{E-E(e)} \times \sum_{k=1}^{\tilde{n}} \int d\tilde{\xi}_k' \langle\tilde{\chi}_k(e)|\tilde{\xi}_k'\rangle \sum_{h=1}^{n} \int d\xi_h''' \langle \mathbf{A}\{\tilde{\phi}_k\tilde{\xi}_k'\}|(H-E)|\mathbf{A}\{\phi_h\xi_h'''\}\rangle\langle\xi_h'''|\chi_h\rangle . \tag{21}$$

The solution is inserted into Eq. (18a):

$$\sum_{j=1}^{n} \int d\xi_j'' \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\mathbf{A}\{\phi_j\xi_j''\}\rangle\langle\xi_j''|\chi_j\rangle + \sum_{j=1}^{\tilde{n}} \int d\tilde{\xi}_j'' \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\mathbf{A}\{\tilde{\phi}_j\tilde{\xi}_j''\}\rangle \sum_e \langle\tilde{\xi}_j''|\tilde{\chi}_j(e)\rangle \frac{1}{E-E(e)} \sum_{k=1}^{\tilde{n}} \int d\tilde{\xi}_k^{IV} \langle\tilde{\chi}_k(e)|\tilde{\xi}_k^{IV}\rangle \times \sum_{h=1}^{n} \int d\xi_h''' \langle \mathbf{A}\{\tilde{\phi}_k\tilde{\xi}_k^{IV}\}|(H-E)|\mathbf{A}\{\phi_h\xi_h'''\}\rangle\langle\xi_h'''|\chi_h\rangle = 0 . \tag{22}$$

The sum over j in the first term runs over the n coupled channels of the no-distortion part of cluster space. The sum over h in the second term does the same. We combine the two sums and get

$$\sum_{j=1}^{n} \int d\xi_j'' [\langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\mathbf{A}\{\phi_j\xi_j''\}\rangle + \sum_e \sum_{c=1}^{\tilde{n}} \int d\xi_c''' \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\mathbf{A}\{\tilde{\phi}_c\tilde{\xi}_c'''\}\rangle\langle\tilde{\xi}_c'''|\tilde{\chi}_c(e)\rangle \frac{1}{E-E(e)} \sum_{k=1}^{\tilde{n}} \int d\xi_k^{IV} \langle\tilde{\chi}_k(e)|\tilde{\xi}_k^{IV}\rangle \times \langle \mathbf{A}\{\tilde{\phi}_k\tilde{\xi}_k^{IV}\}|(H-E)|\mathbf{A}\{\phi_j\xi_j''\}\rangle]\langle\xi_j''|\chi_j\rangle = 0 \qquad (i=1,\ldots,n). \tag{23}$$

This is the dynamical equation of the N-cluster system. From this equation we want to derive properties of composite particle motion and composite particle interaction.

The second term in the square bracket of Eq. (23) starts and ends like the first term, namely with $\langle \mathbf{A}\{\phi_i\xi_i'\}|$ and $|\mathbf{A}\{\phi_i\xi_j''\}\rangle$, respectively. We can therefore interpret the operator

$$\sum_e \sum_{c=1}^{\tilde{n}} \int d\tilde{\xi}_c''' (H-E)|\mathbf{A}\{\tilde{\phi}_c\tilde{\xi}_c'''\}\rangle\langle\tilde{\xi}_c'''|\tilde{\chi}_c(e)\rangle \frac{1}{E-E(e)} \sum_{k=1}^{\tilde{n}} \int d\tilde{\xi}_k^{IV} \langle\tilde{\chi}_k(e)|\tilde{\xi}_k^{IV}\rangle\langle \mathbf{A}\{\tilde{\phi}_k\tilde{\xi}_k^{IV}\}|(H-E) \tag{24}$$

as an effective interaction which arises from the elimination of the distortion part. It may have poles, depending on whether $E(e)$ lies inside or outside of the allowed energy range. When it is sandwiched between $\langle \mathbf{A}\{\phi_i\xi_i'\}|$ and $|\mathbf{A}\{\phi_j\xi_j''\}\rangle$ this operator becomes a (nonlocal) matrix potential which operates on the relative motion states $\langle\xi_j|\chi_j\rangle$.

Equation (23) has the form

$$\sum_{j=1}^{n} [O_{ij}(E) + \tilde{O}_{ij}(E)]|\chi_j\rangle = 0 , \tag{25}$$

where O_{ij} denotes the first term and $\tilde{O}_{ij}$ the second term in the square brackets of Eq. (23). The equation is a coupled channel integro-differential equation for the relative motion functions $\langle\xi_j|\chi_j\rangle$, where j runs from 1 to n.

Let us analyze the operators O_{ij} and $\tilde{O}_{ij}$. At first we consider O_{ii}. Since H and E are symmetric with respect to particle exchange, antisymmetrization has to be carried out only at one side:

$$O_{ii}(E;\xi_i',\xi_i'') \equiv \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\mathbf{A}\{\phi_i\xi_i''\}\rangle = \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\phi_i\xi_i''\rangle . \tag{26}$$

From the properly normalized sum over exchange terms $\mathbf{A}\{\phi_i\xi_i'\}$ we extract $\mathbf{1}\{\phi_i\xi_i'\}$ and call the rest $\mathbf{A}'\{\phi_i\xi_i'\}$. Formally, this reads

$$\mathbf{A} = \mathbf{1} - \mathbf{A}' . \tag{27}$$

For the cluster decomposition of channel i, in natural ordering of particles, the Hamiltonian decomposes into an internal part H_i and an external part

$V^i + T^i$;

$$H = H_i + V^i + T^i . \tag{28}$$

The operator O_{ii} then reads

$$O_{ii}(E;\xi_i',\xi_i'') = \langle (1-\mathbf{A}')\{\phi_i\xi_i'\}|(H_i + V^i + T^i - E)|\phi_i\xi_i''\rangle . \tag{29}$$

From the 1, together with T^i we get the kinetic energy operator for the center of mass motion of the clusters. From the 1 together with V^i we get an interaction $V_{D,i}$ which is called direct interaction. It is the same expression as what is sometimes called double folding interaction in optical model theory. When the nucleon-nucleon potential is local, then this potential is a local one. From the 1 together with H_i we get a sum of cluster eigenenergies or, when H_i contains approximate eigenstates, a sum of cluster energy expectation values. From $\mathbf{A}'$, together with H_i, V^i, T^i and E, a complicated energy-dependent nonlocal potential $k_{ii}(E;\xi_i',\xi_i'')$ is obtained. Putting things together, we have

$$O_{ii}(E;\xi_i',\xi_i'') = \sum_k \frac{-\hbar^2}{2M_k}\Delta_{\xi_i'',k}\delta(\xi_i'-\xi_i'') + V_{D,i}(\xi_i',\xi_i'') + k_{ii}(E;\xi_i',\xi_i'') - E_{\mathrm{rel.},i}\delta(\xi_i'-\xi_i'') . \tag{30}$$

The relative motion energy $E_{\mathrm{rel.},i}$ is obtained by subtraction of the cluster eigenenergies (or expectation values) from the total energy E:

$$E_{\mathrm{rel.},i} = E - \langle\phi_i|H_i|\phi_i\rangle . \tag{30a}$$

The energy dependence of $k_{ii}(E;\xi_i',\xi_i'')$ is rather simple. In terms of the norm operator K_i, defined by

$$K_i(\xi_i',\xi_i'') = \langle \mathbf{A}'\{\phi_i\xi_i'\}|\phi_i\xi_i''\rangle , \tag{31}$$

it is

$$k_{ii}(E;\xi_i',\xi_i'') = \bar{k}_i(\xi_i',\xi_i'') + EK_i(\xi_i',\xi_i'') , \tag{32}$$

both $\bar{k}_{ii}$ and K_i are Hermitian integral operators.

The operator $\tilde{O}_{ii}$ has been obtained by elimination of the correction part in wave function space. It represents the influence of internal degrees of freedom on the interaction of the clusters. In order to see its structure we start from expression (24) and carry out the integration over ξ_c''' and ξ_k^{IV}. This expression then reads

$$\sum_e \sum_{c,k=1}^{\tilde{n}} (H-E)|\mathbf{A}\{\phi_c\tilde{\chi}_c(e)\rangle \frac{1}{E-E(e)} \langle \mathbf{A}\{\phi_k\tilde{\chi}_k(e)\}|(H-E) . \tag{33}$$

With respect to its indices c and k, this expression is a microscopic separable interaction operator of finite rank. But, since we have eliminated continuous degrees of freedom, there is also the continuous label e. Sandwiching the microscopic interaction between $\langle \mathbf{A}\{\phi_i\xi_i'\}|$ and $|\mathbf{A}\{\phi_i\xi_i''\}\rangle$ we get

$$\tilde{O}_{ii}(E;\xi_i',\xi_i'') = \sum_e \sum_{c,k=1}^{\tilde{n}} \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\phi_c\tilde{\chi}_c(e)\rangle \frac{1}{E-E(e)} \times \langle\tilde{\phi}_k\tilde{\chi}_k(e)|(H-E)|\mathbf{A}\{\phi_i\xi_i''\}\rangle . \tag{34}$$

In the two-cluster case, with one-cluster correction functions, it has been shown in Ref. 3, p. 150, that such a singular elimination potential produces a Breit-Wigner resonance whenever the eliminated state is a virtual bound state; correction states which only describe cluster deformations will lead to poles which lie far away from the range of allowed energies.

The off-diagonal elements of the matrix operators O and $\tilde{O}$ are energy-dependent nonlocal interactions:

$$O_{ij}(E;\xi_i',\xi_j'') = \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\phi_j\xi_j''\rangle , \tag{35a}$$

$$\tilde{O}_{ij}(E;\xi_i',\xi_j'') = \sum_e \sum_{c,k=1}^{\tilde{n}} \langle \mathbf{A}\{\phi_i\xi_i'\}|(H-E)|\tilde{\phi}_c\tilde{\chi}_c(e)\rangle \frac{1}{E-E(e)} \times \langle\tilde{\phi}_k\tilde{\chi}_k(e)|(H-E)|\mathbf{A}\{\phi_j\xi_j''\}\rangle . \tag{35b}$$

It has tacitly been assumed that the microscopic Schrödinger equation has a Hermitian Hamiltonian. With two wave packets ψ_{I} and ψ_{II}, taken from the ansatz (4) and real energy E we then have

$$\langle\psi_{\mathrm{I}}|(H-E)|\psi_{\mathrm{II}}\rangle = \langle\psi_{\mathrm{II}}|(H-E)|\psi_{\mathrm{I}}\rangle^* . \tag{36}$$

Going through the derivation of Eq. (25) we see that this leads to the relation

$$\sum_{i,j}\langle\chi_{\mathrm{I},i}|(O_{i,j}+\tilde{O}_{ij})|\chi_{\mathrm{II},j}\rangle = \sum_{i,j}\langle\chi_{\mathrm{II},j}|(O_{ji}+\tilde{O}_{ji})|\chi_{\mathrm{I},i}\rangle^* . \tag{37}$$

Since this relation is true for any two wave packets of our cluster function space, we conclude that

$$O_{ij}(E;\xi_i',\xi_j'') = O_{j,i}^*(E;\xi_j'',\xi_i') , \tag{38a}$$

$$\tilde{O}_{ij}(E;\xi_i',\xi_j'') = \tilde{O}_{ji}^*(E;\xi_j'',\xi_i'') \tag{38b}$$

for all values of i and j. With energy being considered a given parameter, the interaction of composite particles is Hermitian.

When the dynamical equation (23) has been solved for a certain boundary condition, the eliminated functions $\tilde{\chi}_j$ are calculated by Eq. (21) and the microscopic solution is given by Eq. (4). Introducing a column operator (Q_j) for shorter notation we get

$$\psi_E(\boldsymbol{r}) = \sum_j \int d\xi_j' Q_j(E;\boldsymbol{r},\xi_j')\chi_j(\xi_j') \tag{39}$$

with

$$Q_j(E;r,\xi_j') = \langle r|\mathbf{A}\{\phi_j\xi_j'\}\rangle + \sum_i \int d\tilde{\xi}_i'' \sum_e \langle r|\mathbf{A}\{\tilde{\phi}_i\tilde{\xi}_i''\}\rangle\langle\tilde{\xi}_i''|\tilde{\chi}_i(e)\rangle \frac{1}{E-E(e)}$$
$$\times \sum_k \int d\tilde{\xi}_k'''\langle\tilde{\chi}_k(e)|\tilde{\xi}_k'''\rangle\langle\mathbf{A}\{\tilde{\phi}_k\tilde{\xi}_k'''\}|(H-E)|\mathbf{A}\{\phi_j\xi_j'\}\rangle\,. \tag{40}$$

One can see, here, how the boundary condition on χ_i is transferred to the motion of the spectator clusters in distortion states. From the sum and integral over e, only those states contribute which have nonzero overlap with the spectator motion as described by χ_i.

With respect to the total center of mass motion, the separation property of Eq. (23) is the same as that of the original Schrödinger equation. This is due to the fact that antisymmetrization has no effect on the total center of mass coordinate. When the microscopic Hamiltonian is translationally invariant, then the center of mass motion function $\chi_{c.m.}(\xi_{c.m.})$ is a common factor of all functions $\chi_i(\xi_i)$. While the quantum mechanical interpretation of a solution $\chi_i(\xi_i)$ is still open, we are certain that the center of mass function $\chi_{c.m.}$ has all properties of a single particle state, save for the case where the whole system occupies a Pauli excluded state. This feature will be needed in the discussion on asymptotic subsystem behavior.

IV. UNITARITY

A unitarity proof for equations based on Eq. (12) is given in Ref. 3, p. 6 ff. In this proof, the wave function ψ is assumed to be any linear expansion with a discrete and/or a continuous set of expansion coefficients. Since the present ansatz is of that type we can just take over the result.

The solutions of Eq. (12) together with Eq. (3) are orthogonal to each other (after degeneracy has been removed) and diagonalize the Hamiltonian:

$$\langle\psi(e')|\psi(e)\rangle = \delta(e',e)\,, \tag{41a}$$
$$\langle\psi(e')|H|\psi(e)\rangle = E(e)\delta(e',e)\,. \tag{41b}$$

It should be noted that the orthogonality relation holds for the full wave function ψ. This does not imply that it also holds for the relative motion solution χ_i of Eq. (23) or for the solution $\tilde{\chi}_i$ of Eq. (17). The functions χ_i and $\tilde{\chi}_i$ have been introduced as expansion coefficients in a nonorthogonal space. It is tempting to consider χ_i a quantum mechanical wave function which describes the relative motion of composite particles, as well as the center of mass motion of the system. Sometimes, this interpretation will be allowed. But one always has to make sure that it follows from the interpretation of ψ as being the quantum mechanical wave function.

From relations (41a) and (41b), it is concluded in Ref. 2 that the norm of wave packets stays constant in time, which means conservation of probability. When, in addition, the function space allows the construction of initial and final states, one gets conservation of flux and unitarity.

The critical point in the unitarity proof of Ref. 3 is the assumption that scattering states can be treated as square integrable states. This assumption, however, is not only made in cluster theory. In potential scattering theory, for instance, the problem of non-normalizable states is similar and the common technique of radius averaging or asymptotic dampening has the same consequence as wave packet normalization. The infinite configuration space becomes finite while scattering states are still considered to have a continuous spectrum of sharp energies.

A similar assumption will be used in Sec. V when the asymptotic property of the dynamical equation is investigated. It will be assumed that it is possible to physically separate a scattering system into two subsystems in such a way that each subsystem has a sharply defined energy, and yet, the two subsystems do not overlap.

V. ASYMPTOTIC SEPARATION OF THE DYNAMICAL EQUATION

It has been shown in Sec. II that the full wave function factorizes into an antisymmetrized product of two wave functions ψ^A and ψ^B when the scattering system is asymptotically separated into the two subsystems A and B. It is easy to show that, as a consequence of Eqs. (7a) and (7b), Eq. (17) separates into two equations, each one describing one of the subsystems. We are more interested, however, in Eq. (23) because this is the N-cluster equation with eliminated internal degrees of freedom.

In order to study the separation property of Eq. (23) we need projection operators Γ^A and Γ^B, which guarantee that the two subsystems are confined to two nonoverlapping asymptotic regions of the $3N$-dimensional configuration space. The two projection operators are constructed from the solutions of the two subsystem equations:

$$\sum_j [O^A_{ij}(e^A) + \tilde{O}^A_{ij}(e^A)]|\chi^A_j(e^A)\rangle = 0\,, \tag{42}$$

$$\sum_j [O^B_{ij}(e^B) + \tilde{O}^B_{ij}(e^B)]|\chi^B_j(e^B)\rangle = 0\,. \tag{43}$$

We assume that the operators of these equations are directly derived from the wave function ansatz of the subsystems A and B, Eq. (8). The labels e^A, e^B denumerate the two spectra, including the energy eigenvalues $E^A(e^A)$ and $E^B(e^B)$. From the solutions $\chi^A_j(e^A)$, $\chi^B_j(e^B)$ we get the microscopic wave functions $\psi^A(e^A)$ and $\psi^B(e^B)$ by Eq. (39), with operators Q^A_j and Q^B_j instead of Q_j. The microscopic functions form an orthonormal set, as we know from Eq. (41a). In terms of microscopic functions it can be stated more precisely what is meant by asymptotic separation. Let all functions $\psi^A(e^A)$ describe subsystem A as being confined to some area of configuration space.[18] Similarly, let $\psi^B(e^B)$ describe subsystem B as being confined to some other area of configuration space. In order to get two separated subsystems, the two areas must not be infinitely large in all directions. We consider them to be finite and use the same argument as in the Sec. IV, i.e., assume wave packet normalization for scattering states and neglect the energy uncertainty. The operator Γ^A is defined as

$$\Gamma^A_{ij}(\xi^{A\prime}_i, \xi''_j) = \sum_{e^A e^B} \int dr \langle \xi^{A\prime}_i | \chi^A_i(e^A)\rangle \times \langle \psi^B(e^B)\psi^A(e^A)|r\rangle Q_j(E; r, \xi''_j) \tag{44}$$

for all index values i, j which are present in the no-distortion part of the sums of Eq. (8). All values of i and j which are not present in Eq. (8) refer to components of the wave function which are necessarily zero when the system is separated into the two subsystems. For these values of i and j we put $\Gamma^A_{ij} = 0$. The operator Γ^B is defined analogously to Γ^A.

With help from the projection operators Γ^A, Γ^B the asymptotic structure of a solution χ_j of Eq. (23) can be analyzed. The set of functions

$$\langle \xi^{A\prime}_i | \chi_i(E)\rangle^A{}_{\text{asympt.}} = \sum_j \int d\xi''_j \Gamma^A_{ij}(\xi^{A\prime}_i, \xi''_j)\langle \xi''_j | \chi_j(E)\rangle \tag{45}$$

is the asymptotic part of χ_j which describes the motion of subsystem A as a wave packet in some large, remote area.

Similarly, the set of functions

$$\langle \xi'_i | \chi_i(E)\rangle^{A,B} = \sum_j \int d\xi''_j \Gamma^A_{ij}(\xi^{A\prime}_i, \xi''_j)\langle \xi''_j | \chi_j(E)\rangle \times \sum_k \int d\xi'''_k \Gamma^B_{ik}(\xi^{B\prime}_i, \xi'''_k)\langle \xi'''_k | \chi_k(E)\rangle \tag{46}$$

is the asymptotic part of a solution χ_j which describes subsystem A as moving in one asymptotic area while subsystem B is moving in another asymptotic area of configuration space.

The asymptotic property of the dynamical equation (23) is now studied by asking the following: When does the set of functions $\langle \xi'_i | \chi_i(E)\rangle^{A,B}$ satisfy Eq. (23)? The answer is that one of the following three statements must be true:

(i) $\langle \xi'_i | \chi_i(E)\rangle^{A,B}$ is a product of solutions of the subsystem [Eqs. (42) and (43)]

$$\langle \xi'_i | \chi_i(E)\rangle^{A,B} = \langle \xi^{A\prime}_i | \chi^A_i(E^A)\rangle \langle \xi^{B\prime}_i | \chi^B_i(E^B)\rangle \tag{47a}$$

with

$$E = E^A + E^B\,. \tag{47b}$$

(ii) $\langle \xi'_i | \chi_i(E)\rangle^{A,B}$ is a sum (or integral) of such products, each product satisfying Eq. (47b).

(iii) $\langle \xi'_i | \chi_i(E)\rangle^{A,B}$ is identically zero or Pauli-forbidden.

For a proof, one has to insert Eq. (46) into Eq. (23), use the explicit notation of Eqs. (44) and (40), and evaluate the operator products. It is then seen that the projection operators Γ^A and Γ^B have the effect that Eqs. (18)–(23) become operator equations in a product space. Equation (23) is satisfield only when the factors of the product space satisfy Eqs. (42) and (43) under the condition of Eq. (47b). The detailed calculation is rather lengthy and may be skipped here. With the asymptotic separation property, as expressed by Eqs. (46), (47a) and (47b), we now have a powerful tool to analyze the relative motion wave function of composite particles as well as their interaction.

At first, we check whether there are unphysical solutions. Our ansatz, Eq. (3), has correction functions with a continuous degeee of freedom. Among the clusters described by the internal part $\tilde{\phi}_i$ of a correction state, there is at least one unstable cluster, and the relative motion function $\tilde{\chi}_i$ is assumed to be completely free. A function $\mathbf{A}\{\tilde{\phi}_i\tilde{\chi}_i\}$ has all the flexibility needed for an excited cluster to appear, asymptotically, as a composite particle of its own. This, of course, is unphysical. The equation which determines the scattering state, Eq. (23) together with Eq. (39), must not allow such "ghost states," otherwise the theory would be wrong. Indeed, from the asymptotic separation property, one can immediately see that such ghost states will not appear. An isolated ex-

cited cluster defines a subsystem, but its wave function does not satisfy the subsystem equation. From Eqs. (8), (42), (43), and (47a) and (47b) we see that unstable cluster states will appear, asymptotically, only when and where they are needed as correction states in a subsystem wave function.

Let us consider, again, the seven-nucleon system as an example. Choose a separation into subsystems A and B as discussed in Sec. II. From the solution χ_j of the $N=4$ dynamical equation we project out an asymptotic part according to Eq. (46). From Eqs. (47a) and (47b) we see that this part must be a product of an n-α resonating group wave function and a wave function satisfying the Schrödinger equation of n-p scattering, or it must be a superposition of such products. The n-α solution is a distortion corrected scattering state. As many correction states are coupled to the no-distortion state as are needed and as are available by the ansatz. Experience with two-cluster resonating group theory[19] indicates that only a small number of correction states will be needed to obtain quite realistic scattering states; the no-distortion approximation, already, is very good.

In our example, we may leave reality and assume a Hamiltonian which has a bound ^{5}He state. The solution χ_j will then contain an n-p-^{5}He breakup channel. The asymptotic ^{5}He state will satisfy the subsystem equation. It will be a fully corrected ^{5}He bound state and not just a bound state of neutron and α in no-distortion approximation.

The transition to the microscopic seven-particle wave function $\psi_E(r)$ is given by Eq. (39). Since $\psi_E(r)$ is, by definition, a quantum mechanical wave function, it determines the flux as well as the S and the T matrix.

VI. INTERPRETATION OF THE WAVE FUNCTION AND CRITICAL REMARKS

The Schrödinger theory, with a phenomenological interaction, is commonly applied to particles such as nucleons, which are by no means structureless point particles. In most papers, it is tacitly assumed that the obtained wave function has a probability interpretation, i.e., the absolute square of the wave function is considered to be a probability density. When discrepancies arise with charge form factors or Coulomb energy differences, one generally believes that something is wrong with the off-shell behavior of the phenomenological interaction. Some people felt uneasy, though, with the whole concept of a Schrödinger theory with phenomenological potentials. Noyes for instance, suggested throwing overboard the off-shell ambiguity. When the off-shell behavior of an interaction is ambiguous, why not fix it in such a way that particles move on the energy shell all the time? The consequence of this idea is a boundary condition model in zero range limit.[20]

The present theory is based on the assumption that a nonrelativistic Schrödinger theory with fundamental interactions is valid at some microscopic level. It may be the level of quarks in hadron physics, or the level of point particles with mass and charge in atomic physics, or the level of nucleons in cluster physics. As an illustration, the latter example is used in this paper, although the theory is more general. From the first level we get to a second level by deriving a nonrelativistic quantum dynamical wave equation for composite particles. At the second level, quantum dynamics is again described by an equation which is similar to the Schrödinger equation. There are, however, some important differences. The number of composite particles is not conserved, because N composite particles are coupled to $(N-1)$, $(N-2)$, and so on. The interaction, even in the case of a very simple microscopic interaction, is as complicated as the realistic nucleon-nucleon interaction has become in the course of many years of investigation (nonlocality, dependence in various quantum numbers, mixture of repulsion and attraction, three- and more-body forces). The most important feature is that the wave function is no longer a probability amplitude in all regions of configuration space. Let us take a closer look at this feature.

The final solution, in the present theory, is the microscopic wave function ψ. Since the validity of Schrödinger theory has been assumed at the first level, this function has a probability interpretation. In case of doubt, we always have to go back to this mircroscopic wave function ψ. From it we can get the S and T matrix, because the flux of particles follows immediately from the c.m. velocity and c.m. probability density of asymptotic subsystems. At the second level, the wave function is a set of functions $\chi_1, \chi_2, \ldots, \chi_n$. These functions have been introduced as relative motion functions of undistorted clusters, before antisymmetrization. This indicates that they might have something to do with a quantum mechanical wave function describing the motion of composite particles. But we had to introduce excited clusters also, with functions $\tilde{\chi}_1, \tilde{\chi}_2, \ldots, \tilde{\chi}_{\tilde{n}}$ of similar nature. The introduction of these functions is a consequence of the fact that composite particles have internal degrees of freedom. According to Eqs. (18a) and (18b), the internal degrees of freedom are coupled to the relative motion of the composite particles. In the final equation, Eq. (23), the internal degrees of freedom are no longer present explicitly. Their effect has been incorporated in-

to the interaction. After elimination of the distortion degrees of freedom the unknown functions $\chi_1, \chi_2, \ldots \chi_n$ must be considered a storage of information, mainly. The information is obtained by solving Eq. (23), with boundary conditions, and is then used to determine the eliminated functions and the microscopic solution ψ. Moreover, the solutions $\chi_1, \chi_2, \ldots, \chi_n$ are ambiguous, to a certain degree, because part of the motion of undistorted clusters can be packed into distortion space (recall that orthogonality of basis functions was not required). We will investigate this ambiguity in more detail in the next paper. Here it is enough to see that $\chi_1, \ldots, \chi_n$ is definitely not a probability amplitude of the density of clusters in the region where clusters interact. It is planned to show by a numerical example that form factor discrepancies and Coulomb energy discrepancies of similar nature as those encountered with nucleons must arise when an N-cluster relative motion function $\chi_1, \ldots, \chi_n$ is treated as a quantum mechanical wave function at short cluster distances.

Asymptotically, however, the solution $\chi_1, \ldots, \chi_n$ of Eq. (23) does become a quantum mechanical wave function. This conclusion follows from the asymptotic separation property, together with the fact that center of mass motion functions are single particle wave functions. Whenever a cluster, or a bound state of several clusters, has left the region of interaction with other parts of the system it may be considered a subsystem, denoted by A. The nonzero components $\chi_1^A, \ldots, \chi_{n_A}^A$ of the wave function $\chi_1, \ldots, \chi_n$ satisfy Eq. (42). These components still have the center of mass motion $\chi_{\text{c.m.}}(\xi_{\text{c.m.}})$ of the full system as a common factor. But, since subsystem A has now become a composite particle system of its own, the center of mass motion $\chi_{\text{c.m.}}^A(\xi_{\text{c.m.}}^A)$ of the subsystem, also, is a common factor to $\chi_1^A, \ldots, \chi_{n_A}^A$. Particle exchange within the subsystem has no effect on the coordinate $\xi_{\text{c.m.}}^A$. Unless antisymmetrization of the full system has a long range effect on the subsystem, the subsystem c.m. motion $\chi_{\text{c.m.}}^A(\xi_{\text{c.m.}}^A)$ has the properties of a single particle state. Without such a long range effect and with a normalized internal motion of subsystem A, the function

$$\rho(\xi_{\text{c.m.}}^A) = |\chi_{\text{c.m.}}^A(\xi_{\text{c.m.}}^A)|^2 \tag{48}$$

expresses the probability density of finding the center of mass of subsystem A at the position $\xi_{\text{c.m.}}^A$.

The total antisymmetrization has long range effects when two or more clusters are identical. In this case, some of the partial waves are Pauli-forbidden and must be omitted when the probability density is calculated. An example are the odd-parity states in an α-α relative motion. There will be no trouble, in practice, because such states are not generated by Eq. (23), unless the initial condition is chosen carelessly. But one should be aware of the fact that states of wrong exchange symmetry are not excluded by the dynamical equation; they satisfy the equation because they are trivial solutions of the microscopic problem.

In this connection it is interesting to see what one gets from Eq. (23) when N becomes equal to A. One might expect to get back the usual Schrödinger equation because, for $N=A$, the ansatz (3) has no clusters. But we do not get the usual Schrödinger equation. The reason is that Eq. (23) has a knowledge of exchange symmetry while the Schrödinger equation has not. This difference is demonstrated by an example of two noninteracting fermions in a symmetric spin state. After separation of the center of mass motion, Eq. (23) reads, in this case,

$$\int d^3r'' \left[\frac{-\hbar^2}{m}\Delta_{r'} - E\right][\delta(\vec{r}' - \vec{r}'') - \delta(\vec{r}' + \vec{r}'')]\chi(\vec{r}'') = 0, \tag{49}$$

while the Schrödinger equation reads

$$[(-\hbar^2/m)\Delta_{r'} - E]\chi(\vec{r}') = 0. \tag{50}$$

Both equations have the same antisymmetric solution

$$\chi(\vec{r}) = \exp(i\vec{k}\vec{r}) - \exp(-i\vec{k}\vec{r}), \tag{51}$$

with $|\vec{k}| = (Em/\hbar^2)^{1/2}$. But the symmetric solutions are not quite the same. Equation (49) is satisfied by all functions,

$$\chi(\vec{r}) = \exp(i\vec{K}\vec{r}) + \exp(-i\vec{K}\vec{r}), \tag{52}$$

no matter what the value of K is. Equation (50) is satisfied by this function only for $|\vec{K}| = |\vec{k}|$. Equation (49) is a wave equation for two fermions in a symmetric spin state, while Eq. (50) is a quantum dynamical equation for just two particles. For the two fermions, the function of Eq. (52) is a trivial solution for all $\vec{K}$, because it vanishes upon antisymmetrization. In Eq. (49) the long range effect of antisymmetrization is expressed by the nonlocal potential of infinite range:

$$\vec{V}(\vec{r}', \vec{r}'') = [(\hbar^2/m)\Delta_{r'} + E]\delta(\vec{r}' + \vec{r}''). \tag{53}$$

Such potentials also appear in Eq. (23) when clusters are identical. Their presence is not disturbing, once their meaning is understood. Basically, Eqs. (49) and (50) are the same.

A few critical remarks on the present theory may be appropriate. We did not bother to prove the existence of a unique solution of the dynamical equation. With a second order differential equa-

tion, uniqueness is mainly a question of boundary conditions. Even in example 2 of Sec. II, where the function space is overcomplete, uniqueness can probably be achieved by the boundary condition. We also did not prove the existence of the operators which appear in the dynamical equation (23). Formally, they are defined. But their definition includes the construction of a Green's function in a certain restricted function space. In order to construct the Green's function for an N-cluster problem, one has to be able to solve the $(N-1)$ cluster problem, and that leads back to the question of existence of a unique solution. At this point, we have to recall that the present theory is an extension of a well-established, existing theory. For $N=2$ all distortion functions of Eq. (3) are square integrable, except for center of mass motion, and Eq. (23) becomes identical to the resonating group equation. In this case, many numerical examples have been studied, and there is no doubt about the existence of operators and wave functions. Because of this, we are able to solve $N=2$ equations and construct the Green's functions needed for $N=3$. Objections may arise because we formally left the singularity in the Green's function (20). In the $N=3$ case, it is clear what will happen. When the eliminated state is a square integrable subsystem correction multiplied by the center of mass motions of the subsystem and by the wave function of the spectator cluster, then we will get a singular elimination potential for the subsystem. The singularity of the potential will be caused by a denominator $\bar{E}-\langle\tilde{\varphi}|\bar{H}|\tilde{\varphi}\rangle$, where the bar refers to the subsystem and $\tilde{\varphi}$ is the compound or distortion state of the subsystem. The effect of such a potential is well understood (see Ref. 3, p. 150). It leads to a Breit-Wigner resonance of the subsystem. The resonance will be narrow or wide, inside or outside of the allowed energy region, depending on the value of $\langle\tilde{\varphi}|\bar{H}|\tilde{\varphi}\rangle$ and on the coupling to the open channel. The coupling to the relative motion wave function of the undistorted clusters dislocates the singularity of the elimination potential to the complex energy plane, where it becomes a pole of the S matrix. In the $N=3$ case, the Breit-Wigner resonance will be coupled to the motion of the spectator cluster. At large distances, the spectator will be described by an internal function and by either an incoming, an outgoing, or a standing wave, depending on the boundary condition which has been imposed on Eq. (23). Numerical calculations for $N=3$ using a separable interaction approximation together with a Faddeev technique are presently under preparation. For $N\geq 4$, the theory is still a formal one. It allows, however, the investigation of general features of composite particle dynamics.

VII. CONCLUSION

A nonrelativistic quantum dynamical theory of composite particles has been derived from the assumption that the nonrelativistic Schrödinger theory with a given Hamiltonian is valid for the motion of the constituents. For two composite particles, the present theory is identical to resonating group theory. For more than two composite particles, the theory deviates from what is currently considered resonating group theory by the use of distortion states with continuous degrees of freedom. This new feature allows correct scattering states also in the asymptotic region where two or more composite particles together may form an incoming or outgoing state.

The dynamical equation formally is a multichannel Schrödinger equation with a matrix of nonlocal and energy-dependent interactions. The wave function is a multicomponent function of the relative distances of the composite particles and of their center of mass coordinate. The total center of mass motion separates and may be omitted. All internal degrees of freedom of the composite particles as well as all Pauli effects are incorporated in the interaction.

Asymptotically, the relative motion wave function of the composite particles becomes a probability amplitude and the flux of composite particles follows directly from this function. This is true, also, when two or more composite particles form a bound state and the relative motion of the center of mass of this bound state is considered.

The relative motion wave function of composite particles has no probability interpretation in regions where the particles interact. It determines, however, the microscopic wave function which describes the motion of the constituents and which *a priori* has a probability interpretation. The distinction between internal degrees of freedom and relative motion degrees of freedom is not unique. As a consequence, an off-shell ambiguity of the relative motion wave function arises in the interaction region. This off-shell ambiguity has a striking similarity to the off-shell ambiguity of nucleon-nucleon wave functions as described, for instance, by Noyes.[8] Composite particle theory may serve as a nonrelativistic model to study form factor discrepancies and Coulomb energy discrepancies which are based on a probability interpretation of the relative motion wave function within strong-interaction distances.

The present composite particle theory is valid in an energy range which has an upper limit. The limit is given by the threshold of the first channel which is not explicitly taken into account as an open channel. Without this energy limit the theory

goes over into a special version of Schrödinger theory. The special version is characterized by the fact that all wave functions with Pauli-excluded exchange symmetry are redundant solutions. This is a consequence of the incorporation of the Pauli principle into the interaction.

The present theory is described mainly in terms of nuclear fragments as composite particles. Its validity, however, is more general and covers atomic scattering and quark physics. In atomic physics, trouble may arise, in practical applications, from the large number of needed distortion functions. In quark physics, we are still missing a trustworthy microscopic Hamiltonian as well as the confirmation that a nonrelativistic theory is sufficient.

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