K. Wildermuth Y. C. Tang

# A Unified Theory of the Nucleus

K. Wildermuth Y. C. Tang

## A Unified Theory of the Nucleus

With 77 Figures



ACADEMIC PRESS New York San Francisco London 1977

A Subsidiary of Harcourt Brace Jovanovich, Publishers

#### **Preface**

The purpose of this monograph is to describe a microscopic nuclear theory which can be used to consider all low-energy nuclear phenomena from a unified viewpoint. In this theory, the Pauli principle is completely taken into account and translationally invariant wave functions are always employed. Also, this theory is quite flexible; it can be utilized to study reactions initiated not only by nucleons but also by arbitrary composite particles.

Throughout this monograph, we have endeavoured to keep the underlying physical ideas as easily comprehensible as possible. Consequently, it becomes frequently necessary to sacrifice mathematical rigour in favour of clarity in presenting these ideas. In this way, it is our hope that this monograph could be useful to many research physicists in the nuclear field, experimentalists and theorists alike.

In chapters 1 through 4, the formulation of this theory is presented. Numerical examples concerning bound-state, scattering, and reaction calculations are mainly described in chapters 5 through 7. In chapters 8 through 15 we discuss, within the framework of this theory, general properties of nuclear systems. Finally, in chapters 16 and 17, we show in specific cases how one can achieve, without carrying out explicit calculations, a qualitative or even semi-quantitative understanding of these cases by applying the general physical concepts contained inherently in this theory.

Many of our colleagues have offered valuable advice and constructive criticism. These people are: R. E. Brown, D. Clement, F. Gönnenwein, E. Kanellopoulos, P. Kramer, E. Schmid, H. Schultheis, R. Schultheis, G. Staudt, W. Sünkel, and D. R. Thompson. To them we express our most sincere gratitude.

It is also our pleasure to acknowledge W. Pilf, S. Smith, and G. Tollefson for their assistance in the preparation of the manuscript. Finally, we are grateful to our wives, Erika Wildermuth and Helen Tang, for their patience and encouragement throughout the period in which this monograph was written.

K. Wildermuth Y. C. Tang

Tübingen, Germany Minneapolis, Minnesota, U.S.A.

#### Contents

1.	Introduction	1
1.1. 1.2.	General Remarks Difficulties of Some Reaction Theories	. 1
2.	Reformulation of the Schrödinger Equation	6
3.	Discussion of the Basis Wave Functions for Nuclear Systems	9
3.1.	General Remarks	9
3.2.	Qualitative Discussion of Cluster Correlations	9
3.3.	Construction of Oscillator Cluster Wave Functions	11
3.4.	Discussion of <sup>8</sup> Be as an Illustrative Example	14
3.5.	Effects of Antisymmetrization	18
3.5a.	Fermions without Mutual Interaction in a Square-Well Potential	18
3.5b.	The Lowest 4° a-Cluster State of 8Be	19
3.5c.	Mathematical Equivalence of the Lowest <sup>6</sup> Li States Described in the t + <sup>3</sup> He	
	and the d + \alpha Oscillator Cluster Representations	23
3.5d.	Summary	24
3.6.	Applications of Oscillator Cluster Representations to a Qualitative Description of Low-Lying Levels in Light Nuclei	25
3.6a.	<sup>7</sup> Li and <sup>7</sup> Be	25
3.6b.	<sup>6</sup> He, <sup>6</sup> Li, and, <sup>6</sup> Be	27
3.6c.	α-Cluster States of <sup>16</sup> O	28
3.6d.	Brief Remarks	31
3.7.	Construction of Generalized Cluster Wave Functions	32
3.7a.	Introduction of Jacobi Coordinates	35
3.7b.	Introduction of Parameter Coordinates	36
3.7c.	Introduction of Jastrow Factors	38
3.7d.	Summary	40
<b>4</b> .	Formulation of a Unified Microscopic Nuclear Structure and	
	Reaction Theory	41
4.1.	General Remarks	41
4.2.	Specific Examples	42
4.2a.	$n + \alpha$ Scattering	42
4.2b.	d + α Scattering	45
4.2c.	Discussion	47
4.3.	Extension to General Systems	48
5.	Bound-State Calculations	51
5.1.	General Remarks	51
5.2.	Calculation of Matrix Elements	52
5.2a. 5.2b.	Evaluation of Matrix Elements by the Cluster-Coordinate Technique – Example of 8 Be Evaluation of Matrix Elements by the Generator-Coordinate Technique – Example	53
	of <sup>8</sup> Be	58

	•	
Conti	ents	VII
5.3.	Ground and Low Excited States of 6Li	64
5.3a.		64
5.3b.	Calculation With a Nucleon-Nucleon Potential Containing a Hard Core – Accurate	•
	Treatment of the Jastrow Factor	65
5.3e.	Calculation with a Nucleon-Nucleon Potential Containing a Soft Core — Approximate Treatment of the Jastrow Factor	69
5.3d.	Calculation with a Nucleon-Nucleon Potential Containing no Repulsive Core	75
5.3e.	Summary	79
5.4.	Low-Energy $T = 0$ States of $^{12}C$	80
5.5.	Low-Lying Levels of <sup>7</sup> Be	83
<b>5.6</b> .	Concluding Remarks	85
6.	Further Comments About the Pauli Principle	87
6.1.	General Remarks	
6.2.		87
6.3.	Cluster Overlapping and Pauli Principle Energetical Favouring of a Cluster Inside a Large Nucleus	87
		94
7.	Scattering and Reaction Calculations	1.06
7.1.	General Remarks	106
7.2.	Derivation of Coupled Equations	106
7.2a.	Single-Channel Problem	106
7.2b.	1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	112
7.2c.	Reaction Calculations Using Hulthén-Kohn-Type Variational Functions	115
7.3.	Quantitative Results	117
7.3a.	<sup>3</sup> He + α Elastic Scattering	118
7.3b.	$l = 0$ Phase-Shift in $\alpha + \alpha$ scattering	120
7.3c.	Specific Distortion Effects in d + \alpha Scattering	124
7.3d.	Effect of Reaction Channels on <sup>3</sup> He + <sup>3</sup> He Scattering Cross Sections	126
7.3e. 7.3f.	α + 16O Scattering - Utilization of the Generator-Coordinate Technique	129
7.3g.	p + α Scattering Around 3/2* Resonance Level in 5Li	131
7.3g.	α + α Scattering with Specific Distortion Effect and a Nucleon-Nucleon	
7.3h.	Potential Containing a Repulsive Core p + <sup>3</sup> He and n + t Scattering Calculations	134
7.3i.	Coupled-Channel Study of t (p, n) <sup>3</sup> He Reaction	136
7.4.	Concluding Remarks	138
7.7.	Concluding Remarks	140
8.	Introductory Considerations About the Derivation of General	
	Nuclear Properties	142
8.1.	General Remarks	142
8.2.	Introduction of Effective Hamiltonians	144
8.3. 8.4.	Elimination of Linear Dependencies Concluding Remarks	147
0.4.	Concluding Remarks	149
9.	Breit-Wigner Resonance Formulae	150
9.1.	General Remarks	150
9.2.	Single-Level Resonance Formula for Pure Elastic-Scattering	150
9.2a.	Derivation of the Resonance Formula	150
9.2b.	Discussion of the Resonance Formula	154
).2c.	Existence of Sharp Resonances	155
9.2d.	Discussion of a Simple Resonance Model	160

VIII		Content
9.3.	Many-Level Resonance Formula for Pure Elastic-Scattering	162
9.4.	Single-Level Resonance Formula Including Inelastic and Rearrangement Processes	165
9.4a.	Derivation of the Resonance Formula	165
9.4b.	Application of the Resonance Formula to a Specific Example Involving Two	
	Open Channels	168
9.5.	Mutual Influence of Resonance Levels in Inelastic and Rearrangement Processes	174
9.5a.	Derivation of a Two-Level Breit-Wigner Formula	175
9.5b.	A Specific Example	179
9.6.	Behaviour of the Partial Level Width Near a Threshold and Energy-Dependent	104
•	Width Approximation	184
10.	Resonance Reactions and Isobaric-Spin Mixing	186
10.1.	General Remarks	186
10.2.	Isobaric-Spin Mixing in the Compound Region	187
10.2a.		187
10.2b.	The 16.62 and 16.92 MeV States in <sup>8</sup> Be as a Specific Example	192
10.3.	Isobaric-Spin Mixing in the Incoming Channel	195
10.3a.	Qualitative Description	195
10.3b.		197
10.3c.	Brief Discussion in the Case of Many Open Channels	205
11.	Optical-Model Potentials for Composite Particles	206
11.1.	General Remarks	206
1.2.	Optical-Model Description of Elastic-Scattering Processes	207
1.2a.		207
1.2b.	Optical-Model Potential for Pure Elastic Scattering	208
1.2c.	Optical-Model Potential in the Presence of Reaction Channels	214
1.2d.	<b>6</b>	219
1.3.	Specific Examples	221
1.3a.		222
1.3b.	•	224
1.3c.	α + 16 O Scattering	. 227
1.4.	Features of Effective Local Potentials between Nuclei	230
1.4a.	Wave-Function Equivalent Local Potentials	230
1.4b.	Phase-Equivalent Local Potentials	232
2.	Direct Reactions	243
2.1.	General Remarks	243
2.2.	Derivation of the General Formulae	243
	Specific Examples	251
	<sup>3</sup> He (d, p) α Reaction	251
2.3a.		254
2.3a. 2.3b.	<sup>6</sup> Li (p, <sup>3</sup> He) α Reaction	254
2.3a. 2.3b. 2.4.	Influence of the Pauli Principle on Direct-Reactions	255
2.3a. 2.3b. 2.4. 2.4a.	Influence of the Pauli Principle on Direct-Reactions Study of Direct-Reaction Mechanisms in the Plane-Wave Born Approximation	255 256
12.3. 12.3a. 12.3b. 2.4. 2.4a. 2.4b. 2.5.	Influence of the Pauli Principle on Direct-Reactions	255

•

Contents		ΙÌ

Conte	nts	ΙÌ
13.	Some Considerations About Heavy-Ion Transfer Reactions	265
13.1.	General Remarks	265
13.2.	Specific Examples to Study the Influence of Antisymmetrization	266
	α + 6Li Elastic Scattering at Low Energies	267
13.2a. 13.2b.		270
13.20.	Further Discussion of the Odd-Even Feature in the Effective Potential between	
	Nuclei	272
13.4.	Concluding Remarks	274
14.	Collective States	276
14.1.	General Remarks	276
14.2.	Rotational States of Even-Even Nuclei with $K = 0$	276
14.3.	Generalization of Rotational Wave Functions	288
14.4.	Energetical Preference of Rotational Configurations	293
14.5.	Electromagnetic Transitions between Rotational Levels	297
14.6.	Relationship with other Descriptions of Nuclear Rotational States	299
14.7.	Construction of Intrinsic Wave Functions for Quantitative Studies of Collective	
	States in Medium-Heavy and Heavy Nuclei	301
14.8.	Specific Examples	302
14.8a.		302
14.8b.	Rotational States in <sup>22</sup> Ne	303
14.8c.	Backbending	305
14.9.	Concluding Remarks	305
15.	Brief Discussion of Time-Dependent Problems	306
15.1.	General Remarks	306
15.2.	Connection between the Lifetime of a Compound State and Its Level Width	307
15.2a.	Relationship between Phase Shift and Time Delay	307
15.2b.	Quantitative Relationship between the Level Width and the Lifetime of a Compound Nuclear State	309
15.2c.		310
5.3.	Time-Dependent Projection Equation with Time-Dependent Interaction	315
l6.	Qualitative Considerations of Some Nuclear Problems	320
6.1.	General Remarks	320
6.2.	Coulomb-Energy Effects in Mirror Levels	320
6.3.	Reduced Widths and $\gamma$ -Transition Probabilities	325
6.3a.	Reduced Widths of Nuclear Levels	325
6.3b.		323 328
6.4.		
6.5.	Level Spectra of Neighbouring Nuclei Optical Resonances in Nuclear Reactions	331
		333
6.5a.	Optical Resonances in the Incoming Channel	334
6.5b.	Optical Resonances in Reaction Channels	336
7.	Nuclear Fission	340
7.1.	General Remarks	340
<b>7.2</b> .	Substructure Effects in Fission Processes	341
<b>7.3</b> .	Mass Distribution of Fission Fragments	347
7.4.	Deformation Energy of Fissioning Nucleus	349
	•	

X		Contents
17.4a.	Dynamical Consideration of the Fission Process	349
17.4b.	Calculation of the Deformation Energy - Strutinsky Prescription	352
17.4c.	Calculation of the Deformation Energy-Cluster Prescription	357
17.4d.	Discussion	362
18.	Conclusion	365
Appendix A - Cluster Hamiltonians and Jacobi Coordinates		368
Appendix B — Designation of Oscillator States  Appendix C — Demonstration of the Projection Technique		371
		371
Appen	dix D - Connection with Conventional Direct-Reaction Theory	374
Refere	nces	377
Index		388
٠		

**.** 

#### 1. Introduction

#### 1.1. General Remarks

Numerous experimental and theoretical investigations have confirmed the proposal that nuclei are built up of protons and neutrons [HE 32, IV 32]. Therefore it should be possible to derive all the properties of a nucleus consisting of A nucleons, or of a nuclear reaction in which A nucleons participate, from the Schrödinger equation for this A-body system

$$H\Psi(\tilde{r}_{1},...,\tilde{r}_{A};t) = \left[-\frac{\hbar^{2}}{2M}\sum_{i=1}^{A}\nabla_{i}^{2} + V(\tilde{r}_{1},...,\tilde{r}_{A})\right]\Psi(\tilde{r}_{1},...,\tilde{r}_{A};t)$$

$$= i\hbar\frac{\partial}{\partial t}\Psi(\tilde{r}_{1},...,\tilde{r}_{A};t),$$
(1.1)

where  $\tilde{t}_i$  denotes the space, spin, and isobaric-spin coordinates of the i<sup>th</sup> nucleon.

To carry out this program we must overcome two problems:

- (i) We must know the specific form of the nuclear interaction potential energy  $V(\tilde{r}_1, \ldots, \tilde{r}_A)$ .
- (ii) We must solve, at least approximately, the A-body Schrödinger equation.

The form of the nuclear potential is in fact not completely known, although it has become increasingly evident recently that this potential can be considered as primarily a superposition of two-body potentials between all pairs of nucleons [BE 71]. The problem with the two-body potentials proposed earlier was that they could not reproduce the nuclear saturation character, i. e., the property that the nuclear volume must increase proportionally with the nucleon number A. This difficulty has led to speculation [DR 63] that the nuclear interaction might include many-body forces in addition to the two-body terms. Thus, for example, in the case of a three-body problem with an additional three-body force [BR 73], one would have to write the nuclear interaction as

$$V = V_{12} + V_{13} + V_{23} + V_{123}. (1.2)$$

However, over the past twenty years, increasingly reliable two-nucleon potentials have been developed describing the two-nucleon scattering data up to several hundred MeV [BE 71, BR 60, BR 62, HU 62]. In contrast with the earlier two-body interactions, these potentials contain not only strong tensor and Majorana (space-exchange) components, but also velocity-dependent terms or a repulsive core which prevents any two nucleons from approaching each other too closely. Such improved two-body potentials have been found capable of producing saturation [BE 71]. Hence, it has become gradually clear that potentials without large many-body terms, like  $V_{123}$ , are adequate to fit the nuclear data, including the saturation character.

Most of the general considerations which we bring into this monograph remain valid even if the nuclear interaction should contain large many-body terms of short-range character.

2 1. Introduction

In our choice of a nuclear potential, we shall adopt a phenomenological point of view; that is, we shall assume a nuclear potential composed only of two-body forces, and we require only that our two-body potentials be reasonably consistent with the two-nucleon scattering data, give the correct deuteron binding energy, and have the proper nuclear saturation character [WU 62]. The presently unresolved question as to which of the possible potentials meeting these criteria is the correct one will not be considered in this monograph, since it is more a question for relativistic quantum theory. Hence, for our A-nucleon Schrödinger equation, we write

$$H\Psi(\tilde{r}_{1},\ldots,\tilde{r}_{A};t) = \left[-\frac{\hbar^{2}}{2M}\sum_{i=1}^{A}\nabla_{i}^{2} + \sum_{i< j}^{A}\sum_{j=1}^{A}V_{ij}\right]\Psi(\tilde{r}_{1},\ldots,\tilde{r}_{A};t)$$

$$= i\hbar\frac{\partial}{\partial t}\Psi(\tilde{r}_{1},\ldots,\tilde{r}_{A};t). \tag{1.3}$$

For quantitative calculations typical two-nucleon potentials meeting our criteria will be given in Chapter 5.

Our adoption of a potential corresponds to forces which act without propagation delays and hence are not relativistically correct. This neglect of relativistic effects and our consequent use of the non-relativistic Schrödinger equation are reasonable as long as the kinetic energy per nucleon is much less than the nucleon rest mass of about 940 MeV. With this restriction on the energy, we may consider the problem of the nuclear potential as more or less settled, at least for our purposes; for, whatever the outcome of the relativistic theory, it must in the low-energy limit yield a potential in reasonable accord with the phenomenological one.

We shall now turn our attention to the second problem — we wish to develop a flexible and consistent approximation method for solving the A-nucleon Schrödinger equation. The need for flexibility arises, because the properties of nuclei vary considerably from nucleus to nucleus and even from level to level. Hence it is necessary to have a method of great generality such that for each individual nuclear state we can, first, systematically use our physical intuition to include every physical effect that might help to determine the character of the wave function, and then, quantitatively test and improve this approximate wave function to which our intuition has led us.

As will be seen, the method to be discussed in this monograph does meet this requirement. It is in fact a unified theory of the nucleus, since it considers nuclear reactions and nuclear structure from a unified point of view. In addition, with the help of this method, we shall be able to understand the relations between the various nuclear models currently in use. These models have been developed to explain specific nuclear phenomena and very often seem to contradict one another. For the resolution of these contradictions, it will be shown that the Pauli exclusion principle is of fundamental importance, because it reduces to a large extent the differences between different conceptions.

To obtain this method we shall rewrite the many-body Schrödinger equation as a projection equation. But before we do this, we shall discuss why with the usual consideration of the many-body Schrödinger equation, it is in practice not possible to derive such a unified theory of the nucleus.

#### 1.2. Difficulties of Some Reaction Theories

Instead of using the time-dependent Schrödinger equation (1.1) as the starting equation for the treatment of reactions, we can also use the time-independent Schrödinger equation

$$\mathbf{H}\psi = \mathbf{E}\psi,\tag{1.4}$$

because any time-dependent solution  $\Psi$  of eq. (1.1) can be expressed as a linear superposition of the solutions  $\psi$  of eq. (1.4).

As is well known, it is possible only in very special cases to solve exactly eq. (1.4) for A > 2. Therefore, one is generally forced to use approximation methods which allow one to approximate the exact solutions in successive steps. For the derivation of these methods one commonly formulates the Schrödinger equation (1.4) as an integral equation. The advantage of this is that from the beginning the boundary conditions for a given reaction problem can be incorporated into the solution.

To obtain this integral equation (Lippmann-Schwinger equation) one divides the Hamiltonian H into two parts,

$$H = H_0 + H',$$
 (1.5)

where  $H_0$  is the Hamiltonian for the target and the bombarding particle without mutual interaction, and H' describes their mutual interaction. Substituting eq. (1.5) into eq. (1.4) yields

$$(H_0 - E) \psi = -H' \psi,$$
 (1.6)

from which one obtains immediately the following Lippmann-Schwinger equation:

$$\psi = \phi_0 - (H_0 - E - i\epsilon)^{-1} H' \psi.$$
  $\epsilon > 0$  (1.7)

In eq. (1.7),  $\phi_0$  represents a solution of the homogeneous equation

$$(H_0 - E) \phi_0 = 0 ag{1.8}$$

and describes the target and the incoming particle without interaction. The term  $-(H_0-E-i\varepsilon)^{-1}$  H' $\psi$  is responsible for the ensuing scattering and reactions. The infinitesimal part  $-i\varepsilon$  guarantees that only outgoing waves are produced by this term, as is required by physical argument.<sup>†</sup>

Without proceeding any further, one can already recognize the difficulties inherent in eq. (1.7). For this we consider eq. (1.7) in the position representation; that is,

$$\psi = \phi_0(\widetilde{r}_1, \dots, \widetilde{r}_A) - \underset{\widetilde{r}', \widetilde{r}''}{S} G(\widetilde{r}_1, \dots, \widetilde{r}_A; \widetilde{r}'_1, \dots, \widetilde{r}'_A) 
\times \langle \widetilde{r}'_1, \dots, \widetilde{r}'_A | H' | \widetilde{r}''_1, \dots, \widetilde{r}''_A \rangle \psi(\widetilde{r}''_1, \dots, \widetilde{r}''_A),$$
(1.9)

Our emphasis in this section is to point out the essential difficulties associated with reaction theories formulated in a straightforward way from eq. (1.7). Hence, mathematical problems connected with three-body breakup and so on will not be dealt with here.

where the sign S indicates summation over discrete variables and integration over continuous variables. The function  $G(\tilde{r}_1, \ldots, \tilde{r}_A; \tilde{r}'_1, \ldots, \tilde{r}'_A)$  represents the Green's function for the resolvent operator  $-(H_0 - E - i\epsilon)^{-1}$  and has the following form:

$$G(\tilde{r}_{1},\ldots,\tilde{r}_{A};\tilde{r}'_{1},\ldots,\tilde{r}'_{A}) = S_{E_{0}^{\alpha},\lambda_{\alpha}} \langle \tilde{r}_{1},\ldots,\tilde{r}_{A} | E_{0}^{\alpha},\lambda_{\alpha} \rangle \frac{1}{E_{0}^{\alpha} - E - i\epsilon} \langle E_{0}^{\alpha},\lambda_{\alpha} | \tilde{r}'_{1},\ldots,\tilde{r}'_{A} \rangle$$

$$(1.10)$$

In the above equation, the functions  $\langle \tilde{\tau}_1, \ldots, \tilde{\tau}_A | E_0^{\alpha}, \lambda_{\alpha} \rangle$  are orthonormalized solutions of the homogeneous equation (1.8), with  $\lambda_{\alpha}$  denoting collectively the eigenvalues of all those operators which can be diagonalized simultaneously with  $H_0$ .

The representation of  $G(\tilde{r}_1, \dots, \tilde{r}_A; \tilde{r}'_1, \dots, \tilde{r}'_A)$  by means of the orthonormalized eigenfunctions of H<sub>0</sub> has the important consequence that in all approximation methods which one uses to solve eq. (1.9), the wave function  $\psi$  has to be expanded in terms of the orthonormalized eigenfunction set of H<sub>0</sub>. From this it follows that only transitions to those final states which are eigenstates of H<sub>0</sub> can be calculated in a relatively simple manner. For example, let us consider the interaction of two hydrogen atoms and assume for the moment that both the protons and the electrons involved are distinguishable. Then one can calculate the transition probabilities to all those states where the hydrogen atoms are in their ground or energetically allowed excited states and where the two electrons are not exchanged. On the other hand, transitions to final states which are not eigenstates of H<sub>0</sub> cannot be described in a useful way, because these states have to be described ingeneral by a very complicated superposition of eigenstates of H<sub>0</sub>, including highly excited continuum states. In our example here, these are for instance transitions where the reaction products are a H<sup>-</sup> ion plus a H<sup>+</sup> ion, i.e., both electrons belong to one hydrogen nucleus. In nuclear physics, the <sup>6</sup>Li(p, <sup>3</sup>He) <sup>4</sup>He rearrangement reaction is an example of such a transition.

Final states where nothing else occurs except identical particles being exchanged are also not eigenstates of  $H_0$ . Therefore, such exchange transitions also cannot be described in a simple way by a reaction theory which is based on the Lippmann-Schwinger equation (1.7). This means that with such a reaction theory, even a proper consideration of the indistinguishability of identical particles cannot be simply sarried out.

The underlying reason for the above-mentioned difficulty is that the splitting of H into  $H_0$  and H' is not symmetrical in all particle coordinates. This has the consequence that the Green's function  $G(\tilde{\tau}_1, \ldots, \tilde{\tau}_A; \tilde{\tau}'_1, \ldots, \tilde{\tau}'_A)$  is also not symmetrical in these coordinates. For the case of two hydrogen atoms, the Hamiltonian operators H,  $H_0$ , and H' have the following forms:

$$\begin{split} H &= -\frac{\hbar^2}{2\,M_P}\,\,\nabla^2_{R_1} - \frac{\hbar^2}{2\,M_P}\,\,\nabla^2_{R_2} - \frac{\hbar^2}{2\,m_e}\,\,\nabla^2_{r_1} - \frac{\hbar^2}{2\,m_e}\,\,\nabla^2_{r_2} \\ &+ \frac{e^2}{|R_1 - R_2|} - \frac{e^2}{|R_1 - r_1|}\, - \frac{e^2}{|R_1 - r_2|} - \frac{e^2}{|R_2 - r_1|} - \frac{e^2}{|R_2 - r_2|}\, + \frac{e^2}{|r_1 - r_2|}\,\,, \end{split} \tag{1.11}$$

$$H_0 = -\frac{\hbar^2}{2 M_P} \nabla_{\mathbf{R}_1}^2 - \frac{\hbar^2}{2 m_e} \nabla_{\mathbf{r}_1}^2 - \frac{e^2}{|\mathbf{R}_1 - \mathbf{r}_1|} - \frac{\hbar^2}{2 M_P} \nabla_{\mathbf{R}_2}^2 - \frac{\hbar^2}{2 m_e} \nabla_{\mathbf{r}_2}^2 - \frac{e^2}{|\mathbf{R}_2 - \mathbf{r}_2|}$$
(1.12)

$$H' = \frac{e^2}{|\mathbf{R}_1 - \mathbf{R}_2|} - \frac{e^2}{|\mathbf{R}_1 - \mathbf{r}_2|} - \frac{e^2}{|\mathbf{R}_2 - \mathbf{r}_1|} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$
 (1.13)

As is easily seen, H is invariant against a permutation of the proton or electron coordinates, but not  $H_0$  and H'.

One can certainly split H into H<sub>0</sub> and H' in such a way that H<sub>0</sub> describes the reaction products in the final state (outgoing channel) without interaction. But now the description of the particles in the initial state (incoming channel) becomes very complicated. This means that, by means of the Lippmann-Schwinger equation discussed here, the boundary conditions for either the incoming channel or the considered outgoing channel can be fulfilled, but not both together.

For the scattering of nucleons by nuclei, the difficulty associated with the indistinguishability of the nucleons can be removed in the framework of a shell-model reaction theory [MA 69] by truncating the Hilbert space in such a way that the resultant approximate Hamiltonian can be split into  $H_0$  and H' which are both symmetrical with respect to all nucleon coordinates. As a consequence, the corresponding Lippmann-Schwinger equation also becomes symmetrical in these coordinates and it is possible to define a complete set of antisymmetrized orthonormal functions in terms of which the wave function of the system can be expanded. It should be emphasized, however, that this particular reaction theory has a rather limited domain of applicability. It can be used to study elastic, inelastic, and charge-exchange scattering of nucleons, but not processes in which two or more composite particles are involved in either the initial or the final state.

In summary, we wish to make the following remarks. In the usual reaction theories where one splits H into  $H_0$  and H', an orthonormal set of basis functions is defined, in which the wave function of the system has to be expanded. By this procedure the theory is made so inflexible from the beginning that it is in general not possible to introduce the incoming and reaction channels in a symmetrical manner into the integral equation which describes the dynamical behaviour of the system. This has the consequence that one can conveniently introduce only the boundary conditions belonging either to the incoming channel or to the outgoing channel, but not both together. A practical limitation resulting from this is that rearrangement processes cannot be considered. For the treatment of such processes, one has to find a method which allows the handling of the incoming and outgoing channels in a symmetrical way.

#### 2. Reformulation of the Schrödinger Equation

A symmetrical treatment of the incoming and outgoing channels can be done in a basically very simple way by formulating the Schrödinger equation (1.1) in the form of a projection equation (see, e.g., ref. [WI 72])

$$\left\langle \delta \Psi | H + \frac{\hbar}{i} \frac{\partial}{\partial t} | \Psi \right\rangle = 0. \tag{2.1}$$

As usual, the Dirac bracket denotes the integration over spatial coordinates and the summation over spin and isospin coordinates. If  $\delta\Psi$  represents a completely arbitrary variation of  $\Psi$  at a given instant t in the complete Hilbert space, then eq. (2.1) implies that the vector

$$\left(H + \frac{\hbar}{i} \frac{\partial}{\partial t}\right) |\Psi\rangle$$

must be orthogonal to any arbitrary vector in this space. This evidently will be the case only if  $\Psi$  obeys eq. (1.1). Therefore, eq. (2.1) is merely another formulation of the time-dependent Schrödinger equation. However, as we shall see later, eq. (2.1) does allow us to treat the incoming and outgoing channels in a symmetrical way.

If we write \Psi as

$$\Psi = \psi \exp(-iEt/\hbar) \tag{2.2}$$

and insert it into eq. (2.1), we obtain the time-independent Schrödinger equation formulated as a projection equation

$$\langle \delta \psi | H - E | \psi \rangle = 0. \tag{2.3}$$

As has been mentioned previously, we can also use this simpler equation as the starting point for our future considerations.

We shall now briefly discuss some general properties of eq. (2.3), which we shall need at a later stage. Let us make for  $\psi$  the ansatz

$$\psi = \sum_{\mathbf{r}} a_{\mathbf{r}} \phi_{\mathbf{r}} + \int a_{\mathbf{p}} \phi_{\mathbf{p}} d\mathbf{p} \equiv \mathbf{S} a_{\mathbf{k}} \phi_{\mathbf{k}}, \qquad (2.4)$$

where the coefficients  $a_r$  and  $a_p$  are the discrete and continuous linear variational amplitudes for the trial functions  $\phi_r$  and  $\phi_p$ , respectively. By substituting eq. (2.4) into eq. (2.3) and using the fact that  $\delta \psi$  is obtained by an arbitrary variation of the discrete and continuous amplitudes  $a_k$ , i.e.,

$$\delta \psi = \sum_{\mathbf{k}} \delta a_{\mathbf{k}} \phi_{\mathbf{k}}, \tag{2.5}$$

we obtain the following set of coupled equations:

$$\left\langle \phi_{n} \mid H - E \mid S_{k} a_{k} \phi_{k} \right\rangle = 0,$$
 (2.6)

where the subscript n takes on both discrete and continuous values. If the trial functions  $\phi_k$  form a complete set, then the solutions of the coupled equations (2.6) are identical to the solutions of the time-independent Schrödinger equation. We should emphasize that the functions  $\phi_k$  must be linearly independent, but need not be orthogonal to each other. This point is of great importance for our future considerations, because only by choosing in general a nonorthogonal set of functions can one expect to introduce the incoming and outgoing channels symmetrically into the theory. At the same time, the relaxation of the orthogonality requirement also gives us some extra flexibility to choose the set of functions  $\phi_k$  in the most appropriate manner according to the problem under consideration.

If we substitute eq. (2.4) into the time-dependent projection equation (2.1), then we obtain a set of coupled equations similar to eq. (2.6) in the stationary case. The only modification is that the quantity E is replaced by the operator  $-\frac{h}{i}\frac{\partial}{\partial t}$  which acts on the now time-dependent amplitudes  $a_k$ .

In contrast to the trial functions  $\phi_k$ , the eigensolutions of eq. (2.6) are always mutually orthogonal, if all degeneracies are removed. This will be the case even if we restrict the number of variational amplitudes in eq. (2.4). In order to prove this orthogonality property, we consider the following normalized solutions:

$$\psi_l = \sum_{k} a_k^l \phi_k, \qquad (2.7a)$$

$$\psi_{m} = \sum_{k} a_{k}^{m} \phi_{k}, \qquad (2.7b)$$

which belong to the sets of equations

$$\langle \phi_{\mathbf{n}} | \mathbf{H} - \mathbf{E}_{l} | \psi_{l} \rangle = 0, \tag{2.8a}$$

$$\langle \phi_n | H - E_m | \psi_m \rangle = 0. \tag{2.8b}$$

Upon multiplying eq. (2.8a) by  $a_n^{m*}$ , eq. (2.8b) by  $a_n^{l*}$  and summing over all possible values which the index n can assume, we obtain

$$\langle \psi_{\mathbf{m}} | \mathbf{H} - \mathbf{E}_{l} | \psi_{l} \rangle = 0, \tag{2.9a}$$

$$\langle \psi_l | \mathbf{H} - \mathbf{E}_{\mathbf{m}} | \psi_{\mathbf{m}} \rangle = 0. \tag{2.9b}$$

If we now subtract the complex conjugate of eq. (2.9b) from eq. (2.9a), then, due to the hermiticity of H, we obtain the following relations for properly normalized functions  $\psi_l$  and  $\psi_m$ :

$$\langle \psi_l | \psi_m \rangle = \delta(l, m), \tag{2.10}$$

$$\langle \psi_{l} | \mathbf{H} | \psi_{m} \rangle = \langle \psi_{m} | \mathbf{H} | \psi_{l} \rangle = \mathbf{E}_{l} \delta(l, m), \tag{2.11}$$

where the symbol  $\delta(l, m)$  represents the Kronecker symbol for discrete values of l and the Dirac  $\delta$ -function  $\delta(l-m)$  for continuous values of l.

Equations (2.10) and (2.11) show that even when we restrict the number of linear variational parameters, i.e., we only work in a subspace of the Hilbert space, we still obtain the result<sup>†</sup> that (i) any two solutions  $\psi_I$  and  $\psi_m$  are orthonormalized, and (ii) in this subspace the Hamiltonian H can be represented by a real diagonal matrix. These results have the consequence that the normalization of the time-dependent solution of eq. (2.1) remains constant in time. From this it follows that the conservation law of probability current, or in other words the unitarity of the S matrix, is still satisfied, even if we work with a set of functions which does not span the entire Hilbert space.

For numerical calculations, one has to limit the number of linear variational parameters, i.e., the number of trial functions  $\phi_k$  in the ansatz (2.4). It is reasonable to neglect all those terms in eq. (2.4) which can be expected to have a very small amplitude in the final solution of eq. (2.3). To for course, the decision as to which terms will be unimportant is not easy to make and will have to rely on one's experience and physical intuition about the system under investigation (see Chapter 3). Indeed, we know at present of no rigorous rule which could help us in predicting the relative magnitudes of the various variational amplitudes. Therefore, we shall give here only a possibly useful hint which results from the following crude considerations. Let us assume that by some means, we have arrived at a normalized trial function  $\phi_a$ , yielding an energy expectation value fairly close to the eigenvalue of interest. To this function  $\phi_a$  we now add another normalized trial function  $\phi_b$  which, for simplicity, will be assumed to be orthogonal to  $\phi_a$ . A simple calculation then shows that the variational amplitudes a and b satisfy the following relation:

$$\frac{b}{a} \approx -\frac{\langle \phi_b | H | \phi_a \rangle}{\langle \phi_b | H | \phi_b \rangle - \langle \phi_a | H | \phi_a \rangle}. \tag{2.12}$$

From this one sees that |b/a| will be very small if the energy overlapping integral  $|\langle \phi_b | H | \phi_a \rangle|$  is much smaller than the energy difference  $[\langle \phi_b | H | \phi_b \rangle - \langle \phi_a | H | \phi_a \rangle]$ . In the case where  $\phi_a$  and  $\phi_b$  are not entirely orthogonal, a similar consideration will be harder to make, but we do not expect this result to change in any essential way.

Stictly speaking, the proof given here is valid only if all functions  $\phi_k$  are finite-normalizable and hence, belong to a mathematically exact Hilbert space. We shall not discuss the mathematical complications which will appear in our proof if the functions belong partially to a more extended function space (e. g., Banach space), because for all physical situations which we shall describe, we can in principle always work with functions which are normalizable. For practical considerations it is often more convenient to use wave functions  $\phi_k$  which belong to a function space more extended than the Hilbert space.

<sup>††</sup> It should be mentioned that one has to be very careful in omitting such terms, because it can happen that the sum of many  $\phi_k$  with small amplitudes  $a_k$  could contribute significantly to the wave function  $\psi$ . For instance, it is well known that the addition of many small terms does play an important role in connection with the saturation character of the nuclear forces.

### 3. Discussion of the Basis Wave Functions for Nuclear Systems

#### 3.1. General Remarks

The considerations given so far have been quite general. They can be applied not only to nuclear physics, but also to atomic physics, solid-state physics, and other fields of quantum mechanics. The distinction between these different fields lies in the choice of the basis wave functions in terms of which the wave function of the considered physical system is most conveniently expanded. In this chapter, we shall discuss extensively how to choose the proper basis-wave-function set for use in nuclear-physics problems.

The guiding idea for the choice of a proper basis-wave-function set is that the wave function of the system or process which one wishes to describe can be represented by a linear superposition of a small number of terms in this basis set. In this way one obtains a satisfactory description of the physical situation, which is still amenable to quantitative study with present-day computational facilities. More importantly, as we shall see later, a good choice of the basis wave functions is also indispensable for the purpose of obtaining a physical insight into the bound-state structure and reaction mechanisms in a many-particle system.

A proper choice of the basis wave functions depends strongly on the general characteristics of the interaction forces between the particles of which the considered system is composed. In atomic physics, for instance, the interacting atoms can be polarized over large distances due to the long-range nature of the Coulomb interaction. The basic-wave-function sets for atomic systems have therefore to be chosen such that these polarization effects can be included in the description of these systems by a relatively small number of basis functions. In nuclear physics, the situation is quite different. Here the long-range polarization effects on the nuclear participants by the Coulomb forces can be neglected in a good approximation, because the nucleons in a nucleus are tightly bound as a consequence of the great strength of the short-ranged nuclear forces. Therefore, in the choice of basis wave functions for nuclear problems, the emphasis should be on the short-range character of the nuclear interaction and other relevant factors to be discussed in section 3.2, rather than on the presence of the Coulomb repulsion.

#### 3.2. Qualitative Discussion of Cluster Correlations

For nuclear systems two factors predominate in determining the basis wave functions: the character of the nuclear forces and the influence of the Pauli exclusion principle. The important facts about the phenomenological nuclear forces are that they are short-ranged ( $\approx 2$  fm), are strongly attractive over most of this range, but at short distances ( $\lesssim 0.5$  fm) become strongly repulsive. The effect of the Pauli principle in a system of nuclear dimension is to allow low-energy nucleons to move relatively undisturbed throughout the nuclear volume, because these nucleons may not be scattered into other already occupied energy levels.