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Relationship between Feshbach's and Green's Function Theories of the Nucleon–Nucleus Mean Field

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We clarify the relationship and difference between theories of the optical-model potential which had previously been developed in the framework of Feshbach's projection operator approach to nuclear reactions and of Green's function theory, respectively. For definiteness, we consider the nucleon–nucleus system but all results can readily be adapted to the atomic case. The effects of antisymmetrization are properly taken into account. It is shown that one can develop along closely parallel lines the theories of "hole" and "particle" mean fields. The hole one-body Hamiltonians describe the single-particle properties of the system formed when one nucleon is taken away from the target ground state, for instance in knockout or pickup processes. The particle one-body Hamiltonians are associated with the system formed when one nucleon is elastically scattered from the ground state, or is added to it by means of stripping reactions. An infinite number of particle, as well as of hole, Hamiltonians are constructed which all yield exactly the same single-particle wave functions. Many "equivalent" one-body Hamiltonians can coexist because these operators have a complicated structure: they are nonlocal, complex, and energy-dependent. They do not have the same analytic properties in the complex energy plane. Their real and imaginary parts fulfill dispersion relations which may be different. It is shown that hole and particle Hamiltonians can also be constructed by decomposing any vector of the Hilbert space into two parts which are not orthogonal to one another, in contrast to Feshbach's original theory; one interest of this procedure is that the construction and properties of the corresponding hole Hamiltonian can be justified in a mathematically rigorous way. We exhibit the relationship between the hole and particle Hamiltonians and the "mass operator." The latter is associated to the time-ordered Green's function, rather than to its advanced and retarded parts separately as the hole and particle Hamiltonians. Similarities and differences between the hole and particle Hamiltonians and the mass operator are exhibited by constructing their explicit expressions

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in the case of nuclear matter, in the framework of second-order perturbation theory. Particular attention is paid to the connection of the mass operator and the various hole and particle Hamiltonians with observables which can be extracted from stripping, pickup and knockout reactions, in particular the spectroscopic factors and the spectral function. Since many different one-body Hamiltonians exist which all yield the same single-particle wave functions, their relative merits and drawbacks need to be discussed, with particular attention to their relationship to empirical shell- and optical-model potentials and to the possibility of developing practical approximation schemes.

Contents

1. INTRODUCTION

In atomic, as well as in nuclear, physics the success and usefulness of the optical model can hardly be exaggerated. Microscopic theories of the optical-model potential are thus of crucial importance. Feshbach's theory of nuclear reactions played a leading role in the search for this microscopic theory, since it was the first to provide "a proof of the physical existence of an optical potential" [1]. Namely, Feshbach succeeded in deriving a one-body wave equation for the elastic single-particle wave function [2]. Schematically, his theory starts from a coupled-channel formulation of the scattering problem. The nonelastic channels are then "eliminated" with the help of projection operators which separate the elastic and nonelastic components of the wave function. The first version of the theory did not take full account of antisymmetrization effects, but this defect was soon cured [3].

Another theory of the optical-model potential has been developed by Bell and Squires [4], in the framework of the quantum field theoretical approach to many-body physics. Like Feshbach, these authors showed that the elastic single-particle wave function is the solution of a one-body wave equation, in which the potential is the "mass operator" of Green's function theory. Since the analytical properties of the mass operator very much differ from those of Feshbach's potential, these two quantities are intrinsically different [5, 6].

Authors conversant with nuclear reaction theory generally use Feshbach's approach; see, e.g., [7–10]. Authors more familiar with many-body techniques rather adopt Green's function theory; see, e.g., [5, 11–13]. The difference between the two formalisms is so large that it obscures the correspondence between these two types of works. It is thus not only of formal but also of practical interest to establish a link between the two coexisting theories of the optical-model potential. This is the first main purpose of the present work.

Our second main purpose is to exhibit that closely similar techniques can be used for constructing "hole" and "particle" Hamiltonians: (a) The hole Hamiltonians describe the single-particle properties of the bound and scattering eigenstates of the $(A-1)$-nucleon system which is excited when one nucleon is taken away from the A-nucleon ground state, typically by means of pickup or knockout reactions. (b) The particle Hamiltonians describe the single-particle properties of the eigenstates of the $(A+1)$-nucleon system which is formed by scattering one nucleon from the A-nucleon ground state, or by adding one nucleon to this ground state by means of stripping reactions. The optical-model Hamiltonian is a particle Hamiltonian.

The so-called "generalized" optical-model Hamiltonian gives the detailed energy dependence of the elastic scattering amplitude, including the effect of individual resonances [1]. The optical-model Hamiltonian proper only yields the energy average of the elastic amplitude. It can be constructed from the generalized Hamiltonian by means of an averaging procedure [10]. We always deal with generalized optical-model Hamiltonians, but drop the word "generalized."

Above, the expression "single-particle properties" refers to the quantities which play a basic role in the interpretation of one-nucleon transfer reactions. Besides the

single-particle wave functions, the most important of these quantities is the "spectral function" which measures the spectroscopic strength per unit energy interval. In works based on Feshbach's theory, more attention is paid to the single-particle wave function than to the spectral function. In contrast, it is the latter which plays a central role in Green's function theory. By combining the two approaches, our work devotes as much attention to the spectral function as to the single-particle wave function.

The single-particle wave functions needed in microscopic descriptions of one nucleon transfer reactions are the "overlap functions" [9, 14]. Their definition and relevant properties are described in Section 2. The overlap functions are obtained by projecting the eigenstates of the $(A+1)$-nucleon Hamiltonian onto the ground state of the A-nucleon Hamiltonian. This definition hints to the usefulness of Feshbach's projection operator techniques in this context. Feshbach's theory was originally developed in coordinate space [2]. We, rather, adopt the second quantization formalism, since the latter is needed in Green's function theory. For the sake of clarity, we shall occasionally also give the coordinate space representation of some main quantities.

Section 3 deals with hole Hamiltonians. Its main purpose is manifold: (i) Describe how Feshbach's projection operator techniques can be combined with Green's function theory. (ii) Exhibit that there exist many hole Hamiltonians which all yield the overlap functions of the bound states of the $(A-1)$-system. (iii) Show that these hole Hamiltonians only have bound eigenstates. (iv) Discuss the dispersion relations which connect their real and imaginary parts. (v) Derive expressions for the spectral function and the spectroscopic factors in terms of the hole Hamiltonians. (vi) Show that one can construct a hole Hamiltonian by writing the $(A-1)$-nucleon wave function as $\Psi = \tilde{P}^{(h)}\Psi + \tilde{q}^{(h)}\Psi$, where $\tilde{P}^{(h)}$ and $\tilde{q}^{(h)}$ are not orthogonal, in contrast to Feshbach's procedure. Some mathematical properties and proofs are gathered in Appendices B and C.

Section 4 is devoted to particle Hamiltonians. Its manifold purpose is the following: (i) Embed projection operator techniques in the Green's function approach to elastic scattering. (ii) Prove that there exist many particle Hamiltonians which have as eigenstates the bound and "elastic scattering" overlap functions. (iii) Prove that one of these particle Hamiltonians is identical to Feshbach's optical-model Hamiltonian. (iv) Derive the dispersion relations connecting the real to the imaginary parts of these particle Hamiltonians. (v) Express the spectral function and the spectroscopic factors in terms of the particle Hamiltonians. (vi) Show that one can construct a particle Hamiltonian by writing the $(A+1)$-nucleon wave function in the form $\Psi = \tilde{P}^{(p)}\Psi + \tilde{q}^{(p)}\Psi$, where $\tilde{P}^{(p)}$ and $\tilde{q}^{(p)}$ are not orthogonal, in contrast to the procedure introduced by Feshbach in his pioneering work [2, 3]. Mathematical features are gathered in Appendices D and E. In order to render Section 4 self-contained and also to better exhibit the formal analogy between the theories of particle and hole Hamiltonians, its presentation paraphrases that of Section 3 as much as possible.

We mentioned that the mass operator is the quantity which is identified with the optical-model potential in the Green's function theory [4]. In Section 5, we prove

that all the eigenstates of the hole and particle Hamiltonians are also eigenstates of the "one-body" Hamiltonian $h(E)$ obtained by adding the kinetic energy to the mass operator. We show that $h(E)$ enables one to evaluate the spectroscopic factors and the spectral function. Its real and imaginary parts are connected by a dispersion relation which differs from those fulfilled by the hole and particle Hamiltonians. We furthermore exhibit that $h(E)$ is only one among an infinite number of one-body Hamiltonians which share these properties.

In Section 6, we derive explicit expressions for the mass operator and for the hole and particle Hamiltonians, in the case of nuclear matter and in the framework of second-order perturbation theory. In particular, this illustrative example exhibits the usefulness of the "linked-cluster" perturbation expansion of the mass operator. It also indicates that the spatial nonlocality of the hole and particle Hamiltonians is more complicated than that of the mass operator.

Section 7 contains an extended summary and a discussion, in which we attempt to evaluate the relative merits of the various one-body Hamiltonians encountered in Sections 3, 4, and 5.

2. OVERLAP FUNCTIONS

In the present section, we introduce the overlap functions and the "natural orbitals." The overlap functions can be identified with the bound and scattering single-particle wave functions involved in one-nucleon transfer reactions and in elastic scattering processes. The natural orbitals are also of interest, for two main reasons: (a) They provide a convenient single-particle basis. (b) When models are used, one may have to take into account that some natural orbitals are orthogonal to the overlap functions.

2.1. *Many-Body Wave Functions*

We denote by $|\Psi_0^{(A)}\rangle$ the normalized ground state of the A-nucleon system:

$$H^{(A)}\,|\Psi_0^{(A)}\rangle = \mathscr{E}_0^{(A)}\,|\Psi_0^{(A)}\rangle, \qquad \langle \Psi_0^{(A)} \mid \Psi_0^{(A)}\rangle = 1. \tag{2.1}$$

We shall assume that it is not degenerate. It constitutes the target in the reactions that we want to describe (elastic scattering and direct one-nucleon transfer). Transfer reactions excite bound and scattering eigenstates of the $(A \pm 1)$-nucleon Hamiltonians:

$$H^{(A\pm1)}\,|\Psi_\lambda^{(A\pm1)}\rangle = \mathscr{E}_\lambda^{(A\pm1)}\,|\Psi_\lambda^{(A\pm1)}\rangle, \qquad H^{(A\pm1)}\,|\Psi_{\mathscr{E}}^{c(A\pm1)}\rangle = \mathscr{E}^{(A\pm1)}\,|\Psi_{\mathscr{E}}^{c(A\pm1)}\rangle. \tag{2.2a}$$

We shall usually abbreviate the upper index $(A \pm 1)$ by $(\pm)$. We adopt the convention that the upper index $c(\pm)$ means that the channel $c(\pm)$ is the only one that contains an incoming wave; its precise meaning will be specified in Appendix D.

The energies of the bound levels are negative. In general, the following inequalities hold,

$$\mathscr{E}_{\lambda}^{(A+1)} < \mathscr{E}_{0}^{(A)} < \mathscr{E}_{\lambda}^{(A-1)} < \mathscr{E}_{0}^{(A-2)} < 0, \tag{2.2b}$$

where $\mathscr{E}_{0}^{(A-2)}$ is the ground state energy of the $(A-2)$-system. The normalizations are chosen as in [7]:

$$\langle \Psi_{\lambda}^{(\pm)} \mid \Psi_{\lambda'}^{(\pm)} \rangle = \delta_{\lambda\lambda'}, \qquad \langle \Psi_{\mathscr{E}}^{c(\pm)} \mid \Psi_{\mathscr{E}'}^{c(\pm)} \rangle = \delta_{cc'} \delta(\mathscr{E}^{(\pm)} - \mathscr{E}'^{(\pm)}). \tag{2.2c}$$

The set $\{ \Psi_{\lambda}^{(\pm)}, \Psi_{\mathscr{E}}^{(\pm)} \}$ forms a complete basis,

$$\sum_{\lambda(\pm)} |\Psi_{\lambda}^{(\pm)}\rangle\langle \Psi_{\lambda}^{(\pm)}| + \sum_{c(\pm)} \int_{\mathscr{T}_{c}^{(\pm)}}^{\infty} d\mathscr{E} \, |\Psi_{\mathscr{E}}^{c(\pm)}\rangle\langle \Psi_{\mathscr{E}}^{c(\pm)}| = \mathscr{I}^{(A\pm1)}, \tag{2.3a}$$

where $\mathscr{I}^{(A\pm1)}$ is the identity operator in the Hilbert space $\mathscr{H}^{(A\pm1)}$ of the antisymmetric functions of $(A\pm1)$-nucleon coordinates. In (2.3a), the lower limit of integration $\mathscr{T}_{c}^{(\pm)}$ is the threshold energy of the channel $c(\pm)$:

$$\mathscr{T}_{c}^{(+)} \geqslant \mathscr{E}_{0}^{(A)}, \qquad \mathscr{T}_{c}^{(-)} \geqslant \mathscr{E}_{0}^{(A-2)}. \tag{2.3b}$$

We shall often write the completeness relation (2.3a) in the abbreviated form

$$\sum\!\!\!\!\!\!\int d\mathscr{E} \, |\Psi_{\mathscr{E}}^{(A\pm1)}\rangle\langle \Psi_{\mathscr{E}}^{(A\pm1)}| = \mathscr{I}^{(A\pm1)}. \tag{2.3c}$$

2.2. *Overlap Functions*

The overlap functions (in short "the overlaps") are the projections of the $(A\pm1)$-nucleon wave functions on the ground state of the A-nucleon system [9, 14–16]. For the $(A-1)$-system, they are given by

$$\langle \mathbf{r} | \chi_{\lambda}^{(-)} \rangle = \sqrt{A} \, (\Psi_{\lambda}^{(-)} | \Psi_{0}^{(A)} \rangle, \qquad \langle \mathbf{r} | \chi_{\mathscr{E}}^{c(-)} \rangle = \sqrt{A} \, (\Psi_{\mathscr{E}}^{c(-)} \mid \Psi_{0}^{(A)} \rangle, \tag{2.4a}$$

where $(\mid \rangle$ means that the integration runs over the coordinates of $(A-1)$ nucleons. For the $(A+1)$-system, they read

$$\langle \mathbf{r} | \chi_{\lambda}^{(+)} \rangle = \sqrt{A+1} \, (\Psi_{0}^{(A)} \mid \Psi_{\lambda}^{(A)} \rangle, \qquad \langle \mathbf{r} | \chi_{\mathscr{E}}^{c(+)} \rangle = \sqrt{A+1} \, (\Psi_{0}^{(A)} \mid \Psi_{\mathscr{E}}^{c(+)} \rangle, \tag{2.4b}$$

where $(\mid \rangle$ now means that the integration runs over the coordinates of A nucleons. We omit explicit reference to the spin and isospin coordinates. In the second quantization formulation, (2.4a) and (2.4b) take the form

$$\langle \mathbf{r} | \chi_{\lambda}^{(-)} \rangle = \langle \Psi_{\lambda}^{(A-1)} | \, a_{\mathbf{r}} \, | \Psi_{0}^{(A)} \rangle, \qquad \langle \mathbf{r} | \chi_{\mathscr{E}}^{c(-)} \rangle = \langle \Psi_{\mathscr{E}}^{c(A-1)} | \, a_{\mathbf{r}} \, | \Psi_{0}^{(A)} \rangle, \tag{2.5a}$$

$$\langle \mathbf{r} | \chi_{\lambda}^{(+)} \rangle = \langle \Psi_{0}^{(A)} | \, a_{\mathbf{r}} \, | \Psi_{\lambda}^{(A+1)} \rangle, \qquad \langle \mathbf{r} | \chi_{\mathscr{E}}^{c(+)} \rangle = \langle \Psi_{0}^{(A)} | \, a_{\mathbf{r}} \, | \Psi_{\mathscr{E}}^{c(A+1)} \rangle, \tag{2.5b}$$

where $a_{\mathbf{r}}$ is the annihilation operator. By inserting the unit operators (2.3c) in

$$\langle \Psi_0^{(A)} | \, a_{\mathbf{r}}^\dagger a_{\mathbf{r}} + a_{\mathbf{r}} a_{\mathbf{r}}^\dagger \, | \Psi_0^{(A)} \rangle = \delta(\mathbf{r} - \mathbf{r}'), \tag{2.6a}$$

one obtains

$$\sum\!\!\!\!\!\!\int d\mathscr{E} \, |\chi_{\mathscr{E}}^{(-)}\rangle\langle\chi_{\mathscr{E}}^{(-)}| + \sum\!\!\!\!\!\!\int d\mathscr{E} \, |\chi_{\mathscr{E}}^{(+)}\rangle\langle\chi_{\mathscr{E}}^{(+)}| = \mathscr{I}^{(1)}, \tag{2.6b}$$

where $\mathscr{I}^{(1)}$ is the identity operator in the Hilbert space $\mathscr{H}^{(1)}$ of one-particle wave functions. The overlaps associated with the $(A-1)$- and $(A+1)$-systems thus form a complete set. This set is not orthonormal, and the overlaps are not linearly independent.

Let $|\psi_{\mathscr{E}}^{0(A+1)}\rangle$ denote the scattering eigenstate in which the target is in its ground state. The corresponding overlap $|\chi_{\mathscr{E}}^{0(A+1)}\rangle$ can be identified with "the elastic scattering single-particle wave function." The bound overlaps $|\chi_\lambda^{(\pm)}\rangle$ play a central role in the analysis of one-nucleon transfer reactions which feed the bound levels $|\psi_\lambda^{(\pm)}\rangle$ [14].

2.3. *Density Matrix and Natural Orbitals*

We use the same symbol to denote an operator and its representation in some basis, e.g.,

$$N = \int d\mathbf{r} \, d\mathbf{r}' \, |\mathbf{r}\rangle \, N(\mathbf{r}, \mathbf{r}') \langle \mathbf{r}'|, \qquad N(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r}| \, N \, |\mathbf{r}'\rangle = N_{\mathbf{r}\mathbf{r}'}. \tag{2.7}$$

In the coordinate space representation, the one-body "density matrix" is symmetric and given by

$$K(\mathbf{r}, \mathbf{r}') = K_{\mathbf{r}\mathbf{r}'} = \langle \Psi_0^{(A)} | \, a_{\mathbf{r}}^\dagger a_{\mathbf{r}} \, | \Psi_0^{(A)} \rangle. \tag{2.8a}$$

Henceforth, we shall only consider representations in real orthonormal single-particle bases. In the basis $\{\psi_\alpha\}$, one has

$$K_{\alpha\beta} = \langle \Psi_0^{(A)} | \, a_\beta^\dagger a_\alpha \, | \Psi_0^{(A)} \rangle, \tag{2.8b}$$

where

$$a_\alpha = \int d\mathbf{r} \, \langle \psi_\alpha \, | \, \mathbf{r} \rangle \, a_{\mathbf{r}}, \qquad a_\alpha^\dagger = \int d\mathbf{r} \, \langle \mathbf{r} \, | \, \psi_\alpha \rangle \, a_{\mathbf{r}}^\dagger. \tag{2.9}$$

Equations (2.3a) and (2.8b) yield the sum rules

$$K_{\alpha\alpha} = \sum\!\!\!\!\!\!\int d\mathscr{E} \, |\langle \psi_\alpha \, | \, \chi_{\mathscr{E}}^{(-)} \rangle|^2, \qquad 1 - K_{\alpha\alpha} = \sum\!\!\!\!\!\!\int d\mathscr{E} \, |\langle \psi_\alpha \, | \, \chi_{\mathscr{E}}^{(+)} \rangle|^2. \tag{2.10a}$$

The natural orbitals are the normalized eigenstates of the density matrix

$$K\,|\omega_\nu\rangle = n_\nu\,|\omega_\nu\rangle, \qquad \langle\omega_\nu\,|\,\omega_{\nu'}\rangle = \delta_{\nu\nu'}, \tag{2.10b}$$

where n_ν is the occupation probability of the natural orbital $|\omega_\nu\rangle$ in the ground state $|\Psi_0^{(A)}\rangle$. One has

$$0 \leqslant n_\nu \leqslant 1. \tag{2.10c}$$

In nature, occupancies $n_\nu = 0$ or 1 are most unlikely to exist. Below, their possible occurrence will nevertheless be considered because practical calculations use an approximation for $|\Psi_0^{(A)}\rangle$. One may then have $n_\nu = 0$ or $n_\nu = 1$. We call $|\omega_{\nu(0)}\rangle$ and $|\omega_{\nu(1)}\rangle$ the corresponding natural orbitals. According to (2.10a),

$$\langle\omega_{\nu(0)}\,|\,\chi_{\mathscr{E}}^{(-)}\rangle = 0, \qquad \langle\omega_{\nu(1)}\,|\,\chi_{\mathscr{E}}^{(+)}\rangle = 0. \tag{2.11}$$

These relations imply that

$$K\,|\chi_{\mathscr{E}}^{(-)}\rangle = K^{(\neq 0)}\,|\chi_{\mathscr{E}}^{(-)}\rangle, \qquad K\,|\chi_{\mathscr{E}}^{(+)}\rangle = K^{(\neq 1)}\,|\chi_{\mathscr{E}}^{(+)}\rangle, \tag{2.12a}$$

where

$$K_{\mathbf{r}\mathbf{r}'}^{(\neq 0)} = \sum_{n_\nu \neq 0} n_\nu \omega_\nu(\mathbf{r})\,\omega_\nu^*(\mathbf{r}'), \qquad K_{\mathbf{r}\mathbf{r}'}^{(\neq 1)} = \sum_{n_\nu \neq 1} n_\nu \omega_\nu(\mathbf{r})\,\omega_\nu^*(\mathbf{r}'). \tag{2.12b}$$

2.4. *Hilbert Spaces*

Section 3 will be devoted to the overlaps $|\chi_{\mathscr{E}}^{(-)}\rangle$ and related quantities. According to (2.11), we shall thus deal with single-particle states or operators which are "contained" in the truncated Hilbert space $\mathscr{H}_{(\neq 0)}^{(1)}$ spanned by the natural orbitals with nonvanishing occupation probabilities. By "contained" we mean that they have the form

$$F = \sum_{n_\nu \neq 0} |\omega_\nu\rangle\langle\omega_\nu\,|\,F\rangle, \qquad \mathscr{O} = \sum_{\substack{n_\nu \neq 0 \\ n_{\nu'} \neq 0}} |\omega_\nu\rangle\langle\omega_\nu|\,\mathscr{O}\,|\omega_{\nu'}\rangle\langle\omega_{\nu'}| \tag{2.13a}$$

and that they only act on vectors of $\mathscr{H}_{(\neq 0)}^{(1)}$. In $\mathscr{H}_{(\neq 0)}^{(1)}$ the unit operator is given by

$$\mathscr{I}_{(\neq 0)}^{(1)}(\mathbf{r}, \mathbf{r}') = \sum_{n_\nu \neq 0} \omega_\nu(\mathbf{r})\,\omega_\nu^*(\mathbf{r}'). \tag{2.13b}$$

Section 4 will be devoted to the overlaps $|\chi_{\mathscr{E}}^{(+)}\rangle$ and related quantities. According to (2.11), we shall thus deal with single-particle states or operators which are contained in the truncated Hilbert space $\mathscr{H}_{(\neq 1)}^{(1)}$, formed by excluding the natural

orbitals with $n_v = 1$ from the full Hilbert space. The corresponding identity operator is

$$\mathscr{I}^{(1)}_{(\neq 1)}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') = \sum_{n_v = 1} \omega_v(\mathbf{r})\, \omega_v^*(\mathbf{r}'). \tag{2.14}$$

In Section 5 we shall construct Hamiltonians which have as eigenstates the overlaps $|\chi_\lambda^{(-)}\rangle$, $|\chi_\lambda^{(+)}\rangle$, and $|\chi_{\mathscr{E}}^{0(+)}\rangle$. There, we shall deal with single-particle states or operators defined on the full Hilbert space,

$$\mathscr{H}^{(1)} = \mathscr{H}^{(1)}_{(\neq 0)} + \mathscr{H}^{(1)}_{(\neq 1)}. \tag{2.15}$$

3. HOLE ONE-BODY HAMILTONIANS

In the present section, we combine Feshbach's projection operator approach with the many-body Green's function theory to construct hole Hamiltonians. These have as eigenstates the overlaps $|\chi_\lambda^{(-)}\rangle$ corresponding to the bound levels of the $(A-1)$-system. They do not have as eigenstates the overlaps $|\chi_{\mathscr{E}}^{c(-)}\rangle$ associated with scattering states of the $(A-1)$-system. This is not a severe drawback, because the latter overlaps have only limited practical interest. Indeed, in the continuous energy domain the most important physical quantity is the "hole spectral function," which measures the single-particle strength per unit energy interval. It plays a central role in the interpretation of knockout reactions [17]. We shall see that the hole spectral function can be evaluated from the hole Hamiltonians.

We shall see that the hole Hamiltonians are not fully specified by the requirements that they should have the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates and should enable one to evaluate the hole spectral function. We shall thus be led to investigate many "equivalent" but different hole Hamiltonians.

(i) Sections 3.2–3.10 are devoted to the hole Hamiltonian "proper", $h^{(h)}(E)$. This operator has the specific property that its "resolvent" is the "hole Green's function" of many-body theory. Its real and imaginary parts are hermitian, but its real part diverges linearly at large energy.

(ii) In Section 3.11, we show that one can readily construct from $h^{(h)}(E)$ many other Hamiltonians which also have the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates. However, they present the main drawback that their real and imaginary parts are not hermitian. Among them, the "Feshbach-type" Hamiltonian has the merit that it remains finite at large energy.

(iii) In Section 3.13, we construct a hole Hamiltonian whose real and imaginary parts are hermitian, and which remains finite at large energy. This will be achieved by decomposing any vector of the Hilbert space into two components which are not orthogonal to one another, in contrast to Feshbach's original method.

(iv) In Section 3.15, we exhibit that, actually, there exist an infinite number of Hamiltonians which all have the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates and enable one to evaluate the hole spectral function.

Above, we did not introduce the concept of a "hole potential," although we shall be dealing with overlaps $|\chi_\lambda^{(-)}\rangle$ which are expected to be closely related to single-particle states in an empirical shell-model potential. The reason is that the hole Hamiltonians only have bound eigenstates (Section 3.9) so that it would not be natural to write them as sums of a kinetic energy and a potential operator.

3.1. *Hole Green's and Spectral Functions*

We briefly recall a few definitions and properties. Details can, for instance, be found in [18]. The single-particle energies are defined as

$$E_\lambda^{(-)} = \mathscr{E}_0^{(A)} - \mathscr{E}_\lambda^{(-)}, \qquad E = \mathscr{E}_0^{(A)} - \mathscr{E}^{(-)}. \tag{3.1a}$$

We shall likewise use

$$T_c^{(-)} = \mathscr{E}_0^{(A)} - \mathscr{T}_c^{(-)} \tag{3.1b}$$

for characterizing threshold energies, see (2.3a). In the following, we drop the specification "single-particle" unless confusion might arise. The interest of these energies is twofold. First, they can be associated with the eigenvalues of a one-body Hamiltonian. Second, they provide a common energy scale for the $(A-1)$- and $(A+1)$-systems, as will become clear in Section 5.

For a z complex, the hole Green's function is defined by

$$G^{(h)}(\mathbf{r}, \mathbf{r}'; z) = \langle \Psi_0^{(A)} |\, a_{\mathbf{r}'}^\dagger (z + H - \mathscr{E}_0^{(A)})^{-1}\, a_{\mathbf{r}} \,|\, \Psi_0^{(A)} \rangle. \tag{3.2}$$

It is a symmetric function of $\mathbf{r}$ and $\mathbf{r}'$. By using the completeness relation (2.3a), one gets

$$G^{(h)}(z) = \int_{-\infty}^{\infty} dE' \, \frac{S^{(h)}(E')}{z - E'}, \tag{3.3a}$$

where

$$S^{(h)}(E) = \sum_\lambda |\chi_\lambda^{(-)}\rangle\langle\chi_\lambda^{(-)}|\, \delta(E - E_\lambda^{(-)}) + \sum_c |\chi_E^{c(-)}\rangle\langle\chi_E^{c(-)}| \tag{3.3b}$$

is the hole spectral function. This quantity plays a central role in the interpretation of pickup or knockout reactions, as well as in studies of the nuclear response

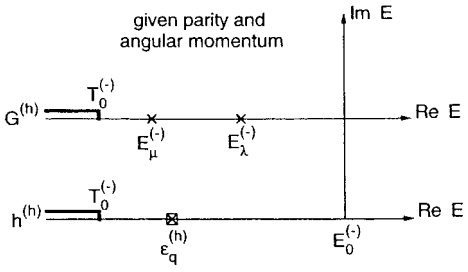

FIG. 1. Sketch of the analytic properties of the hole Green's function and of the hole Hamiltonian in the complex energy plane. The thick lines represent left-hand cuts. The crosses correspond to poles on the real axis. For given angular momentum and parity, only very few such poles exist.

function; see, e.g., [19–24]. It vanishes for energies larger than the single-particle energy associated with the ground state energy $\mathscr{E}_0^{(A-1)} = \mathscr{E}_0^{(-)}$ of the $(A-1)$-system:

$$S^{(h)}(E) = 0 \qquad \text{for} \quad E > E_0^{(-)}, \tag{3.4a}$$

$$E_0^{(-)} = \mathscr{E}_0^{(A)} - \mathscr{E}_0^{(-)}. \tag{3.4b}$$

According to (2.5a) and (2.8a), it fulfills the sum rule:

$$\int_{-\infty}^{E_0^{(-)}} dE\, S^{(h)}(E) = K^{(\neq 0)}. \tag{3.4c}$$

The value of $G^{(h)}(E)$ for E real will conventionally be defined as

$$G^{(h)}(E) = \lim_{\eta \to +0} G^{(h)}(E - i\eta) = G^{(h)}(E - i\eta). \tag{3.5a}$$

Henceforth, the limit $\eta \to +0$ will usually no longer be recalled explicitly.

According to (3.3b), the hole Green's function can be written as the sum of "discrete" and "continuum" contributions:

$$G^{(h)}(E) = G_{dt}^{(h)}(E) + G_{ct}^{(h)}(E), \tag{3.5b}$$

$$G_{dt}^{(h)}(E) = \sum_{\lambda} \frac{|\chi_\lambda^{(-)}\rangle\langle\chi_\lambda^{(-)}|}{E - E_\lambda^{(-)} - i\eta}, \qquad G_{ct}^{(h)}(E) = \sum_{c} \int_{-\infty}^{T_c^{(-)}} dE' \, \frac{|\chi_{E'}^{c(-)}\rangle\langle\chi_{E'}^{c(-)}|}{E - E' - i\eta}. \tag{3.5c}$$

As sketched in Fig. 1, it has a branch cut which runs above the real axis and extends from $-\infty$ up to the threshold $T_0^{(-)}$ associated with nucleon emission from the $(A-1)$-system:

$$T_0^{(-)} = \mathscr{E}_0^{(A)} - \mathscr{T}_0^{(-)}, \qquad \text{where} \quad \mathscr{T}_0^{(-)} = \mathscr{E}_0^{(A-2)} \tag{3.5d}$$

(see (2.2b)). According to (3.3a), one has

$$S^{(h)}(E)=\frac{1}{2i\pi}\{G^{(h)}(E-i\eta)-G^{(h)}(E+i\eta)\}=\frac{1}{2i\pi}\{G^{(h)}(E-i\eta)-G^{(h)}(E-i\eta)^{\dagger}\}. \tag{3.6}$$

3.2. *The Hole Hamiltonian*

For a z complex, we define the "hole Hamiltonian" $h^{(h)}(z)$ by

$$[z-h^{(h)}(z)]\,G^{(h)}(z)=1. \tag{3.7a}$$

When two operators are related in that way, we shall call $G^{(h)}(z)$ the resolvent of $h^{(h)}(z)$. For E real, we adopt the limit

$$h^{(h)}(E)=\lim_{\eta\to+0} h^{(h)}(E-i\eta). \tag{3.7b}$$

At the present stage, our interest in the hole Hamiltonian is fully justified by the fact that it has the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates:

$$h^{(h)}(E_\lambda^{(-)}\,|\chi_\lambda^{(-)}\rangle=E_\lambda^{(-)}\,|\chi_\lambda^{(-)}\rangle. \tag{3.7c}$$

This can readily be derived from (3.5c) and (3.7a); see, e.g., [18]. We shall discuss it further in Section 3.10.

The hole Green's function and the hole Hamiltonian are symmetric in the coordinate space representation. Hence, their hermitian and antihermitian parts are real. The operators $G^{(h)}(z)$ and $h^{(h)}(z)$ are "hermitian-analytic":

$$G^{(h)}(E-i\eta)=G^{(h)}(E+i\eta)^{\dagger},\quad h^{(h)}(E-i\eta)=h^{(h)}(E+i\eta)^{\dagger}\qquad \text{for any}\quad \eta\neq 0. \tag{3.7d}$$

When one uses for $|\Psi_0^{(A)}\rangle$ a model in which some natural orbitals have a vanishing occupation probability, (2.11) implies that

$$G^{(h)}(E)\,|\omega_{\nu(0)}\rangle=0. \tag{3.8a}$$

Therefore, the hole Green's function, the hole spectral function, and the hole Hamiltonian are contained within the Hilbert space $\mathscr{H}^{(1)}_{(\neq 0)}$ in the sense described in connection with (2.13a) and (2.13b). For instance, (3.7a) should then be written in the more detailed form

$$[z-h^{(h)}(z)]\,G^{(h)}(z)=\mathscr{I}^{(1)}_{(\neq 0)}. \tag{3.8b}$$

We now express the hole spectral function in terms of the hole Hamiltonian. Equations (3.6), (3.7a), and (3.7b) yield

$$S^{(h)}(E) = (2i\pi)^{-1} \{ [E - h^{(h)}(E) - i\eta]^{-1} - [E - (h^{(h)}(E))^{\dagger} + i\eta]^{-1} \}. \tag{3.9a}$$

Let us write $h^{(h)}(E)$ as the sum of its real and imaginary parts:

$$h^{(h)}(E - i\eta) = \mathrm{Re}\, h^{(h)}(E) + iW^{(h)}(E), \tag{3.9b}$$

$$W^{(h)}(E) = (2i)^{-1} \{ h^{(h)}(E) - [h^{(h)}(E)]^{\dagger} \}. \tag{3.9c}$$

Equations (3.7a) and (3.9a) give

$$S^{(h)}(E) = S^{(h)}_{dt}(E) + S^{(h)}_{ct}(E), \tag{3.10a}$$

where

$$S^{(h)}_{dt}(E) = G^{(h)}(E - i\eta) \frac{\eta}{\pi} [G^{(h)}(E - i\eta)]^{\dagger}, \tag{3.10b}$$

$$S^{(h)}_{ct}(E) = \frac{1}{\pi} G^{(h)}(E - i\eta)\ W^{(h)}(E) [G^{(h)}(E - i\eta)]^{\dagger}. \tag{3.10c}$$

As in (3.5c), the indices *dt* and *ct* refer to discrete and continuum. This notation is justified because we shall show that

$$S^{(h)}_{dt}(E) = \sum_{\lambda} |\chi^{(-)}_{\lambda}\rangle \langle \chi^{(-)}_{\lambda}|\ \delta(E - E^{(-)}_{\lambda}); \tag{3.10d}$$

see (3.57c) below. Equations (3.3b) and (3.10a) then give

$$S^{(h)}_{ct}(E) = \sum_{c} |\chi^{c(-)}_{E}\rangle \langle \chi^{c(-)}_{E}| = \sum_{c} S^{(h)}_{c(-)}(E). \tag{3.10e}$$

Equation (3.10c) shows that the imaginary part $W^{(h)}(E)$ vanishes if and only if $S^{(h)}_{ct}(E) = 0$. According to (3.1a) and (3.3b) this occurs for E larger than the threshold energy $T^{(-)}_0$ for nucleon emission from the $(A-1)$-system:

$$W^{(h)}(E) = 0 \qquad \text{for} \quad E > T^{(-)}_0. \tag{3.10f}$$

Equation (3.10c) also implies that, for $E < T^{(-)}_0$, the diagonal elements of $W^{(h)}(E)$ are positive, which we express as

$$W^{(h)}(E) > 0 \qquad \text{for} \quad E < T^{(-)}_0. \tag{3.10g}$$

As sketched in Fig. 1, the branch cut of $h^{(h)}(E)$ thus runs above the real axis and extends from $-\infty$ up to $T^{(-)}_0$.

3.3. *Hole Projection Operator*

We decompose any vector of the Hilbert space $\mathscr{H}^{(A-1)}$ into two orthogonal parts with the help of two hermitian projection operators $P^{(h)}$ and $Q^{(h)}$:

$$P^{(h)} + Q^{(h)} = \mathscr{I}^{(A-1)}, \qquad P^{(h)}Q^{(h)} = 0. \tag{3.11}$$

In analogy with Feshbach's theory of nucleon scattering [3] we require the "hole projection operator" $P^{(h)}$ to have the following property:

$$P^{(h)} \, |\Psi^{(A-1)}\rangle = a_{u^{(-)}} \, |\Psi_0^{(A)}\rangle \qquad \text{for all} \quad |\Psi^{(A-1)}\rangle. \tag{3.12a}$$

We now investigate to what extent (3.11) and (3.12a) specify $P^{(h)}$ and $|u^{(-)}\rangle$. We first show that there exists a simple relation between $|u^{(-)}\rangle$ and the overlap $|\chi^{(-)}\rangle$ defined by (2.5a). Using (3.12a), a sufficient condition for fulfilling (3.11) is

$$\langle (1 - P^{(h)}) \, \Psi^{(A-1)}| \, a_{\mathbf{r}} \, |\Psi_0^{(A)}\rangle = 0 \qquad \text{for all } \mathbf{r}. \tag{3.12b}$$

Equations (3.12a) and (3.12b) give

$$\chi^{(-)}(\mathbf{r}) = \int d\mathbf{r}' \, \langle \Psi_0^{(A)}| \, a_{\mathbf{r}}^{\dagger} a_{\mathbf{r}} \, |\Psi_0^{(A)}\rangle \, u^{(-)}(\mathbf{r}'), \tag{3.13a}$$

which amounts to

$$|\chi^{(-)}\rangle = K \, |u^{(-)}\rangle. \tag{3.13b}$$

Since $|\chi^{(-)}\rangle$ is well-defined, (3.13b) fully determines $|u^{(-)}\rangle$, provided that K has an inverse. This is most likely the case when one uses the exact $|\Psi_0^{(A)}\rangle$.

However, a problem arises when one adopts for $|\Psi_0^{(A)}\rangle$ a model in which K has vanishing eigenvalues. Then, $P^{(h)}$ and $u^{(-)}(\mathbf{r})$ are not fully specified by (3.12a). Indeed,

$$a_{\nu(0)} \, |\Psi_0^{(A)}\rangle = 0, \tag{3.14}$$

where $a_{\nu(0)}$ is the annihilation operator of the natural orbital $\omega_{\nu(0)}(\mathbf{r})$ whose occupancy vanishes. Equation (3.14) shows that any amount of $|\omega_{\nu(0)}\rangle$ can be admixed into $|u^{(-)}\rangle$ without affecting the requirement (3.12a). An additional condition must then be imposed in order to uniquely define $|u^{(-)}\rangle$. In the spirit of Feshbach's theory of nucleon scattering [3] this additional condition will be chosen as we now describe.

The quantity of main physical interest is the overlap $|\chi^{(-)}\rangle$. According to (2.11), the latter is orthogonal to $|\omega_{\nu(0)}\rangle$. It is thus sufficient to restrict oneself to the Hilbert space $\mathscr{H}^{(1)}_{(\neq 0)}$ defined in connection with (2.13b). Therefore, we replace (3.13b) by

$$|\chi^{(-)}\rangle = K^{(\neq 0)} \, |u^{(-)}\rangle, \tag{3.15a}$$

where $K^{(\neq 0)}$ is given by (2.12b). Then, the quantity

$$|u^{(-)}\rangle = \{K^{(\neq 0)}\}^{-1} |\chi^{(-)}\rangle \tag{3.15b}$$

is uniquely defined. The condition that we added to (3.12a) in order to fully specify $|u^{(-)}\rangle$ and $P^{(h)}$ is thus

$$\langle \omega_{\nu(0)} | u^{(-)}\rangle = 0. \tag{3.15c}$$

Let us now construct an explicit expression for the projection operator $P^{(h)}$. In order to facilitate comparison with Feshbach's scattering theory, we adopt the coordinate space representation. The defining relations (3.12a) and (3.15b) successively yield

$$P^{(h)} |\Psi^{(A-1)}\rangle = \int d\mathbf{r}\, a_{\mathbf{r}} |\Psi_0^{(A)}\rangle [u^{(-)}(\mathbf{r})]^* \tag{3.16a}$$

$$= \int d\mathbf{r}\, d\mathbf{r}'\, a_{\mathbf{r}} |\Psi_0^{(A)}\rangle [K^{(\neq 0)}]^{-1}_{\mathbf{r}\mathbf{r}'} [\chi^{(-)}(\mathbf{r}')]^* \tag{3.16b}$$

$$= \int d\mathbf{r}\, d\mathbf{r}'\, a_{\mathbf{r}} |\Psi_0^{(A)}\rangle [K^{(\neq 0)}]^{-1}_{\mathbf{r}\mathbf{r}'} \langle \Psi_0^{(A)} | a^{\dagger}_{\mathbf{r}'} |\Psi^{(A-1)}\rangle. \tag{3.16c}$$

The hole projection operator is thus given by

$$P^{(h)} = \int d\mathbf{r}\, d\mathbf{r}'\, a_{\mathbf{r}} |\Psi_0^{(A)}\rangle [K^{(\neq 0)}]^{-1}_{\mathbf{r}\mathbf{r}'} \langle \Psi_0^{(A)}| a^{\dagger}_{\mathbf{r}'}. \tag{3.17}$$

In the natural orbital basis, $K^{(\neq 0)}$ is diagonal and $P^{(h)}$ takes the simple form given in [25], namely

$$P^{(h)} = \sum_{n_\nu \neq 0} a_\nu |\Psi_0^{(A)}\rangle \frac{1}{n_\nu} \langle \Psi_0^{(A)}| a^{\dagger}_{\nu}. \tag{3.18}$$

3.4. *Hole Hamiltonian in Terms of Projection Operators*

We now construct an expression for the hole Hamiltonian $h^{(h)}(E)$ in terms of the projection operators $P^{(h)}$ and $Q^{(h)}$. We replace by $(P^{(h)} + Q^{(h)})$ the unit operator $\mathscr{I}^{(A-1)}$ which appears as the middle factor in the identity

$$(z + H)^{-1}\, \mathscr{I}^{(A-1)} (z + H) = \mathscr{I}^{(A-1)}, \tag{3.19a}$$

where z is a complex energy. By multiplying the resulting relation from the left by $P^{(h)}$ and then from the right successively by $P^{(h)}$ and $Q^{(h)}$, we find

$$P^{(h)}(z+H)^{-1}\,P^{(h)}(z+P^{(h)}HP^{(h)})+P^{(h)}(z+H)^{-1}\,Q^{(h)}HP^{(h)}=P^{(h)}, \quad (3.19b)$$

$$P^{(h)}(z+H)^{-1}\,Q^{(h)}(z+Q^{(h)}HQ^{(h)})\,Q^{(h)}+P^{(h)}(z+H)^{-1}\,P^{(h)}HQ^{(h)}=0. \quad (3.19c)$$

We extract $P^{(h)}(z+H)^{-1}\,Q^{(h)}$ from (3.19c) and insert the result into (3.19b). This gives

$$P^{(h)}(z+H)^{-1}\,P^{(h)}\mathscr{O}^{(h)}(z)\,P^{(h)}=P^{(h)}, \quad (3.20a)$$

where

$$\mathscr{O}^{(h)}(z)=z+P^{(h)}HP^{(h)}-P^{(h)}HQ^{(h)}(z+Q^{(h)}HQ^{(h)})^{-1}\,Q^{(h)}HP^{(h)}. \quad (3.20b)$$

In order to obtain a relation between one-body operators, we multiply (3.20a) from the left by $\langle\,\Psi_0^{(A)}|\,a_{\mathbf{r}'}^{\dagger}$ and from the right by $a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle$. Noting that

$$P^{(h)}a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle=a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle, \qquad \langle\,\Psi_0^{(A)}|\,a_{\mathbf{r}'}^{\dagger}P^{(h)}a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle=K^{(\neq 0)}_{\mathbf{r}\mathbf{r}'}, \quad (3.21)$$

we find that

$$\int d\mathbf{s}\,d\mathbf{s}'\,G^{(h)}(\mathbf{s}',\mathbf{r}';z+\mathscr{E}_0^{(A)})(K^{(\neq 0)})^{-1}_{\mathbf{s}\mathbf{s}'}$$

$$\times\langle\,\Psi_0^{(A)}|\,a_{\mathbf{s}}^{\dagger}\mathscr{O}^{(h)}(z)\,a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle=K^{(\neq 0)}_{\mathbf{r}\mathbf{r}'}. \quad (3.22a)$$

We introduce the one-body operator

$$\langle\mathbf{r}|\,O^{(h)}(z)\,|\mathbf{r}'\rangle=\langle\,\Psi_0^{(A)}|\,a_{\mathbf{r}'}^{\dagger}\mathscr{O}^{(h)}(z)\,a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle. \quad (3.22b)$$

By first transposing (3.22a) and then multiplying the result from the left by $[K^{(\neq 0)}]^{-1}$, we obtain

$$(K^{(\neq 0)})^{-1}\,O^{(h)}(z)(K^{(\neq 0)})^{-1}\,G^{(h)}(z+\mathscr{E}_0^{(A)})=\mathscr{I}^{(1)}_{(\neq 0)}. \quad (3.23)$$

This equation has the same form as (3.8b). By setting $z=E-\mathscr{E}_0^{(A)}-i\eta$, it yields the expression that we were searching for the hole Hamiltonian, namely,

$$h^{(h)}(E)=E[\,\mathscr{I}^{(1)}_{(\neq 0)}-(K^{(\neq 0)})^{-1}]+(K^{(\neq 0)})^{-1}\,[\,R^{(h)}+D^{(h)}(E-i\eta)\,](K^{(\neq 0)})^{-1}, \quad (3.24)$$

where, in the coordinate space representation,

$$R^{(h)}_{\mathbf{r}\mathbf{r}'}=\langle\,\Psi_0^{(A)}|\,a_{\mathbf{r}'}^{\dagger}[a_{\mathbf{r}},H]\,|\Psi_0^{(A)}\rangle, \quad (3.25)$$

$$D^{(h)}_{\mathbf{r}\mathbf{r}'}(E-i\eta)=\langle\,\Psi_0^{(A)}|\,a_{\mathbf{r}'}^{\dagger}HQ^{(h)}\{E+Q^{(h)}HQ^{(h)}-\mathscr{E}_0^{(A)}-i\eta\}^{-1}\,Q^{(h)}Ha_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle. \quad (3.26)$$

In keeping with (3.7b), we shall often write

$$D^{(h)}(E) = \lim_{\eta \to +0} D^{(h)}(E - i\eta). \tag{3.27a}$$

For the sake of simplicity, we shall usually omit the label ($\neq 0$). For instance, we shall write (3.24) in the form

$$h^{(h)}(E) = E(1 - K^{-1}) + K^{-1}R^{(h)}K^{-1} + K^{-1}D^{(h)}(E)\, K^{-1}. \tag{3.27b}$$

Equations (3.5c) and (3.27b) yield

$$\{E_\lambda^{(-)}K^{-1} - K^{-1}R^{(h)}K^{-1} - K^{-1}D^{(h)}(E_\lambda^{(-)})\, K^{-1}\}\ |\chi_\lambda^{(-)}\rangle = 0, \tag{3.27c}$$

which amounts to (3.7c).

3.5. *Mean Removal Energy*

The operator $R^{(h)}$ is independent of energy and is hermitian. By writing explicitly the commutator in (3.25) and by inserting the expression (2.3a) of the unit operator $\mathscr{I}^{(A-1)}$, we obtain

$$R^{(h)}_{\mathbf{r}\mathbf{r}'} = \sum_{\lambda(-)}^{\int} \langle \Psi_0^{(A)} |\, a^\dagger_{\mathbf{r}'}\, | \Psi_\lambda^{(-)} \rangle [\mathscr{E}_0^{(A)} - \mathscr{E}_\lambda^{(-)}] \langle \Psi_\lambda^{(-)} |\, a_{\mathbf{r}}\, | \Psi_0^{(A)} \rangle. \tag{3.28a}$$

The middle factor is the single-particle energy $E_\lambda^{(-)}$. Equations (3.3b) and (3.28a) yield the following "sum rule":

$$R^{(h)} = \int_{-\infty}^{E_0^{(-)}} ES^{(h)}(E)\, dE. \tag{3.28b}$$

Let us consider some arbitrary single-particle basis $\{\psi_\alpha\}$. According to (3.2) and (3.3b) the diagonal element $S^{(h)}_{\alpha\alpha}(E)$ measures the probability per unit energy interval of finding the $(A-1)$-system with the excitation energy $E^* = E_0^{(-)} - E$ after having taken out one nucleon with wave function $\psi_\alpha(\mathbf{r})$ from the A-nucleon ground state. Therefore, $R^{(h)}_{\alpha\alpha}$ is the "centroid" energy of those states of the $(A-1)$-system which are fed when one nucleon with wave function $\psi_\alpha(\mathbf{r})$ is removed from $|\Psi_0^{(A)}\rangle$. This centroid is intimately related to a definition of the shell-model potential which had been advocated by Brandow [26], see also [27–29]. When only two-body forces exist, the sum rule [30–34]

$$\mathscr{E}_0^{(A)} = \tfrac{1}{2}\left[\langle \mathscr{T} \rangle + \sum_\alpha R^{(h)}_{\alpha\alpha} \right] \tag{3.29}$$

holds, where $\langle \mathscr{T} \rangle$ is the kinetic energy of the ground state $|\Psi_0^{(A)}\rangle$:

$$\langle \mathscr{T} \rangle = \sum_{\alpha\beta} \langle \alpha | T | \beta \rangle K_{\alpha\beta}. \tag{3.30}$$

Here and below, T is the one-body kinetic energy operator. Koltun [27] derived a linked-cluster perturbation expansion for the "mean removal energy" $R^{(h)}_{\alpha\alpha}/K_{\alpha\alpha}$.

3.6. *High Energy Behaviour of the Hole Hamiltonian and Sum Rules*

Because of the first term on the right-hand side of (3.27b), the hole Hamiltonian $h^{(h)}(E)$ diverges at large E. We now show that this high energy behaviour can be derived without making use of projection operators. According to (3.3a), (3.4c) and (3.28b), at large E one has

$$G^{(h)}(E) \sim E^{-1}(K + E^{-1}R^{(h)}). \tag{3.31a}$$

By inserting this in

$$h^{(h)}(E) = E - [G^{(h)}(E)]^{-1}, \tag{3.31b}$$

one obtains

$$h^{(h)}(E) \sim E(1 - K^{-1}) + K^{-1}R^{(h)}K^{-1}. \tag{3.31c}$$

This is in keeping with (3.27b), since $D^{(h)}(E) \sim E^{-1}$.

According to (3.31a), the contour integral of $G^{(h)}(z)$ over a closed large circle in the complex z-plane is equal to

$$\int_{\text{circle}} dz\, G^{(h)}(z) = 2i\pi K. \tag{3.32a}$$

By indenting the contour around the singularities of $G^{(h)}(z)$, this yields

$$(2i\pi)^{-1} \int_{-\infty}^{E_0^{(-)}} dE \{ G^{(h)}(E - i\eta) - G^{(h)}(E + i\eta) \} = K, \tag{3.32b}$$

which is compatible with Eqs. (3.4c) and (3.6), as it should be. Equations (3.5b) and (3.32b) show that one can write the density matrix as the sum of discrete and continuum contributions:

$$K = K^{(h)}_{dt} + K^{(h)}_{ct}, \tag{3.32c}$$

$$K^{(h)}_{dt} = \sum_{\lambda} |\chi^{(-)}_{\lambda}\rangle\langle\chi^{(-)}_{\lambda}|, \tag{3.32d}$$

$$K^{(h)}_{ct} = (2i\pi)^{-1} \int_{-\infty}^{T_0^{(-)}} dE \{ G^{(h)}_{ct}(E - i\eta) - G^{(h)}_{ct}(E - i\eta)^{\dagger} \}. \tag{3.32e}$$

3.7. *Independent Particle Model*

In the independent particle model, each nucleon only feels an energy-independent potential U, possibly nonlocal. Schematically, the corresponding Hamiltonian H_U reads

$$H_U^{(A)} = \sum_{j=1}^{A} h_U(j), \tag{3.33a}$$

$$h_U(j) = T(j) + U(j). \tag{3.33b}$$

Let φ_α and φ_E denote the bound and scattering eigenstates of h_U, normalized as in (2.2c):

$$h_U\varphi_\alpha = e(\alpha)\,\varphi_\alpha, \qquad h_U\varphi_E = E\varphi_E, \tag{3.33c}$$

$$\langle \varphi_\alpha \,|\, \varphi_\beta \rangle = \delta_{\alpha\beta}, \qquad \langle \varphi_E \,|\, \varphi_{E'} \rangle = \delta(E - E'). \tag{3.33d}$$

In this model, the density matrix is diagonal and the φ_α's are the natural orbitals as well as the overlap functions. Their occupation probabilities n_α are either equal to unity or vanish. The A orbits φ_α with $n_\alpha = 1$ form the "Fermi sea," and will be denoted by $\alpha \in F$. The ground state $|\Phi_U^{(A)}\rangle$ is a Slater determinant formed with these "occupied" orbits. The hole Green's function reads

$$G_U^{(h)}(E) = \sum_{\alpha \in F} \frac{|\varphi_\alpha\rangle\langle\varphi_\alpha|}{E - e(\alpha) - i\eta}. \tag{3.34a}$$

At large E, it approaches K_U/E where

$$K_U = \sum_{\alpha \in F} |\varphi_\alpha\rangle\langle\varphi_\alpha|. \tag{3.34b}$$

The hole spectral function is equal to

$$S_U^{(h)}(E) = \sum_{\alpha \in F} |\varphi_\alpha\rangle\langle\varphi_\alpha|\,\delta(E - e(\alpha)). \tag{3.34c}$$

It fulfills the sum rule

$$\int_{-\infty}^{\infty} dE\, S_U^{(h)}(E) = \frac{1}{2i\pi} \int_{-\infty}^{\infty} dE[\, G_U^{(h)}(E - i\eta) - G_U^{(h)}(E - i\eta)^\dagger] = K_U. \tag{3.34d}$$

The matrix elements $\langle \varphi_\alpha |\, G_U^{(h)}\, |\varphi_\beta\rangle$ vanish for states φ_α or φ_β which lie outside the Fermi sea. Hence, the inverse of $G_U^{(h)}$ is not defined on the full Hilbert space.

Likewise for the hole Hamiltonian, which reduces to the following energy-independent operator

$$h_U^{(h)} = R_U^{(h)} = \sum_{\alpha \in F} |\varphi_\alpha\rangle\langle\varphi_\alpha|\, e(\alpha). \tag{3.34e}$$

Note that $h_U^{(h)}$ does not have any scattering eigenstate.

The independent particle model illustrates some of the differences between the hole Green's function $G_U^{(h)}(E)$ and the familiar Green's function $g_U^{(-)}(E)$ of potential scattering theory. For comparison with the above, for E real we define $g_U^{(-)}(E)$ as the limit

$$g_U^{(-)}(E) = (E - h_U - i\eta)^{-1}. \tag{3.35a}$$

In the free case ($U = 0$) it reduces to

$$g_0^{(-)}(E) = (E - k^2/2m - i\eta)^{-1}. \tag{3.35b}$$

The spectral expansion of $g_U^{(-)}(E)$ reads

$$g_U^{(-)}(E) = \sum_\alpha \frac{|\varphi_\alpha\rangle\langle\varphi_\alpha|}{E - e(\alpha) - i\eta} + \int_{-\infty}^{\infty} dE' \, \frac{|\varphi_{E'}\rangle\langle\varphi_{E'}|}{E - E' - i\eta}. \tag{3.35c}$$

At large E, one has

$$g_U^{(-)}(E) \sim 1/E, \tag{3.35d}$$

while (3.34a) shows that $G_U^{(h)}(E) \sim K_U/E$. Relatedly,

$$\frac{1}{2i\pi} \int_{-\infty}^{\infty} dE [\, g_U^{(-)}(E - i\eta) - g_U^{(-)}(E - i\eta)^\dagger] = 1, \tag{3.35e}$$

which should be contrasted with (3.34d). These differences reflect the incomplete nature of the Hilbert space $\mathscr{H}^{(1)}_{\in F}$ as compared to $\mathscr{H}^{(1)}$. Indeed, (3.35e) expresses the fact that the set $\{\varphi_{\alpha \in F}\}$ forms a complete basis in $\mathscr{H}^{(1)}_{\in F}$. In other words, the origin of the difference between $h_U^{(h)}$ and h_U lies in the fact that, as specified right after (3.8a), the hole Hamiltonian is contained within the Hilbert space $\mathscr{H}^{(1)}_{(\neq 0)}$. The latter coincides with $\mathscr{H}^{(1)}_{\in F}$ in the independent particle model.

3.8. *Dispersion Relation for the Hole Hamiltonian*

We first derive an expression of $W^{(h)}(E)$ in terms of the eigenstates of $Q^{(h)}HQ^{(h)}$. These belong to either the discrete or the continuous spectrum,

$$Q^{(h)}HQ^{(h)}\, |\Phi_q^{(h)}\rangle = (\mathscr{E}_0^{(A)} - \varepsilon_q^{(h)})\, |\Phi_q^{(h)}\rangle, \tag{3.36a}$$

$$Q^{(h)}HQ^{(h)}\, |\Phi_{\mathscr{E}}^{c(-)}\rangle = (\mathscr{E}_0^{(A)} - \varepsilon^{(h)})\, |\Phi_{\mathscr{E}}^{c(-)}\rangle, \tag{3.36b}$$

where $\mathscr{E} = \mathscr{E}_0^{(A)} - \varepsilon^{(h)}$. The quantities $\varepsilon^{(h)}$ and $\varepsilon_q^{(h)}$ correspond to single-particle energies. We adopt the same normalization as in (2.2c). The use of the same symbol $c(-)$ for the degeneracy index as for the scattering eigenstates $|\Psi_{\mathscr{E}}^{c(-)}\rangle$ will be justified in connection with Eq. (C.17) of Appendix C.

The set of the nonvanishing expectation values of $Q^{(h)}HQ^{(h)}$ with respect to all the configurations of $(A-1)$ nucleons is contained in the set of the expectation values of H. Therefore, the smallest eigenvalue of $Q^{(h)}HQ^{(h)}$ must be larger than the smallest eigenvalue of H. This implies that the following inequalities hold:

$$\varepsilon^{(h)} \leqslant T_0^{(-)} < E_0^{(-)}, \qquad \varepsilon_q^{(h)} < E_0^{(-)}. \tag{3.36c}$$

We recall that $E_0^{(-)}$ and $T_0^{(-)}$ correspond to the ground state of the $(A-1)$-nucleon system and to its threshold for nucleon emission, respectively.

By introducing the operator $\sum_c |\Phi^{(h)}\rangle\langle\Phi^{(h)}|$ in (3.26), one finds that, in any single-particle representation $\{\psi_\alpha\}$,

$$\operatorname{Im} D_{\alpha\alpha'}^{(h)}(E) = \pi \sum_c \int_{-\infty}^{T_0^{(-)}} d\varepsilon^{(h)} [\mathscr{J}_{\alpha'}^{c(-)}(\varepsilon^{(h)})]^* \mathscr{J}_{\alpha}^{c(-)}(\varepsilon^{(h)})\, \delta(E - \varepsilon^{(h)}), \tag{3.37}$$

where

$$\mathscr{J}_{\alpha}^{c(-)}(\varepsilon^{(h)}) = \langle \Phi_{\mathscr{E}}^{c(-)} |\, Q^{(h)} H a_\alpha \,|\Psi_0^{(A)}\rangle. \tag{3.38}$$

Equation (3.37) confirms the properties (3.10f) and (3.10g). The following dispersion relation connects the real and imaginary parts of the hole Hamiltonian,

$$\operatorname{Re} h^{(h)}(E) = E(1 - K^{-1}) + K^{-1} R^{(h)} K^{-1} + \sum_q K^{-1} \frac{|\mathscr{J}_q^{(h)}\rangle\langle\mathscr{J}_q^{(h)}|}{E - \varepsilon_q^{(h)}} K^{-1} - \frac{\mathscr{P}}{\pi} \int_{-\infty}^{T_0^{(-)}} dE' \frac{\operatorname{Im} h^{(h)}(E')}{E' - E}, \tag{3.39}$$

where $\mathscr{P}$ denotes a "principal value" and

$$\mathscr{J}_{q\alpha}^{(h)} = \langle \Phi_q^{(h)} |\, Q^{(h)} H a_\alpha \,|\Psi_0^{(A)}\rangle = \langle \alpha |\, \mathscr{J}_q^{(h)}\rangle. \tag{3.40}$$

3.9. *Hole Mass Operator*

In the present section, we write the hole Hamiltonian as the sum of a kinetic energy and a potential operator. The latter will be called the "hole mass operator" by analogy with the mass operator proper, which is associated with the time-ordered Green's function (Section 5). Our purpose is threefold. First, we draw attention on the fact that the definition of the kinetic energy operator requires some caution when one uses for $|\Psi_0^{(A)}\rangle$ a model in which the occupancy of some natural orbitals vanishes. Second, we exhibit that the hole Hamiltonian has no scattering eigenstate, so that the properties of the hole mass operator are quite different from

those of a typical finite-depth potential, in particular of those of the phenomenological shell-model potential. Third, we discuss the bilinear expansion of the hole Green's function.

3.9.1. *Kinetic and Interaction Contributions to* $R^{(h)}$

The full many-body Hamiltonian is the sum of kinetic and interaction contributions:

$$H = \mathscr{T} + \mathscr{V}. \tag{3.41a}$$

By inserting (3.41a) in the expression (3.25) of $R^{(h)}$ one finds

$$R^{(h)} = \mathscr{T}^{(h)} + \mathscr{V}^{(h)}, \tag{3.41b}$$

where

$$\mathscr{T}^{(h)}_{\mathbf{r}\mathbf{r}'} = \langle \Psi_0^{(A)} |\, a^\dagger_{\mathbf{r}'}[\, a_{\mathbf{r}}, \mathscr{T}\,] \,| \Psi_0^{(A)} \rangle = -\frac{1}{2m} \nabla^2_{\mathbf{r}} K^{(\neq 0)}_{\mathbf{r}\mathbf{r}'}, \tag{3.41c}$$

$$\mathscr{V}^{(h)}_{\mathbf{r}\mathbf{r}'} = \langle \Psi_0^{(A)} |\, a^\dagger_{\mathbf{r}'}[\, a_{\mathbf{r}}, \mathscr{V}\,] \,| \Psi_0^{(A)} \rangle. \tag{3.41d}$$

It should be noted that $\mathscr{T}^{(h)}$ and $\mathscr{V}^{(h)}$ are not hermitian, although their sum $R^{(h)}$ is hermitian.

3.9.2. *Hole Mass Operator*

When the kinetic energy operator T acts on a function of $\mathscr{H}^{(1)}_{(\neq 0)}$, the result in general does not belong to that Hilbert space. Therefore, it is appropriate to introduce the following "modified" kinetic energy operator:

$$T^{(\neq 0)} = \sum_{\substack{n_\nu \neq 0 \\ n_{\nu'} \neq 0}} |\omega_\nu\rangle\langle\omega_\nu|\, T\, |\omega_{\nu'}\rangle\langle\omega_{\nu'}|. \tag{3.42}$$

We define the hole mass operator as the difference between the hole Hamiltonian and this modified kinetic energy operator:

$$M^{(h)}(E) = h^{(h)}(E) - T^{(\neq 0)}. \tag{3.43}$$

Below we drop the $(\neq 0)$ index, as we did in (3.27b). The explicit expression of $M^{(h)}(E)$ is given by (3.24):

$$M^{(h)}(E) = E - T - EK^{-1} + K^{-1}R^{(h)}K^{-1} + K^{-1}D^{(h)}(E)\, K^{-1}. \tag{3.44}$$

Its real and imaginary parts are both hermitian. They are connected by a dispersion relation, which is readily derived from (3.39). By using (3.41b) one gets

$$M^{(h)}(E) = [\,1 - K^{-1}\,][\,E - T\,] + K^{-1}[\,\mathscr{V}^{(h)} + D^{(h)}(E)\,]\, K^{-1}. \tag{3.45}$$

The expression (3.45) is not convenient because $K^{-1}T$ and $\mathscr{V}^{(h)}$ are not hermitian.

3.9.3. *Limitation*

Let us consider a typical one-body Hamiltonian $h = T + U$. When U has a finite range, h reduces to T at large distance. Hence, it has scattering eigenstates at positive energy. We now sketch a proof that this feature does not hold for the hole Hamiltonian $h^{(h)}(E)$, because it only has bound eigenstates.

If $h^{(h)}(E)$ would have a scattering eigenstate $|\varphi_{\mathbf{k}}(E)\rangle$, the latter would be a solution of the Lippmann–Schwinger equation ($E_k = k^2/2m$),

$$\langle \mathbf{r} \,|\, \varphi_{\mathbf{k}}(E)\rangle = -i\eta \,\langle \mathbf{r}|\, (E_k - h^{(h)}(E) - i\eta)^{-1} \,|\mathbf{k}\rangle, \tag{3.46a}$$

where $\langle \mathbf{r} \,|\, \mathbf{k}\rangle$ is a plane wave. The right-hand side of (3.46a) can be written as

$$\begin{aligned} -i\eta \,\langle \mathbf{r}|\, (E - h^{(h)}(E) - i\eta)^{-1} + (E_k - h^{(h)}(E) - i\eta)^{-1} \\ \times (E - E_k)(E - h^{(h)}(E) - i\eta)^{-1} \,|\mathbf{k}\rangle. \end{aligned} \tag{3.46b}$$

This is equal to

$$-i\eta\{\, G^{(h)}(\mathbf{r}, \mathbf{k}; E - i\eta) + \langle \mathbf{r}|\, (E_k - h^{(h)}(E) - i\eta)^{-1} \,(E - E_k)\, G^{(h)}(E - i\eta) \,|\mathbf{k}\rangle\,\}, \tag{3.46c}$$

where $G^{(h)}(\mathbf{r}, \mathbf{k}; E - i\eta)$ is the Fourier transform of $G^{(h)}(\mathbf{r}, \mathbf{r}'; E - i\eta)$. The limit $\eta \to +0$ vanishes, since $G^{(h)}(\mathbf{r}, \mathbf{k}; E - i\eta)$ and $G^{(h)}(E - i\eta)\,|\mathbf{k}\rangle$ are both normalizable. This confirms that $h^{(h)}(E)$ does not have scattering eigenstates.

3.9.4. *Bilinear Expansion of the Hole Green's Function*

We showed that all the eigenstates of $h^{(h)}(E)$ can be normalized. Theorems given in Section 12.5 of [35] indicate that the basic origin of this property is that the hole Green's function is a Hilbert–Schmidt operator; hence it is also compact (see Appendix B). Let us introduce the eigenvalues and eigenstates of $h^{(h)}(E)$ for fixed E:

$$h^{(h)}(E)\,|\varphi_\alpha^{(h)}(E)\rangle = e_\alpha^{(h)}(E)\,|\varphi_\alpha{}^{(h)}(E)\rangle, \qquad \langle \tilde{\varphi}_\alpha^{(h)}(E)|\, h^{(h)}(E) = \langle \tilde{\varphi}_\alpha^{(h)}(E)|\, e_\alpha^{(h)}(E), \tag{3.47a}$$

$$\langle \varphi_\alpha^{(h)}(E) \,|\, \varphi_\alpha^{(h)}(E)\rangle = 1, \qquad \langle \tilde{\varphi}_\beta^{(h)}(E) \,|\, \varphi_\alpha^{(h)}(E)\rangle = \delta_{\beta\alpha}. \tag{3.47b}$$

In general, the eigenvalues $e_\alpha^{(h)}(E)$ are complex:

$$e_\alpha^{(h)}(E) = \langle \varphi_\alpha^{(h)}(E)|\, \mathrm{Re}\, h^{(h)}(E)\,|\varphi_\alpha^{(h)}(E)\rangle + i\,\langle \varphi_\alpha^{(h)}(E)|\, W^{(h)}(E)\,|\varphi_\alpha^{(h)}(E)\rangle. \tag{3.48a}$$

The results of Section 3.2 show that

$$\mathrm{Im}\, e_\alpha^{(h)}(E) > 0 \qquad \text{for} \quad E < T_0^{(-)}, \tag{3.48b}$$

$$\mathrm{Im}\, e_\alpha^{(h)}(E) = 0 \qquad \text{for} \quad E > T_0^{(-)}. \tag{3.48c}$$

We assume that the eigenstates of $h^{(h)}(E)$ form a complete biorthogonal set [36–38]

$$\sum_{\alpha} |\varphi_{\alpha}^{(h)}(E)\rangle\langle\tilde{\varphi}_{\alpha}^{(h)}(E)| = 1. \tag{3.49}$$

According to (3.7a), the bilinear expansion of $G^{(h)}(E-i\eta)$ reads

$$G^{(h)}(E-i\eta) = \sum_{\alpha} \frac{|\varphi_{\alpha}^{(h)}(E)\rangle\langle\tilde{\varphi}_{\alpha}^{(h)}(E)|}{E-e_{\alpha}^{(h)}(E)-i\eta}. \tag{3.50}$$

This expansion is quite different from that given by (3.5b) and (3.5c). In particular, (3.5c) contains an integral which is responsible for the branch cut of $G^{(h)}(E)$. In contrast, in (3.50) the sum only runs over discrete eigenvalues. In (3.50) the existence of a branch cut is hidden in the complex nature of the eigenvalues $e_{\alpha}^{(h)}(E)$. For instance, the spectral function can still be evaluated from (3.6), but it now reads

$$S^{(h)}(E) = \frac{1}{2i\pi} \sum_{\alpha} \left[\frac{|\varphi_{\alpha}^{(h)}(E)\rangle\langle\tilde{\varphi}_{\alpha}^{(h)}(E)|}{E-e_{\alpha}^{(h)}(E)-i\eta} - \frac{|\tilde{\varphi}_{\alpha}^{(h)}(E)\rangle\langle\varphi_{\alpha}^{(h)}(E)|}{E-[e_{\alpha}^{(h)}(E)]^{*}+i\eta} \right]. \tag{3.51}$$

3.10. *Spectroscopic Factors*

We first introduce the following "normalized" overlap

$$|\lambda^{(-)}\rangle = [\mathscr{S}_{\lambda}^{(-)}]^{-1/2} |\chi_{\lambda}^{(-)}\rangle, \qquad \langle\lambda^{(-)}|\lambda^{(-)}\rangle = 1, \tag{3.52}$$

where

$$\mathscr{S}_{\lambda}^{(-)} = \langle\chi_{\lambda}^{(-)}|\chi_{\lambda}^{(-)}\rangle. \tag{3.53a}$$

The latter quantity can be written as

$$\mathscr{S}_{\lambda}^{(-)} = \langle\Psi_0^{(A)}| a_{\lambda}^{\dagger} |\Psi_{\lambda}^{(-)}\rangle\langle\Psi_{\lambda}^{(-)}| a_{\lambda} |\Psi_0^{(A)}\rangle, \tag{3.53b}$$

where $a_{\lambda}^{\dagger}$ and a_{λ} are creation and annihilation operators. Equation (3.53b) shows that $\mathscr{S}_{\lambda}^{(-)}$ is the probability of exciting the bound level $|\Psi_{\lambda}^{(-)}\rangle$ when one removes from $|\Psi_0^{(A)}\rangle$ one nucleon with wave function $\lambda^{(-)}(\mathbf{r})$. Thus, $\mathscr{S}_{\lambda}^{(-)}$ can be identified with the "spectroscopic factor" of the level $|\Psi_{\lambda}^{(-)}\rangle$. Let us now prove in two different ways that $\mathscr{S}_{\lambda}^{(-)}$ can be calculated from the hole Hamiltonian:

(a) By introducing the operators $P^{(h)}$ and $Q^{(h)}$ in (2.2a), one readily obtains

$$(\mathscr{E}_{\lambda}^{(-)} - P^{(h)}HP^{(h)})\, P^{(h)} |\Psi_{\lambda}^{(-)}\rangle = P^{(h)}HQ^{(h)} |\Psi_{\lambda}^{(-)}\rangle, \tag{3.54a}$$

$$(\mathscr{E}_{\lambda}^{(-)} - Q^{(h)}HQ^{(h)})\, Q^{(h)} |\Psi_{\lambda}^{(-)}\rangle = Q^{(h)}HP^{(h)} |\Psi_{\lambda}^{(-)}\rangle. \tag{3.54b}$$

The solution of (3.54b) is given by

$$Q^{(h)}\,|\Psi_\lambda^{(-)}\rangle = (\mathscr{E}_\lambda^{(-)} - Q^{(h)}HQ^{(h)})^{-1}\,Q^{(h)}HP^{(h)}\,|\Psi_\lambda^{(-)}\rangle. \tag{3.54c}$$

By substituting (3.54c) in the normalization condition

$$\langle \Psi_\lambda^{(-)}|\,P^{(h)} + Q^{(h)}\,|\Psi_\lambda^{(-)}\rangle = 1, \tag{3.54d}$$

one finds

$$\langle \Psi_\lambda^{(-)}|\,P^{(h)} + P^{(h)}HQ^{(h)}(\mathscr{E}_\lambda^{(-)} - Q^{(h)}HQ^{(h)})^{-2}\,Q^{(h)}HP^{(h)}\,|\Psi_\lambda^{(-)}\rangle = 1. \tag{3.54e}$$

By using (3.17) and (3.26), this gives

$$\mathscr{S}_\lambda^{(-)}\,\langle\lambda^{(-)}|\,K^{-1}\left\{1 - \left[\frac{1}{dE}\,D^{(h)}(E)\right]_{E=E_\lambda^{(-)}} K^{-1}\right\}|\lambda^{(-)}\rangle = 1. \tag{3.55a}$$

In view of (3.24), this yields the expression that we are looking for, namely,

$$\mathscr{S}_\lambda^{(-)} = \left[\,1 - \langle\lambda^{(-)}|\,\frac{d}{dE}\,h^{(h)}(E)\,|\lambda^{(-)}\rangle\,\right]^{-1}_{E=E_\lambda^{(-)}}. \tag{3.55b}$$

(b) Another derivation is based on the "Hellmann–Feynman theorem," of which an extension is given in Appendix A. According to (3.50), the poles $E_\lambda^{(-)}$ of $G^{(h)}(E)$ are located at the roots of

$$E_\lambda^{(-)} = e_\lambda^{(h)}(E_\lambda^{(-)}) \qquad \text{with} \quad E_\lambda^{(-)} > T_0^{(-)}. \tag{3.56a}$$

One has

$$\lim_{E\to E_\lambda^{(-)}} (E - E_\lambda^{(-)})\,G^{(h)}(E) = s_\lambda^{(-)}\,|\varphi_\lambda^{(h)}\rangle\langle\tilde{\varphi}_\lambda^{(h)}|, \tag{3.56b}$$

where

$$\begin{aligned} &|\varphi_\lambda^{(h)}\rangle = |\varphi_\lambda^{(h)}(E_\lambda^{(-)})\rangle, \qquad |\tilde{\varphi}_\lambda^{(h)}\rangle = |\tilde{\varphi}_\lambda^{(h)}(E_\lambda^{(-)})\rangle, \\ &s_\lambda^{(-)} = \left[\,1 - \frac{d}{dE}\,e_\lambda^{(h)}(E)\right]^{-1}_{E=E_\lambda^{(-)}}. \end{aligned} \tag{3.56c}$$

Since $h^{(h)}(E)$ is real and hermitian for $E > T_0^{(-)}$, one has

$$|\varphi_\lambda^{(h)}\rangle = |\lambda^{(-)}\rangle = |\tilde{\varphi}_\lambda^{(h)}\rangle. \tag{3.56d}$$

The Hellmann–Feynman theorem (A.3b) states that

$$\frac{d}{dE} e_\lambda^{(h)}(E) = \langle \tilde{\varphi}_\lambda^{(h)}(E)| \frac{d}{dE} h^{(h)}(E) \, |\varphi_\lambda^{(h)}(E)\rangle. \tag{3.56e}$$

The expression (3.55b) of the spectroscopic factor results from (3.5c) and (3.56b)–(3.56e).

We are now in a position to give the promised proof of (3.10d). When inserting the bilinear expansion (3.50) in the right-hand side of (3.10b), only those terms with $e_\alpha(E)$ real do contribute. Using the notation (3.47a) and (3.47b) one finds that

$$S_{dt}^{(h)}(E) = \eta\pi^{-1} \sum_\alpha |\varphi_\lambda^{(h)}(E)\rangle \{ [E - e_\alpha^{(h)}(E)]^2 + \eta^2 \}^{-1} \langle \varphi_\alpha^{(h)}(E)|. \tag{3.57a}$$

This quantity can be written as

$$\sum_\alpha \delta[E - e_\alpha^{(h)}(E)] \, |\varphi_\alpha^{(h)}(E)\rangle\langle \varphi_\alpha^{(h)}(E)| = \sum_\lambda \frac{|\lambda^{(-)}\rangle\langle\lambda^{(-)}|}{1 - (d/dE)\, e_\lambda^{(h)}(E)} \, \delta(E - E_\lambda^{(-)}), \tag{3.57b}$$

where we used (3.56c) and (3.56d). It follows that

$$S_{dt}^{(h)}(E) = \sum_\lambda \mathscr{I}_\lambda^{(-)} \, |\lambda^{(-)}\rangle\langle\lambda^{(-)}| \, \delta(E - E_\lambda^{(-)}), \tag{3.57c}$$

which amounts to (3.10d) as announced.

3.11. *Feshbach-type Hole Hamiltonians*

Other Schrödinger-type equations for $|\chi_\lambda^{(-)}\rangle$ can be obtained by multiplying (3.27c) on the left by any energy-independent, but possibly nonlocal, operator $\mathscr{N}$. Indeed, this yields

$$[E_\lambda^{(-)} - h_{\mathscr{N}}^{(h)}(E_\lambda^{(-)})] \, |\chi_\lambda^{(-)}\rangle = 0, \tag{3.58a}$$

with

$$h_{\mathscr{N}}^{(h)}(E) = E(1 - \mathscr{N}K^{-1}) + \mathscr{N}K^{-1}[R^{(h)} + D^{(h)}(E)] \, K^{-1}. \tag{3.58b}$$

The resolvent $G_{\mathscr{N}}^{(h)}(E)$ defined by

$$[E - h_{\mathscr{N}}^{(h)}(E)] \, G_{\mathscr{N}}^{(h)}(E) = 1 \tag{3.58c}$$

is related to the hole Green's function by

$$G_{\mathscr{N}}^{(h)}(E) = G^{(h)}(E) \, \mathscr{N}^{-1}. \tag{3.58d}$$

The hole Hamiltonian proper $h^{(h)}(E)$ corresponds to $\mathscr{N}=1$. It is directly related to the hole spectral function, and its real and imaginary parts are symmetric in the coordinate space representation. However, these properties are accompanied by the peculiar feature that $h^{(h)}(E)$ diverges at large E. This divergence can be eliminated by setting $\mathscr{N}=K$ in (3.58b), which then becomes

$$h_{\mathscr{F}}^{(h)}(E)=Kh^{(h)}(E)+E(1-K) \tag{3.59a}$$

$$=[R^{(h)}+D^{(h)}(E)]\,K^{-1} \tag{3.59b}$$

$$=T+(\mathscr{V}^{(h)}+D^{(h)})\,K^{-1}. \tag{3.59c}$$

Despite the appearance of the kinetic energy operator T in the latter relation, $h_{\mathscr{F}}^{(h)}(E)$ has no scattering eigenstate. The lower index $\mathscr{F}$ stands for Feshbach-type. This notation is motivated by the fact that $h_{\mathscr{F}}^{(h)}(E)$ is akin to a Hamiltonian which had been introduced by Feshbach in his pioneering work on the optical-model potential. This will become apparent in Section 4.14.

The Hamiltonian $h_{\mathscr{F}}^{(h)}(E)$ is not hermitian-analytic; i.e., it does not fulfill a relation similar to (3.7d). Its real and imaginary parts are not symmetric in the coordinate space representation; this is exhibited by the factor K^{-1} in (3.59b). The left-hand bound eigenstate of $h_{\mathscr{F}}^{(h)}(E_\lambda^{(-)})$ is given by

$$\langle\tilde{\lambda}_{\mathscr{F}}^{(-)}|=c_{\mathscr{F}}^{\lambda(-)}\langle\lambda^{(-)}|\,K^{-1},\qquad c_{\mathscr{F}}^{\lambda(-)}=\langle\lambda^{(-)}|\,K^{-1}\,|\lambda^{(-)}\rangle^{-1}, \tag{3.60a}$$

where the coefficient $c_{\mathscr{F}}^{\lambda(-)}$ has been determined from Eqs. (A.1c) and (A.1e) of Appendix A. According to (3.58d), the relationship between the resolvent $G_{\mathscr{F}}^{(h)}(E)$ defined by

$$[E-h_{\mathscr{F}}^{(h)}(E)]\,G_{\mathscr{F}}^{(h)}(E)=1, \tag{3.60b}$$

and the hole Green's function is

$$G_{\mathscr{F}}^{(h)}(E)=G^{(h)}(E)\,K^{-1}. \tag{3.60c}$$

From (3.55b) and (3.59a), one finds the following expression for the spectroscopic factor:

$$\mathscr{S}_\lambda^{(-)}=\left\{\langle\lambda^{(-)}|\,K^{-1}\left[1-\frac{d}{dE}h_{\mathscr{F}}^{(h)}(E)\right]|\lambda^{(-)}\rangle\right\}^{-1}_{E=E_\lambda^{(-)}}. \tag{3.60d}$$

The difference between this formula and a simpler one given in [39, 40] is due to the fact that, in these papers, the effects of antisymmetrization and of ground state correlations were not fully taken into account. One advantage of $h_{\mathscr{F}}^{(h)}(E)$ over $h^{(h)}(E)$

is that it remains finite at large energy. Its real and imaginary parts are connected by the dispersion relation

$$\mathrm{Re}\, h^{(h)}_{\mathscr{F}}(E) = R^{(h)} K^{-1} + \sum_q \frac{|\mathscr{J}^{(h)}_q\rangle\langle\mathscr{J}^{(h)}_q|}{E-\varepsilon^{(h)}_q} K^{-1} - \frac{\mathscr{P}}{\pi}\int_{-\infty}^{T_0^{(-)}} dE' \frac{\mathrm{Im}\, h^{(h)}_{\mathscr{F}}(E')}{E'-E}. \quad (3.60e)$$

This seems simpler than (3.39), but this apparent simplicity is somewhat deceptive because the real and imaginary parts of $h^{(h)}_{\mathscr{F}}(E)$ are not hermitian.

3.12. *Choice of the Single-Particle Wave Function*

One could choose to identify the single-particle wave function with $|u^{(-)}\rangle$ instead of $|\chi^{(-)}\rangle$. These two quantities are related by (3.13b). One readily derives a wave equation for $|u^{(-)}_\lambda\rangle$ once an equation for $|\chi^{(-)}_\lambda\rangle$ has been found. Indeed,

$$\bar{h}^{(h)}_\chi(E)\,|\chi^{(-)}_E\rangle = E\,|\chi^{(-)}_E\rangle \quad (3.61a)$$

amounts to

$$\bar{h}^{(h)}_u(E)\,|u^{(-)}_E\rangle = E\,|u^{(-)}_E\rangle, \quad (3.61b)$$

where

$$\bar{h}^{(h)}_u(E) = \bar{h}^{(h)}_\chi(E)\,K - E(K-1). \quad (3.61c)$$

We dropped the index λ, for simplicity. Let us consider two examples:

(a) According to (3.27b) and (3.61c), the $u^{(-)}$-Hamiltonian associated with $h^{(h)}(E)$ is equal to

$$h^{(h)}_u(E) = K^{-1}[R^{(h)} + D^{(h)}(E)]. \quad (3.62a)$$

This operator is not symmetric in the coordinate space representation and remains finite at large energy. It is the transpose of the Feshbach-type hole Hamiltonian:

$$h^{(h)}_u(E) = [h^{(h)}_{\mathscr{F}}(E)]^{\mathrm{T}}. \quad (3.62b)$$

(b) According to (3.59b) and (3.61c), the $u^{(-)}$-Hamiltonian associated with $h^{(h)}_{\mathscr{F}}$ is given by

$$h^{(h)}_{\mathscr{F},u} = R^{(h)} + D^{(h)}(E) - E(K-1). \quad (3.63)$$

This operator is symmetric in the coordinate space representation and diverges at large energy.

Therefore, the mathematical properties of the hole Hamiltonian and of the Feshbach-type Hamiltonian are interchanged when one describes the single-particle wave function by $|u^{(-)}\rangle$ instead of $|\chi^{(-)}\rangle$. in the present paper we ascribed a

privileged role to the overlap functions $|\chi^{(-)}\rangle$ for the following three main reasons. First, these are the single-particle wave functions which most naturally appear in the description of pickup and knockout processes [9, 14]. Second, it is in terms of the overlaps that the spectroscopic factors and the hole spectral function are most directly expressed. Third, $|\chi_\lambda^{(-)}\rangle$, as well as $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$, are eigenvectors of the mass operator (plus kinetic energy), which provides a unified description of the single-particle properties of the $(A-1)$- and $(A+1)$-systems (Section 5).

3.13. *Kerman-type Hole Hamiltonian*

The difficulty that the Feshbach-type Hamiltonian $h_{\mathscr{F}}^{(h)}(E)$ is not hermitian-analytic was encountered in the case of elastic scattering theory. It led some authors to modify the definition of the single-particle scattering wave function at finite distance in such a way that the corresponding one-body Hamiltonian becomes hermitian-analytic [10, 41–44]. We now describe a similar modification in the present hole case. We define the normalized wave function

$$|\lambda_{\mathscr{K}}^{(-)}\rangle = [c_{\mathscr{F}}^{\lambda(-)}]^{1/2}\, K^{-1/2}\, |\lambda^{(-)}\rangle, \tag{3.64a}$$

where $c_{\mathscr{F}}^{\lambda(-)}$ is given by (3.60a). The symbol $\mathscr{K}$ refers to Kerman [41]. It is readily checked from (3.27c) that $|\lambda_{\mathscr{K}}^{(-)}\rangle$ is an eigenstate of the following "Kerman-type" hole Hamiltonian:

$$h_{\mathscr{K}}^{(h)}(E) = K^{-1/2} h_{\mathscr{F}}^{(h)}(E)\, K^{1/2} \tag{3.64b}$$

$$= K^{1/2} h^{(h)}(E)\, K^{1/2} + E(1-K) \tag{3.64c}$$

$$= K^{-1/2}[\, R^{(h)} + D^{(h)}(E)\,]\, K^{-1/2}. \tag{3.64d}$$

This Hamiltonian has the following three main merits: (i) It approaches a constant at large E. (ii) Its real and imaginary parts are symmetric in the coordinate space representation. (iii) Its real and imaginary parts are connected by a simple dispersion relation. Its has the following drawbacks: (a) Its eigenstate $\lambda_{\mathscr{K}}^{(-)}(\mathbf{r})$ differs from $\lambda^{(-)}(\mathbf{r})$ at finite distance; this is relevant for analyses of direct one-nucleon transfer reactions. (b) Its connection to the spectroscopic factors and to the spectral function is not as direct as in the case of the hole Hamiltonian $h^{(h)}(E)$:

$$\mathscr{S}_\lambda^{(-)} = \langle \lambda_{\mathscr{K}}^{(-)}|\, K\, |\lambda_{\mathscr{K}}^{(-)}\rangle \left[\langle \lambda_{\mathscr{K}}^{(-)}|\, 1 - \frac{d}{dE} h_{\mathscr{K}}^{(h)}(E)\, |\lambda_{\mathscr{K}}^{(-)}\rangle \right]^{-1}_{E=E_\lambda^{(-)}}. \tag{3.65a}$$

The first factor is due to the normalization coefficient $c_{\mathscr{F}}^{\lambda(-)}$. The hole spectral function reads

$$S^{(h)}(E) = (2i\pi)^{-1}\, K^{1/2}\{\, G_{\mathscr{K}}^{(h)}(E-i\eta) - G_{\mathscr{K}}^{(h)}(E-i\eta)^\dagger\}\, K^{1/2}, \tag{3.65b}$$

where $G^{(h)}_{\mathscr{K}}(E)$ is the resolvent of $h^{(h)}_{\mathscr{K}}(E)$:

$$[E - h^{(h)}_{\mathscr{K}}(E)]\, G^{(h)}_{\mathscr{K}}(E) = 1. \tag{3.65c}$$

One has

$$G^{(h)}_{\mathscr{K}}(E) = K^{-1/2} G^{(h)}(E)\, K^{-1/2}. \tag{3.65d}$$

3.14. *A New "Hole-type" Hamiltonian*

The hole Hamiltonian $h^{(h)}(E)$ diverges at large E. In contrast, the Feshbach-type Hamiltonian remains finite at large energy. However, its real and imaginary parts are not symmetric in the coordinate space representation. It is mainly in order to eliminate this drawback that a Kerman-type Hamiltonian was introduced in Section 3.13, at the expense that its bound eigenstates differ from the overlap functions at finite radial distance. In the present section, we shall construct a hole-type Hamiltonian $\tilde{h}^{(h)}(E)$ which is free of these drawbacks. We shall exhibit the nature of the price which has to be paid for fulfilling simpler properties. This operator $\tilde{h}^{(h)}(E)$ will be derived by means of a variant of Feshbach's method, in which every vector of the Hilbert space $\mathscr{H}^{(A-1)}$ will be decomposed into two parts which are not orthogonal to one another. One of our main motivations for studying it in detail is that it lends itself to a rigorous mathematical treatment (Appendices B and C).

3.14.1. *Operators $\tilde{P}^{(h)}$ and $\tilde{Q}^{(h)}$*

Since

$$\tilde{P}^{(h)} = \int d\mathbf{r}\, a_{\mathbf{r}}\, |\psi^{(A)}_0\rangle\langle\psi^{(A)}_0|\, a^{\dagger}_{\mathbf{r}}, \qquad \tilde{q}^{(h)} = \mathscr{I}^{(A-1)} - \tilde{P}^{(h)} \tag{3.66a}$$

are both positive definite,

$$\tilde{Q}^{(h)} = \sqrt{\tilde{q}^{(h)}} \tag{3.66b}$$

exists. The operators $\tilde{P}^{(h)}$ and $\tilde{Q}^{(h)}$ are hermitian. However, in contrast to $P^{(h)}$ and $Q^{(h)}$, they are not projection operators:

$$[\tilde{P}^{(h)}]^2 \neq \tilde{P}^{(h)}, \qquad [\tilde{Q}^{(h)}]^2 \neq \tilde{Q}^{(h)}. \tag{3.66c}$$

One has

$$\tilde{P}^{(h)} + \tilde{Q}^{(h)}\tilde{Q}^{(h)} = \mathscr{I}^{(A-1)}. \tag{3.66d}$$

An explicit expression for $\tilde{Q}^{(h)}$ is readily obtained from (3.66a) and (3.66b),

$$\tilde{Q}^{(h)} = 1 - L^{(h)}, \tag{3.67a}$$

where

$$L^{(h)} = \int d\mathbf{r}\, d\mathbf{r}'\, a_{\mathbf{r}}\, |\psi_0^{(A)}\rangle\langle \mathbf{r}|\, \beta^{(h)}\, |\mathbf{r}'\rangle\langle \psi_0^{(A)}|\, a_{\mathbf{r}'}^{+}, \tag{3.67b}$$

with

$$\beta^{(h)} = (1+\sqrt{1-K})^{-1} = (1-\sqrt{1-K})/K. \tag{3.67c}$$

One has

$$\tilde{P}^{(h)} + \tilde{Q}^{(h)} = 1 - \int d\mathbf{r}\, d\mathbf{r}'\, a_{\mathbf{r}}\, |\psi_0^{(A)}\rangle\langle \mathbf{r}|\, (\beta^{(h)}-1)\, |\mathbf{r}'\rangle\langle \psi_0^{(A)}|\, a_{\mathbf{r}'}^{\dagger}. \tag{3.67d}$$

3.14.2. *Construction of the Hole-type Hamiltonian*

Let us successively apply $\tilde{P}^{(h)}$ and $\tilde{Q}^{(h)}$ to

$$\mathscr{E}^{(-)}\, |\Psi_{\mathscr{E}}^{(-)}\rangle = H\, |\psi_{\mathscr{E}}^{(-)}\rangle, \tag{3.68a}$$

where $|\psi_{\mathscr{E}}^{(-)}\rangle$ is a bound or a scattering eigenstate. Using (3.66d), one finds

$$\mathscr{E}^{(-)}\tilde{P}^{(h)}\, |\psi_{\mathscr{E}}^{(-)}\rangle = \tilde{P}^{(h)}H\tilde{P}^{(h)}\, |\psi_{\mathscr{E}}^{(-)}\rangle + \tilde{P}^{(h)}H\tilde{Q}^{(h)}\tilde{Q}^{(h)}\, |\psi_{\mathscr{E}}^{(-)}\rangle, \tag{3.68b}$$

$$\mathscr{E}^{(-)}\tilde{Q}^{(h)}\, |\psi_{\mathscr{E}}^{(-)}\rangle = \tilde{Q}^{(h)}H\tilde{P}^{(h)}\, |\psi_{\mathscr{E}}^{(-)}\rangle + \tilde{Q}^{(h)}H\tilde{Q}^{(h)}\tilde{Q}^{(h)}\, |\psi_{\mathscr{E}}^{(-)}\rangle. \tag{3.68c}$$

We first use these coupled equations in the case of a bound eigenstate $|\psi_{\lambda}^{(-)}\rangle$. When solving (3.68c) for $\tilde{Q}^{(h)}\, |\psi_{\lambda}^{(-)}\rangle$, two situations can occur: (a) The energy $\mathscr{E}_{\lambda}^{(-)}$ is embedded in the continuous spectrum of $\tilde{Q}^{(h)}H\tilde{Q}^{(h)}$. (b) The energy $\mathscr{E}_{\lambda}^{(-)}$ lies outside the continuous spectrum of $\tilde{Q}^{(h)}H\tilde{Q}^{(h)}$. It can be shown that both cases lead to the same solution. For simplicity, here we shall only consider case (b). Equation (3.68c) gives

$$\tilde{Q}^{(h)}\, |\psi_{\lambda}^{(-)}\rangle = (\mathscr{E}_{\lambda}^{(-)} - \tilde{Q}^{(h)}H\tilde{Q}^{(h)})^{-1}\, \tilde{Q}^{(h)}H\tilde{P}^{(h)}\, |\psi_{\lambda}^{(-)}\rangle. \tag{3.68d}$$

The right-hand side does not change if one replaces $\mathscr{E}_{\lambda}^{(-)}$ by either one of the two limiting prescriptions $\mathscr{E}_{\lambda}^{(-)} \to \mathscr{E}_{\lambda}^{(-)} \mp i\eta$. We shall choose the sign $(-i\eta)$ so that the hole-type Hamiltonian $\tilde{h}^{(h)}(E)$ which will be defined below has analytic properties similar to those of the hole Hamiltonian $h^{(h)}(E)$. By introducing (3.68d) in (3.68b), one obtains

$$[\mathscr{E}_{\lambda}^{(-)} - \tilde{P}^{(h)}H - \tilde{P}^{(h)}H\tilde{Q}^{(h)}\{\mathscr{E}_{\lambda}^{(-)} - \tilde{Q}^{(h)}H\tilde{Q}^{(h)} - i\eta\}^{-1}\, \tilde{Q}^{(h)}H]\, \tilde{P}^{(h)}\, |\psi_{\lambda}^{(-)}\rangle = 0, \tag{3.68e}$$

where the sign in front of $i\eta$ is arbitrary.

We now derive a one-body wave equation for the overlap $|\chi_\lambda^{(-)}\rangle$. According to (3.66a) and to the definition (2.8a) of the density matrix one has

$$\tilde{P}^{(h)} a_{\mathbf{r}} \, |\psi_0^{(A)}\rangle = \int d\mathbf{r}' \, K_{\mathbf{r}\mathbf{r}'} a_{\mathbf{r}'} \, |\psi_0^{(A)}\rangle, \tag{3.69}$$

$$\langle \psi_0^{(A)} | \, a_{\mathbf{r}'}^\dagger \tilde{P}^{(h)} \, |\psi_\lambda^{(-)}\rangle = \int d\mathbf{r} \, \langle \chi_\lambda^{(-)} | \, \mathbf{r} \rangle \, K_{\mathbf{r}\mathbf{r}'}. \tag{3.70}$$

This suggests multiplying (3.68e) from the left by $\langle \psi_0^{(A)} | \, a_{\mathbf{r}'}^\dagger$ and from the right by K^{-1}. We transpose the result and find that

$$E_\lambda^{(-)} \chi_\lambda^{(-)}(\mathbf{r}) = \int d\mathbf{r}' \, \tilde{h}^{(h)}(\mathbf{r}, \mathbf{r}'; E_\lambda^{(-)} - i\eta) \, \chi_\lambda^{(-)}(\mathbf{r}'), \tag{3.71}$$

where

$$\tilde{h}^{(h)}(\mathbf{r}, \mathbf{r}'; E - i\eta) = \mathscr{E}_0^{(A)} \delta(\mathbf{r} - \mathbf{r}') - \langle \psi_0^{(A)} | \, a_{\mathbf{r}'}^\dagger H a_{\mathbf{r}} \, |\psi_0^{(A)}\rangle + \tilde{D}_{\mathbf{r}\mathbf{r}'}^{(h)}(E - i\eta), \tag{3.72}$$

$$\tilde{D}_{\mathbf{r}\mathbf{r}'}^{(h)}(E - i\eta) = \langle \psi_0^{(A)} | \, a_{\mathbf{r}'}^\dagger H \tilde{Q}^{(h)} (E + \tilde{Q}^{(h)} H \tilde{Q}^{(h)} - \mathscr{E}_0^{(A)} - i\eta)^{-1} \, \tilde{Q}^{(h)} H a_{\mathbf{r}} \, |\psi_0^{(A)}\rangle. \tag{3.73}$$

We shall call $\tilde{h}^{(h)}(E - i\eta)$ the hole-type Hamiltonian. It can also be expressed as

$$\tilde{h}^{(h)}(\mathbf{r}, \mathbf{r}'; E - i\eta) = \mathscr{E}_0^{(A)} [\, \delta(\mathbf{r} - \mathbf{r}') - K_{\mathbf{r}\mathbf{r}'} \,] + R_{\mathbf{r}\mathbf{r}'}^{(h)} + \tilde{D}_{\mathbf{r}\mathbf{r}'}^{(h)}(E - i\eta) \tag{3.74a}$$

$$= R_{\mathbf{r}\mathbf{r}'}^{(h)} + \langle \psi_0^{(A)} | \, H a_{\mathbf{r}} a_{\mathbf{r}'}^\dagger \, |\psi_0^{(A)}\rangle + \tilde{D}_{\mathbf{r}\mathbf{r}'}^{(h)}(E - i\eta). \tag{3.74b}$$

Unless confusion might arise, we shall write, for E real,

$$\tilde{h}^{(h)}(E) = \tilde{h}^{(h)}(E - i\eta), \qquad \tilde{D}^{(h)}(E) = \tilde{D}^{(h)}(E - i\eta). \tag{3.75}$$

Equation (3.71) shows that $\tilde{h}^{(h)}(E)$ is equivalent to the hole Hamiltonian $h^{(h)}(E)$ in the sense that both operators have the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates, with eigenvalues $E_\lambda^{(-)}$. They also share the properties that their real and imaginary parts are hermitian and that they only have bound eigenstates. In the case of $\tilde{h}^{(h)}(E)$, the origin of the latter property is that, apart from a constant, this Hamiltonian is a Hilbert–Schmidt operator (see Appendix B.2). Unlike $h^{(h)}(E)$, however, the hole-type Hamiltonian $\tilde{h}^{(h)}(E)$ approaches a constant at large E.

3.14.3. *Resolvent of the Hole-type Hamiltonian*

For a z complex, the resolvent $\tilde{G}^{(h)}(z)$ of $\tilde{h}^{(h)}(z)$ is defined by

$$[\, z - \tilde{h}^{(h)}(z) \,] \, \tilde{G}^{(h)}(z) = 1. \tag{3.76}$$

We now derive the relationship between $\tilde{G}^{(h)}(E-i\eta)$ and the hole Green's function $G^{(h)}(E-i\eta)$, for $\eta \neq 0$. Let us insert the unit operator $\mathscr{I}^{(A-1)}$ from (3.66d) in the following identity (z complex)

$$(z+H)\,\mathscr{I}^{(A-1)}(z+H)^{-1}=1. \tag{3.77a}$$

We get

$$(z+H\tilde{P}^{(h)}+H\tilde{Q}^{(h)}\tilde{Q}^{(h)})(z+H)^{-1}=1. \tag{3.77b}$$

By multiplying this relation by $\tilde{Q}^{(h)}$ from the left, we obtain

$$(z+\tilde{Q}^{(h)}H\tilde{Q}^{(h)})\;\tilde{Q}^{(h)}(z+H)^{-1}=\tilde{Q}^{(h)}[\,1-H\tilde{P}^{(h)}(z+H)^{-1}], \tag{3.77c}$$

which yields

$$\tilde{Q}^{(h)}(z+H)^{-1}=(z+\tilde{Q}^{(h)}H\tilde{Q}^{(h)})^{-1}\;\tilde{Q}^{(h)}[\,1-H\tilde{P}^{(h)}(z+H)^{-1}]. \tag{3.77d}$$

We introduce the latter result in (3.77b) and find that

$$\begin{aligned}&[\,z+H\tilde{P}^{(h)}-H\tilde{Q}^{(h)}(z+\tilde{Q}^{(h)}H\tilde{Q}^{(h)})^{-1}\;\tilde{Q}^{(h)}H\tilde{P}^{(h)}](z+H)^{-1}\\&\quad=1-H\tilde{Q}^{(h)}(z+\tilde{Q}^{(h)}H\tilde{Q}^{(h)})^{-1}\;\tilde{Q}^{(h)}.\end{aligned} \tag{3.77e}$$

In order to obtain a relation between one-body operators, we multiply (3.77e) from the left by $\langle\psi_0^{(A)}|\,a_{\mathbf{r}}^{\dagger}$ and from the right by $a_{\mathbf{r}}\,|\psi_0^{(A)}\rangle$. We set $z=E-\mathscr{E}_0^{(A)}-i\eta$, with $\eta\neq 0$. With the help of the expressions (3.66a) and (3.72) of $\tilde{P}^{(h)}$ and $\tilde{h}^{(h)}(E)$ this leads to

$$G^{(h)}(E-i\eta)[\,E-\tilde{h}^{(h)}](E-i\eta)-i\eta\,]=K-\hat{F}^{(h)}(E-i\eta), \tag{3.78a}$$

where

$$\hat{F}^{(h)}(\mathbf{r},\mathbf{r}';E-i\eta)=\langle\psi_0^{(A)}|\,a_{\mathbf{r}'}^{\dagger}H\tilde{Q}^{(h)}[\,E+\tilde{Q}^{(h)}H\tilde{Q}^{(h)}-\mathscr{E}_0^{(A)}-i\eta\,]^{-1}\;\tilde{Q}^{(h)}a_{\mathbf{r}}\,|\psi_0^{(A)}\rangle. \tag{3.78b}$$

Equations (3.76) and (3.78a) yield

$$G^{(h)}(E-i\eta)=[\,K-\hat{F}^{(h)}(E-i\eta)\,]\;\tilde{G}^{(h)}(E-i\eta). \tag{3.78c}$$

We now show that the relationship between the hole Green's function $G^{(h)}(E-i\eta)$ and the hole-type Green's function $\tilde{G}^{(h)}(E-i\eta)$ is much simpler than (3.78c) appears to indicate. First note that, according to (3.72),

$$\tilde{D}_{\mathbf{r}\mathbf{r}'}^{(h)}(E-i\eta)=\tilde{h}_{\mathbf{r}\mathbf{r}'}^{(h)}(E-i\eta)-\mathscr{E}_0^{(A)}\delta(\mathbf{r}-\mathbf{r}')+\langle\psi_0^{(A)}|\,a_{\mathbf{r}'}^{\dagger}Ha_{\mathbf{r}}\,|\psi_0^{(A)}\rangle. \tag{3.79}$$

By inserting the unit operator (3.66c) between the operators H and $a_{\mathbf{r}}$ inside the matrix element on the right-hand side of (3.73), one readily finds that

$$\begin{aligned}\tilde{D}^{(h)}_{\mathbf{r}\mathbf{r}'}(E-i\eta) = &\langle \psi_0^{(A)} |\, a^\dagger_{\mathbf{r}'} H(1-\tilde{P}^{(h)})\, a_{\mathbf{r}}\, |\psi_0^{(A)}\rangle \\ &+ \langle \psi_0^{(A)} |\, a^\dagger_{\mathbf{r}'} H\tilde{Q}^{(h)} \frac{1}{E+\tilde{Q}^{(h)}H\tilde{Q}^{(h)} - \mathscr{E}_0^{(A)} - i\eta} \\ &\times [\,\tilde{Q}^{(h)}H\tilde{P}^{(h)} - (E-\mathscr{E}_0^{(A)} - i\eta)\,\tilde{Q}^{(h)}]\, a_{\mathbf{r}}\, |\psi_0^{(A)}\rangle. \end{aligned} \tag{3.80}$$

Equations (3.69), (3.78b), (3.79), and (3.80) yield

$$(1-K)[\tilde{h}^{(h)}(E-i\eta) - \mathscr{E}_0^{(A)}] = -(E-\mathscr{E}_0^{(A)} - i\eta)\,\hat{F}(E-i\eta). \tag{3.81a}$$

We multiply this relation from the right by $\tilde{G}^{(h)}(E-i\eta)$ and find, with the use of (3.76),

$$[\,1-K+\hat{F}(E-i\eta)\,]\,\tilde{G}(E-i\eta) = (E-\mathscr{E}_0^{(A)} - i\eta)^{-1}\,(1-K). \tag{3.81b}$$

By inserting this result in (3.78c), we obtain the simple relationship that we were looking for, namely,

$$\tilde{G}^{(h)}(E-i\eta) = G^{(h)}(E-i\eta) + (E-\mathscr{E}_0^{(A)} - i\eta)^{-1}\,(1-K). \tag{3.82}$$

Explicitly, this reads

$$\tilde{G}^{(h)}(E-i\eta) = G^{(h)}(E-i\eta) + \frac{1-\sum |\omega_\nu\rangle\, n_\nu\, \langle\omega_\nu|}{E-\mathscr{E}_0^{(A)} - i\eta}, \tag{3.83}$$

where we expressed K in terms of the natural orbitals; see (2.12b). Hence, $\tilde{G}^{(h)}(E-i\eta)$ has the same singularities as $G(E-i\eta)$, except an additional pole of infinite degeneracy located at $E=\mathscr{E}_0^{(A)}+i\eta$. As specified in (2.2b), $\mathscr{E}_0^{(A)}$ is large and negative; it is typically on the order of -1000 MeV.

3.14.4. *High Energy Behaviour and Sum Rules*

Equations (3.73) and (3.74a) show that, at large E,

$$\tilde{h}^{(h)}(E) \sim \mathscr{E}_0^{(A)}(1-K) + R^{(h)}. \tag{3.84}$$

According to (3.76), $\tilde{G}^{(h)}(z)$ thus behaves as

$$\tilde{G}^{(h)}(z) \sim z^{-1}\{1 + z^{-1}[\,(1-K)\,\mathscr{E}_0^{(A)} + R^{(h)}]\}. \tag{3.85a}$$

This result can also be obtained from (3.31a) and (3.82). Indeed, these yield

$$\tilde{G}^{(h)}(z) \sim z^{-1}(K + z^{-1}R^{(h)}) + z^{-1}(1 + z^{-1}\mathscr{E}_0^{(A)})(1-K). \tag{3.85b}$$

The high energy behaviour $\tilde{G}^{(h)}(z) - z^{-1}$ is in striking contrast with that of the hole Green's function, namely $G^{(h)}(z) \sim K/z$; see (3.31a). We now derive sum rules by performing contour integrals, as we did in connection with (3.32a) and (3.32b), Since $\tilde{G}^{(h)}(z) \sim z^{-1}$ at large z, its contour integral over a large closed circle in the complex z-plane is equal to

$$\int_{\text{circle}} dz\, \tilde{G}^{(h)}(z) = 2i\pi. \tag{3.86a}$$

By indenting the contour around the singularities of $\tilde{G}^{(h)}$, which are all located on the real axis, (3.86a) yields

$$(2i\pi)^{-1} \int_{-\infty}^{E_0^{(-)}} dE[\,\tilde{G}^{(h)}(E - i\eta) - \tilde{G}^{(h)}(E - i\eta)^{\dagger}\,] = 1. \tag{3.86b}$$

In order to discuss the striking difference between this result and (3.32b), let us define a hole-type spectral function as

$$\tilde{S}^{(h)}(E) = (2i\pi)^{-1}[\,\tilde{G}^{(h)}(E - i\eta) - \tilde{G}^{(h)}(E - i\eta)^{\dagger}\,]; \tag{3.87}$$

compare with (3.6). According to (3.82), one has

$$\tilde{S}^{(h)}(E) = S^{(h)}(E) + \lim_{n \to +0} \frac{1}{\pi} \frac{\eta}{[\,(E - \mathscr{E}_0^{(A)})^2 + \eta^2\,]} (1 - K) \tag{3.88a}$$

$$= S^{(h)}(E) + (1 - K)\, \delta(E - \mathscr{E}_0^{(A)}). \tag{3.88b}$$

Hence, the hole-type spectral function is equal to the hole spectral function at all energies except at E. Equation (3.86b) yields

$$\int_{-\infty}^{E_0^{(-)}} dE\, \tilde{S}^{(h)}(E) = 1. \tag{3.89}$$

3.14.5. *The Spectroscopic Factor in Terms of the "Hole-type" Hamiltonian*

Equation (3.82) implies that $\tilde{G}^{(h)}(E)$ and $G^{(h)}(E)$ both have poles at the single-particle energies $E_\lambda^{(-)}$ of the bound states $|\psi_\lambda^{(-)}\rangle$ of the $(A-1)$-system. By multiplying (3.82) by $(E - E_\lambda^{(-)} - i\eta)$ and then taking the limit $E \to E_\lambda^{(-)} + i\eta$, one obtains

$$|\lambda^{(-)}\rangle\, \mathscr{S}_\lambda^{(-)}\, \langle \lambda^{(-)}| = |\lambda^{(-)}\rangle\, \tilde{\mathscr{S}}_\lambda^{(-)}\, \langle \lambda^{(-)}|, \tag{3.90}$$

where $\mathscr{S}_\lambda^{(-)}$ is defined by (3.55b) while, according to the Hellmann–Feynman theorem (A.3a),

$$\tilde{\mathscr{S}}_\lambda^{(-)} = \left[\, \langle \lambda^{(-)}|\, 1 - \frac{d}{dE} \tilde{h}^{(h)}(E)\, |\lambda^{(-)}\rangle \,\right]^{-1}_{E = E_\lambda^{(-)}}. \tag{3.91}$$

Equation (3.90) and the equality $\mathscr{S}_\lambda^{(-)} = \tilde{\mathscr{S}}_\lambda^{(-)}$ imply that

$$\left[\langle \lambda^{(-)} | \frac{d}{dE} \tilde{h}^{(h)}(E) \, | \lambda^{(-)} \rangle \right]_{E = E_\lambda^{(-)}} = \left[\langle \lambda^{(-)} | \frac{d}{dE} h^{(h)}(E) \, | \lambda^{(-)} \rangle \right]_{E = E_\lambda^{(-)}}. \tag{3.92}$$

3.14.6. *Limit towards the Real Axis*

We now define $\tilde{G}^{(h)}(E)$ for E real and also summarize (3.5a), (3.7b), and (3.75):

$$\tilde{G}^{(h)}(E) = \lim_{\eta \to +0} \tilde{G}^{(h)}(E - i\eta), \qquad G^{(h)}(E) = \lim_{\eta \to +0} G^{(h)}(E - i\eta), \tag{3.93a}$$

$$\tilde{h}^{(h)}(E) = \lim_{\eta \to +0} \tilde{h}^{(h)}(E - i\eta), \qquad h^{(h)}(E) = \lim_{\eta \to +0} h^{(h)}(E - i\eta). \tag{3.93b}$$

The consistency of the results obtained in Sections 3.4–3.10 indicate that

$$G^{(h)}(E) = \lim_{\eta \to +0} \frac{1}{E - h^{(h)}(E - i\eta) - i\eta} = \lim_{\eta \to +0} \frac{1}{E - h^{(h)}(E) - i\eta}, \tag{3.94a}$$

$$\lim_{\eta \to +0} h^{(h)}(E - i\eta) \, G^{(h)}(E - i\eta) = h^{(h)}(E) \, G^{(h)}(E). \tag{3.94b}$$

We now argue that relations similar to (3.94a) and (3.94b) are not valid in the case of $\tilde{G}^{(h)}(E)$ and $\tilde{h}^{(h)}(E)$ at $E = \mathscr{E}_0^{(A)}$, and more specifically that

$$\begin{aligned} \tilde{G}^{(h)}(\mathscr{E}_0^{(A)}) &= \lim_{\eta \to +0} \frac{1}{\mathscr{E}_0^{(A)} - \tilde{h}^{(h)}(\mathscr{E}_0^{(A)} - i\eta) - i\eta} \\ &\neq \lim_{\eta \to +0} \frac{1}{\mathscr{E}_0^{(A)} - \tilde{h}^{(h)}(\mathscr{E}_0^{(A)}) - i\eta}. \end{aligned} \tag{3.95}$$

In other words, we shall show that $\tilde{G}^{(h)}(\mathscr{E}_0^{(A)})$ is not the resolvent of $\tilde{h}^{(h)}(\mathscr{E}_0^{(A)})$,

$$\lim_{\eta \to +0} \tilde{G}^{(h)}(\mathscr{E}_0^{(A)} - i\eta) \neq \lim_{\eta \to +0} [\mathscr{E}_0^{(A)} - \tilde{h}^{(h)}(\mathscr{E}_0^{(A)}) - i\eta]^{-1}. \tag{3.96}$$

We prove this *ab absurdo*, i.e., by reducing this opposite statement to the absurd. If $\tilde{G}^{(h)}(\mathscr{E}_0^{(A)})$ would be the resolvent of $\tilde{h}^{(h)}(\mathscr{E}_0^{(A)})$, according to (3.82) there would exist an operator

$$\tilde{\mathscr{C}}^{(h)} = \mathscr{E}_0^{(A)} - \tilde{h}^{(h)}(\mathscr{E}_0^{(A)}) \tag{3.97a}$$

which would fulfill the relation

$$\lim_{\eta \to +0} \left[\frac{1}{\tilde{\mathscr{C}}^{(h)} - i\eta} - \frac{1}{\mathscr{E}_0^{(A)} - h^{(h)}(\mathscr{E}_0^{(A)}) - i\eta} - \frac{1 - K}{-i\eta} \right] = 0 \tag{3.97b}$$

and would have a biorthogonal set of normalizable vectors belonging to the eigenvalue zero. Note the appearance of $\tilde{h}^{(h)}(\mathscr{E}_0^{(A)})$ in $\tilde{\mathscr{C}}^{(h)}$, as opposed to that of $h^{(h)}(\mathscr{E}_0^{(A)})$ in the second term of (3.97b). We now show that (3.97b) is not possible. Let $\{|\varphi_q^{(h)}\rangle, |\tilde{\varphi}_q^{(h)}\rangle\}$ be the biorthogonal set of normalizable vectors, belonging to the eigenvalue zero, of $\tilde{\mathscr{C}}^{(h)}$ and $\tilde{\mathscr{C}}^{(h)\dagger}$, respectively. Then,

$$\langle \tilde{\varphi}_q^{(h)} \mid \varphi_r^{(h)} \rangle = \delta_{qr}, \tag{3.98a}$$

$$\frac{1}{\tilde{\mathscr{C}}^{(h)} - i\eta} = -\frac{1}{i\eta} \sum_q |\varphi_q^{(h)}\rangle\langle \tilde{\varphi}_q^{(h)}| + \rho^{(h)}(\eta), \tag{3.98b}$$

where $\rho^{(h)}(\eta)$ has a finite limit when $\eta \to +0$. The second term within the square brackets in (3.97b) also has a finite limit when $\eta \to +0$, since $\mathscr{E}_0^{(A)}$ is not a discrete eigenvalue of $h^{(p)}(\mathscr{E}_0^{(A)})$. By inserting (3.98b) into (3.97b), assumed to be correct, the latter would yield

$$1 - K = \sum_q |\varphi_q^{(h)}\rangle\langle \tilde{\varphi}_q^{(h)}|. \tag{3.99a}$$

Equations (3.98a) and (3.99a) would give

$$(1 - K)\, |\varphi_q^{(h)}\rangle = |\varphi_q^{(h)}\rangle. \tag{3.99b}$$

This is an "absurd" relation since all quantities with which we deal are contained in the Hilbert space $\mathscr{H}^{(1)}_{(\neq 0)}$ from which the natural orbitals with eigenvalue zero are excluded; see (2.11) and (2.13b). This confirms *ab absurdo* the validity of the statements (3.95)–(3.96). One consequence is that one may not derive expressions for $\tilde{S}^{(h)}(E)$ by means of the methods that we had used in conjunction with (3.10b) and (3.10c).

3.14.7. *Analytic Properties of the Hole-type Hamiltonian*

We now explicitly exhibit that $h^{(h)}(E)$ and $\tilde{h}^{(h)}(E)$ have similar analytical properties and derive a dispersion relation between the real and imaginary parts of $\tilde{h}^{(h)}(E)$. In Appendix B.4, we prove that $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$ is self-adjoint. Let us introduce its scattering and bound eigenstates,

$$\tilde{Q}^{(h)} H \tilde{Q}^{(h)}\, |\tilde{\Phi}_q^{(h)}\rangle = (\mathscr{E}_0^{(A)} - \tilde{\varepsilon}_q^{(h)})\, |\tilde{\Phi}_q^{(h)}\rangle, \tag{3.100a}$$

$$\tilde{Q}^{(h)} H \tilde{Q}^{(h)}\, |\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle = (\mathscr{E}_0^{(A)} - \tilde{\varepsilon}^{(h)})\, |\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle, \tag{3.100b}$$

where $\mathscr{E} = \mathscr{E}_0^{(A)} - \tilde{\varepsilon}^{(h)}$. We adopt the same normalization as in (2.2c). The quantities $\tilde{\varepsilon}^{(h)}$ and $\tilde{\varepsilon}_q^{(h)}$ correspond to single-particle energies. The upper degeneracy index c can be identified with the channel index. Indeed, it is shown in Eq. (C.11a) that the scattering eigenstates of $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$ are given by $|\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle = \Omega_{\tilde{Q}}^{(h)}\, |\Psi_{\mathscr{E}}^{c(-)}\rangle$, where

$|\Psi_{\mathscr{E}}^{c(-)}\rangle$ is the eigenstate of H and $\Omega_{\tilde{Q}}^{(h)}$ is a generalized Møller operator. The unit operator reads

$$1 = \sum_q |\tilde{\Phi}_q^{(h)}\rangle\langle\tilde{\Phi}_q^{(h)}| + \sum_c \int_{-\infty}^{T_0^{(-)}} d\tilde{\varepsilon}\, |\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle\langle\tilde{\Phi}_{\mathscr{E}}^{c(-)}|. \tag{3.101}$$

The imaginary part of the hole-type operator $\tilde{h}^{(h)}(E)$ defined by (3.72) and (3.75) is thus given by ($\mathscr{E} = \mathscr{E}_0^{(A)} - E$):

$$\tilde{W}^{(h)}(\mathbf{r}, \mathbf{r}'; E) = \pi \sum_c \langle \Psi_0^{(A)}|\, a_{\mathbf{r}'}^\dagger H\tilde{Q}^{(h)}\, |\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle\langle\tilde{\Phi}_{\mathscr{E}}^{c(-)}|\, \tilde{Q}^{(h)} H a_{\mathbf{r}}\, |\Psi_0^{(A)}\rangle. \tag{3.102}$$

Defining

$$\langle \mathbf{r}\,|\,\tilde{\mathscr{J}}^{c(-)}(E)\rangle = \tilde{\mathscr{J}}_{\mathbf{r}}^{c(-)}(E) = \langle\tilde{\Phi}_{\mathscr{E}}^{c(-)}|\, \tilde{Q}^{(h)} H a_{\mathbf{r}}\, |\Psi_0^{(A)}\rangle, \tag{3.103}$$

one gets

$$\tilde{W}^{(h)}(\mathbf{r}, \mathbf{r}'; E) = \pi \sum_c [\,\tilde{\mathscr{J}}_{\mathbf{r}'}^{c(-)}(E)]^* [\,\tilde{\mathscr{J}}_{\mathbf{r}}^{c(-)}(E)] \qquad \text{for} \quad E < T_0^{(-)}, \tag{3.104}$$

$$\tilde{W}^{(h)}(E) = 0 \qquad \text{for} \quad E > T_0^{(-)}. \tag{3.105}$$

The latter relation is in keeping with (C.6) and (C.7).

Theorem VIII.2 of [45] shows that the resolvent $(z - \mathscr{E}_0^{(A)} + \tilde{Q}^{(h)} H \tilde{Q}^{(h)})^{-1}$ is an analytic function of z in the complementary set of the spectrum of $[\,\tilde{Q}^{(h)} H \tilde{Q}^{(h)} - \mathscr{E}_0^{(A)}]$. We thus conclude from (3.72) and (3.105) that, except for polar singularities at $\tilde{\varepsilon}_q^{(h)}$, the hole-type Hamiltonian $\tilde{h}^{(h)}(E)$ is analytic in the complex E-plane cut from $-\infty$ to $T_0^{(-)}$. These analytical properties are similar to those of the hole Hamiltonian $h^{(h)}(E)$. We recall, however, that $\tilde{h}^{(h)}(E)$ remains finite at large E, in contrast to $h^{(h)}(E)$. The real and imaginary parts of

$$\tilde{h}^{(h)}(E) = \mathrm{Re}\,\tilde{h}^{(h)}(E) + i\tilde{W}^{(h)}(E) \tag{3.106}$$

fulfill the dispersion relation

$$\mathrm{Re}\,\tilde{h}^{(h)}(E) = \mathscr{E}_0^{(A)}(1 - K) + R^{(h)} + \sum_q \frac{|\tilde{\mathscr{J}}_q^{(h)}\rangle\langle\tilde{\mathscr{J}}_q^{(h)}|}{E - \tilde{\varepsilon}_q^{(h)}} - \frac{\mathscr{P}}{\pi}\int_{-\infty}^{T_0^{(-)}} dE'\, \frac{\tilde{W}^{(h)}(E')}{E' - E}, \tag{3.107}$$

where

$$\langle \mathbf{r}\,|\,\tilde{\mathscr{J}}_q^{(h)}\rangle = \langle\tilde{\Phi}_q^{(h)}|\, \tilde{Q}^{(h)} H a_{\mathbf{r}}\, |\Psi_0^{(A)}\rangle. \tag{3.108}$$

3.15. *A Wider Class of Hole Hamiltonians*

Let $\hat{C}^{(h)}(z)$ be an operator which, as a function of z, is analytic in a domain which includes the real energies $E < E_0^{(-)}$. Define

$$\hat{G}^{(h)}(E-i\eta) = G^{(h)}(E-i\eta) + \hat{C}^{(h)}(E-i\eta). \tag{3.109a}$$

It is readily checked that, if it exists, the operator

$$\hat{h}^{(h)}(E) = E - [\hat{G}^{(h)}(E-i\eta)]^{-1} \tag{3.109b}$$

has the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates:

$$\hat{h}^{(h)}(E_\lambda^{(-)})\,|\chi_\lambda^{(-)}\rangle = E_\lambda^{(-)}\,|\chi_\lambda^{(-)}\rangle. \tag{3.109c}$$

Furthermore, the hole spectral function is given by an equation formally identical to (3.6), namely,

$$S^{(h)}(E) = (2i\pi)^{-1} = [\hat{G}^{(h)}(E-i\eta) - \hat{G}^{(h)}(E+i\eta)] \qquad \text{for} \quad E < E_0^{(-)}. \tag{3.109d}$$

A considerable freedom thus exists in the definition of the hole Hamiltonian. This encompasses $\tilde{h}^{(h)}(E)$. Indeed, the resolvent $\tilde{G}^{(h)}(E)$ as given by (3.82) is of the form (3.109a), except at the isolated energy $E = \mathscr{E}_0^{(A)}$. In general, the modified Hamiltonians $\hat{h}^{(h)}(E)$ will not have simple mathematical properties, unless additional conditions are imposed on $\hat{C}^{(h)}(z)$. This will be discussed in Section 5.7, in a broader context.

3.16. *Overview*

We have constructed and investigated various hole Hamiltonians which all enable one to evaluate the single-particle properties of the $(A-1)$-system, i.e., those observables which can in principle be measured by means of pickup or knockout reactions. We combined techniques and concepts of Feshbach's and Green's function theories. Our terminology and presentation have been strongly influenced by the fact that we shall use similar methods to study particle Hamiltonians, which yield single-particle information on the $(A+1)$-system. For instance, this is why in Sections 3.11 and 3.13 we dubbed $h_{\mathscr{F}}^{(h)}(E)$ and $h_{\mathscr{K}}^{(h)}(E)$ Feshbach-type and Kerman-type Hamiltonians. Some freedom exists in choosing a definition for the single-particle wave functions. We identified them with the overlap functions, for reasons given in Section 3.12.

We studied four main types of hole Hamiltonians, namely: (i) The hole Hamiltonian proper $h^{(h)}(E)$ (Sections 3.2–3.10), (ii) the Feshbach-type Hamiltonian $h_{\mathscr{F}}^{(h)}(E)$ (Section 3.11), (iii) the Kerman-type Hamiltonian $h_{\mathscr{K}}^{(h)}$ (Section 3.13), (iv) the hole-type Hamiltonian $\tilde{h}^{(h)}(E)$ (Section 3.14). These Hamiltonians were all required to yield information on the following three main observables: (a) The

overlaps $|\chi_\lambda^{(-)}\rangle$, i.e., the projections of the bound levels $|\Psi_\lambda^{(-)}\rangle$ of the $(A-1)$-system on the ground state $|\Psi_0^{(A)}\rangle$ of the A-nucleon system; (b) the spectroscopic factors $\mathscr{S}_\lambda^{(-)}$ of these bound levels; (c) the hole spectral function, which measures the single-particle strength per unit energy interval in the $(A-1)$-system.

Let us generically denote the hole Hamiltonians by $h_{\mathscr{R}}^{(h)}(E)$. They all have the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates, except $h_{\mathscr{K}}^{(h)}(E)$. They are all nonlocal, energy-dependent, and complex. They are analytic in the complex energy plane, except for poles located on the real axis and for a left-hand cut. The latter runs along the real axis; it extends from $-\infty$ up to the threshold energy $T_0^{(-)}$ associated with nucleon emission from the $(A-1)$-system. All these hole Hamiltonians thus fulfill similar dispersion relations. In the case of the Feshbach-type Hamiltonian, the dispersion relation connects quantities which are not symmetric in the coordinate space representation. In contrast, the real and imaginary parts of $h^{(h)}(E)$, $\tilde{h}^{(h)}(E)$, and $h_{\mathscr{K}}^{(h)}(E)$ are symmetric in this representation.

The hole Green's function is the resolvent of $h^{(h)}(E)$. It is intimately connected to the hole spectral function $S^{(h)}(E)$. The latter is the quantity of main physical interest. It can readily be calculated from $h^{(h)}(E)$, $h_{\mathscr{F}}^{(h)}(E)$, and $h_{\mathscr{K}}^{(h)}(E)$, as well as from $\tilde{h}^{(h)}(E)$. In the latter case, however, one must leave out a spurious contribution to the spectral function, located at the large negative energy $E=\mathscr{E}_0^{(A)}$ of the target ground state.

In Section 3.15, we pointed out that there exist many Hamiltonians, besides $h^{(h)}(E)$ and $\tilde{h}^{(h)}(E)$, which also have the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates and, moreover, enable one to calculate the hole spectral function. We shall return to this freedom in Section 5.7.

4. PARTICLE ONE-BODY HAMILTONIANS

4.1. *Introduction*

In the present section, we combine Feshbach's projection operator approach with the many-body Green's function theory to construct particle Hamiltonians. In order to better exhibit analogies and differences with our preceding study of hole Hamiltonians, we closely follow the presentation of Section 3, that we intentionally paraphrase as much as possible. This also renders the present Section 4 self-contained. One main qualitative difference with Section 3 is that, in addition to the overlaps $|\chi_\lambda^{(+)}\rangle$ associated with the bound levels of the $(A+1)$-system, the particle Hamiltonians also have as eigenstates the "elastic" overlaps

$$\chi_E^{0(+)}(\mathbf{r}) = \langle \mathbf{r} | \chi_E^{0(+)} \rangle = \langle \Psi_0^{(A)} | \, a_{\mathbf{r}} \, | \Psi_{\mathscr{E}}^{0(A+1)} \rangle, \tag{4.1}$$

where $|\Psi_{\mathscr{E}}^{0(A+1)}\rangle$ denotes the scattering wave function in which the target is its ground state $|\Psi_0^{(A)}\rangle$. A precise definition of $|\Psi_{\mathscr{E}}^{0(A+1)}\rangle$ is given in Appendix D. The

index E attached to $|\chi_E^{0(+)}\rangle$ is the asymptotic kinetic energy of the incident nucleon. It is related to $\mathscr{E}^{(A+1)}$ by

$$E = \mathscr{E}^{(A+1)} - \mathscr{E}_0^{(A)}. \tag{4.2}$$

We shall abbreviate $\mathscr{E}^{(A+1)}$ by $\mathscr{E}^{(+)}$ and, moreover, often drop the upper index of $\mathscr{E}^{(+)}$.

Thus, the particle Hamiltonians $h_{(p)}(E)$ will have the following eigenstates

$$h_{(p)}(E_\lambda^{(+)})\,|\chi_\lambda^{(+)}\rangle = E_\lambda^{(+)}\,|\chi_\lambda^{(+)}\rangle, \tag{4.3a}$$

$$h_{(p)}(E)\,|\chi_E^{0(+)}\rangle = E\,|\chi_E^{0(+)}\rangle, \tag{4.3b}$$

with $E_\lambda^{(+)} < 0$ and $E > 0$. While (4.3a) is similar to (3.7c), Eq. (4.3b) has no analog in the hole case. We shall also require the particle Hamiltonians to enable one to evaluate the spectroscopic factors as well as the particle spectral function, which measures the single-particle strength per unit energy interval in the $(A+1)$-system. We shall see that the particle Hamiltonians are not fully specified by these requirements. We shall thus be led to investigate many equivalent but different Hamiltonians.

(i) Sections 4.3–4.13 are devoted to the particle Hamiltonian proper. This operator $h^{(p)}(E)$ has the specific property that its resolvent is the "particle Green's function" of many-body theory. Its real and imaginary parts are hermitian, but its real part diverges linearly at large energy.

(ii) In Section 4.14, we show that one can readily construct from $h^{(p)}(E)$ many other Hamiltonians which also have the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$ as eigenstates. They present the main drawback that their real and imaginary parts are not hermitian. We shall demonstrate that Feshbach's optical-model Hamiltonian [3] belongs to this family; it has the merit that it remains finite at large energy.

(iii) In Section 4.16, we construct a particle Hamiltonian whose real and imaginary parts are hermitian and which remains finite at large energy. This will be achieved by decomposing any vector of the Hilbert space into two components which are not orthogonal to one another, in contrast to Feshbach's original method.

(iv) In Section 4.18, we exhibit that, actually, there exist an infinite number of Hamiltonians which all have the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$ as eigenstates and enable one to evaluate the particle spectral function.

4.2. *Particle Green's and Spectral Functions*

We recall several definitions and properties. Details can be found in [18], for instance. "Single-particle energies" associated with the bound levels and thresholds of the $(A+1)$-system are defined as

$$E_\lambda^{(+)} = \mathscr{E}_\lambda^{(+)} - \mathscr{E}_0^{(A)}, \qquad T_c^{(+)} = \mathscr{T}_c^{(+)} - \mathscr{E}_0^{(A)}; \tag{4.4a}$$

see (2.3a), (4.2), and (4.3a). The smallest value of $T_c^{(+)}$ will be denoted by $T_0^{(+)}$; since it corresponds to the elastic channel,

$$T_0^{(+)} = 0. \tag{4.4b}$$

The single-particle energy of the ground state of the $(A+1)$-system is

$$E_0^{(+)} = \mathscr{E}_0^{(A+1)} - \mathscr{E}_0^{(A)} < 0, \tag{4.4c}$$

where the last inequality follows from (2.2b). In the following, we shall drop the specification "single-particle" unless confusion might arise. The interest of these energies is twofold. First, they can be associated with the eigenvalues of a one-body Hamiltonian; see (4.3a) and (4.3b). Second, they provide a common energy scale for the $(A-1)$- and $(A+1)$-systems. This will become clear in Section 5.

For a z complex, the particle Green's function is defined as

$$G^{(p)}(\mathbf{r}, \mathbf{r}'; z) = \langle \Psi_0^{(A)} \mid a_{\mathbf{r}} \{ z - H + \mathscr{E}_0^{(A)} \}^{-1} a_{\mathbf{r}'}^{\dagger} \mid \Psi_0^{(A)} \rangle. \tag{4.5a}$$

It is a symmetric function of $\mathbf{r}$ and $\mathbf{r}'$. The completeness relation (2.3a) yields

$$G^{(p)}(z) = \int_{-\infty}^{\infty} dE' \, \frac{S^{(p)}(E')}{z - E'}, \tag{4.5b}$$

where $S^{(p)}(E)$ is the "particle spectral function"

$$S^{(p)}(E) = \sum_{\lambda} |\chi_{\lambda}^{(+)}\rangle\langle\chi_{\lambda}^{(+)}| \, \delta(E - E_{\lambda}^{(+)}) + \sum_{c} |\chi_E^{c(+)}\rangle\langle\chi_E^{c(+)}| \tag{4.6a}$$

$$= (2i\pi)^{-1} \{ G^{(p)}(E - i\eta) - G^{(p)}(E + i\eta) \}; \tag{4.6b}$$

compare with (3.6). According to (4.5a) and (4.5b), the function $G^{(p)}(z)$ is analytic in the whole complex z-plane, except on the real axis, where it has poles at $E_{\lambda}^{(+)}$ and a branch cut which extends from 0 to $+\infty$. This is depicted in Fig. 2. Thus, one can write (4.6b) as

$$S^{(p)}(E) = (2i\pi)^{-1} \{ G^{(p)}(E + i\eta)^{\dagger} - G^{(p)}(E + i\eta) \}. \tag{4.6c}$$

The particle spectral function vanishes for E smaller than the energy $E_0^{(+)}$ of the ground state of the $(A+1)$-system:

$$S^{(p)}(E) = 0 \qquad \text{for} \quad E < E_0^{(+)}. \tag{4.6d}$$

According to (2.5b) and (2.8a), it fulfills the sum rule

$$\int_{E_0^{(+)}}^{\infty} dE \, S^{(p)}(E) = 1 - K, \tag{4.7a}$$

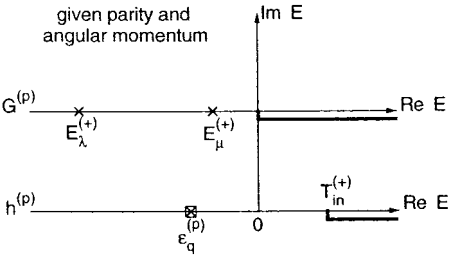

FIG. 2. Sketch of the analytic properties of the particle Green's function and of the particle Hamiltonian in the complex energy plane. The thick lines represent right-hand cuts. The crosses correspond to poles on the real axis. For given angular momentum and parity, only very few such poles exist.

where K is the one-body density matrix (2.8a). When one uses an approximation for the ground state $|\Psi_0^{(A)}\rangle$, Eq. (4.7a) may have to be written in the more detailed form:

$$\int_{E_0^{(+)}}^{\infty} dE\, S^{(p)}(E) = \mathscr{I}^{(1)}_{(\neq 1)} - K^{(\neq 1)}. \tag{4.7b}$$

The appearance of $\mathscr{I}^{(1)}_{(\neq 1)}$ and of the truncated density matrix $K^{(\neq 1)}$ is due to (2.11) which states that the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{c(+)}\rangle$ are orthogonal to those natural orbitals whose occupancy is equal to unity. Hence, the particle Green's function and all related quantities are contained within the truncated Hilbert space $\mathscr{H}^{(1)}_{(\neq 1)}$, in the sense discussed in connection with (2.13a).

For E real, $G^{(p)}(E)$ will be defined as the limit

$$G^{(p)}(E) = \lim_{\eta \to +0} G^{(p)}(E + i\eta). \tag{4.8}$$

Note the difference with the limit (3.5a) that we had adopted for the hole Green's function $G^{(h)}(E)$. In the latter case, the $(E - i\eta)$ limit was adopted in order to simplify the connection with the time-ordered Green's function (Section 5). In the particle case, the $(E + i\eta)$ limit is more convenient for relating $G^{(p)}(E)$ to elastic scattering properties, because it is related to the "outgoing wave boundary condition."

The particle spectral function is the sum of "discrete" and "continuum" contributions, respectively, associated with bound and scattering states of the $(A+1)$-system:

$$S^{(p)}(E) = S^{(p)}_{dt}(E) + S^{(p)}_{ct}(E), \tag{4.9a}$$

$$S^{(p)}_{dt}(E) = \sum_\lambda |\chi_\lambda^{(+)}\rangle\langle\chi_\lambda^{(+)}|\, \delta(E - E_\lambda^{(+)}), \tag{4.9b}$$

$$S^{(p)}_{ct}(E) = \sum_c |\chi_E^{c(+)}\rangle\langle\chi_E^{c(+)}| = \sum_c S^{(p)}_{c(+)}(E). \tag{4.9c}$$

Correspondingly,

$$G^{(p)}(E) = G^{(p)}_{dt}(E) + G^{(p)}_{ct}(E), \tag{4.9d}$$

$$G^{(p)}_{dt}(E) = \sum_{\lambda} \frac{|\chi^{(+)}_{\lambda}\rangle\langle\chi^{(+)}_{\lambda}|}{E - E^{(+)}_{\lambda} + i\eta}, \tag{4.9e}$$

$$G^{(p)}_{ct}(E) = \sum_{c} \int_{T^{(+)}_{c}}^{\infty} dE' \frac{|\chi^{c(+)}_{E'}\rangle\langle\chi^{c(+)}_{E'}|}{E - E' + i\eta}. \tag{4.9f}$$

4.3. *The Particle Hamiltonian and Its Bound Eigenstates*

For a z complex, we define the "particle Hamiltonian" $h^{(p)}(z)$ as that operator whose resolvent is $G^{(p)}(z)$:

$$[z - h^{(p)}(z)]\, G^{(p)}(z) = 1. \tag{4.10a}$$

It is hermitian-analytic. For E real, we adopt the limit

$$h^{(p)}(E) = \lim_{\eta \to +0} h^{(p)}(E + i\eta), \tag{4.10b}$$

so that

$$[E - h^{(p)}(E)]\, G^{(p)}(E) = 1. \tag{4.10c}$$

The particle Hamiltonian $h^{(p)}(E)$ is symmetric in the coordinate space representation. At the present stage, our interest in the particle Hamiltonian is fully justified by the fact that the bound overlaps $|\chi^{(+)}_{\lambda}\rangle$ are eigenstates of $h^{(p)}(E)$:

$$h^{(p)}(E^{(+)}_{\lambda})\, |\chi^{(+)}_{\lambda}\rangle = E^{(+)}_{\lambda}\, |\chi^{(+)}_{\lambda}\rangle. \tag{4.11}$$

This can readily be derived from (4.9e) and (4.10c). The particle Hamiltonian thus fulfills the requirement (4.3a).

When one uses for $|\psi^{(A)}_0\rangle$ a model in which the occupation probabilities of some natural orbitals are equal to unity, (2.11) implies that

$$G^{(p)}(E)\, |\omega_{\nu(1)}\rangle = 0. \tag{4.12}$$

Then, (4.10c) should be written in the more detailed form

$$[E - h^{(p)}(E)]\, G^{(p)}(E) = \mathscr{I}^{(1)}_{(\neq 1)}. \tag{4.13}$$

4.4. *Elastic Single-Particle Wave Functions*

In the present section, we show that the requirement (4.3b) is fulfilled by the particle Hamiltonian $h^{(p)}(E)$. Previous proofs were based on time-dependent scattering theory

[5, 15, 46]. The latter will be used in Appendix E, in a broader context. Here, we would rather use the "very cryptic" [47] but probably more familiar language of stationary collision theory. This will be convenient to show later on that there exist many other Hamiltonians which have the elastic overlap $|\chi_E^{0(+)}\rangle$ as an eigenstate (Sections 4.17, 4.18, and 5.7).

4.4.1. *Lippmann–Schwinger Equation for the Particle Hamiltonian*

We write the particle Hamiltonian as the sum of the kinetic energy operator T and of a potential-type operator $M^{(p)}(E)$ that we dub "the particle mass operator":

$$h^{(p)}(E) = T + M^{(p)}(E). \tag{4.14}$$

The eigenstates of T are plane waves:

$$T\,|\mathbf{k}\rangle = E_k\,|\mathbf{k}\rangle, \tag{4.15a}$$

$$E_k = k^2/2m, \tag{4.15b}$$

$$\langle \mathbf{r}\,|\,\mathbf{k}\rangle = (2\pi)^{-3/2}\,e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{4.15c}$$

We introduce the scattering eigenstates of $h^{(p)}(E)$:

$$h^{(p)}(E_k)\,|\varphi_{\mathbf{k}}\rangle = E_k\,|\varphi_{\mathbf{k}}\rangle. \tag{4.16a}$$

The lower index $\mathbf{k}$ on $|\varphi_{\mathbf{k}}\rangle$ refers to the asymptotic boundary condition that, at large distance,

$$\langle \mathbf{r}\,|\,\varphi_{\mathbf{k}}\rangle \sim \langle \mathbf{r}\,|\,\mathbf{k}\rangle + \mathrm{out}(\mathbf{r}), \tag{4.16b}$$

where out($\mathbf{r}$) denotes outgoing waves. According to the Lippmann–Schwinger equation,

$$|\varphi_{\mathbf{k}}\rangle = |\mathbf{k}\rangle + (E_k - h^{(p)}(E_k) + i\eta)^{-1}\,M^{(p)}(E_k)\,|\mathbf{k}\rangle \tag{4.16c}$$

$$= i\eta G^{(p)}(E_k + i\eta)\,|\mathbf{k}\rangle. \tag{4.16d}$$

In the coordinate space representation, (4.16d) reads

$$\langle \mathbf{r}\,|\,\varphi_{\mathbf{k}}\rangle = i\eta \int d\mathbf{r}'\; G^{(p)}(\mathbf{r}, \mathbf{r}'; E_k + i\eta)\,e^{i\mathbf{k}\cdot\mathbf{r}'}. \tag{4.16e}$$

We pointed out in Section 2.4 that the one-body quantities considered in the present Section 4 must be contained within the Hilbert space $\mathscr{H}^{(1)}_{(\neq 1)}$. When the kinetic energy operator T acts on a function of $\mathscr{H}^{(1)}_{(\neq 1)}$, the result in general does

not belong to that Hilbert space. Therefore, it is appropriate to introduce the modified kinetic energy operator

$$T^{(\neq 1)} = \left\{1 - \sum_{\nu} |\omega_{\nu(1)}\rangle\langle\omega_{\nu(1)}|\right\} T \left\{1 - \sum_{\nu} |\omega_{\nu(1)}\rangle\langle\omega_{\nu(1)}|\right\}, \tag{4.17}$$

where $|\omega_{\nu(1)}\rangle$ are natural orbitals whose occupation numbers are equal to unity. Correspondingly, the plane wave (4.15c) should then be replaced by the eigenstate of $T^{(\neq 1)}$. We shall no longer mention this type of modification, since it does not give rise to any basic difficulty.

4.4.2. *Lippmann–Schwinger Equation for the* $(A+1)$*-Body Problem*

The relevant properties of the scattering eigenstates of the $(A+1)$-nucleon Hamiltonian are surveyed in Appendix D. In the present section, we only consider the elastic scattering eigenstate $|\Psi_{\mathbf{k}}^{0(+)}\rangle$ in which the target is in the ground state $|\Psi_0^{(A)}\rangle$:

$$H\,|\Psi_{\mathbf{k}}^{0(+)}\rangle = \mathscr{E}_k^0\,|\Psi_{\mathbf{k}}^{0(+)}\rangle. \tag{4.18a}$$

The lower index $\mathbf{k}$ refers to the incident plane wave $|\mathbf{k}\rangle$. In spatial coordinates, $|\Psi_{\mathbf{k}}^{0(+)}\rangle$ has the following asymptotic behaviour at large distance:

$$\langle \mathbf{r}, \xi\,|\,\Psi_{\mathbf{k}}^{0(+)}\rangle \sim (A+1)^{-1/2}\,\mathscr{A}\{[\langle \mathbf{r}\,|\,\mathbf{k}\rangle + \mathrm{out}(\mathbf{r})]\;\Psi_0^{(A)}(\xi)\}. \tag{4.18b}$$

Here, the symbol ξ generically denotes the coordinates $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A$ of the target, while $\mathscr{A}$ is the antisymmetrization operator. In keeping with (D.9b), the total energy is equal to

$$\mathscr{E}_k^0 = \mathscr{E}_0^{(A)} + E_k. \tag{4.18c}$$

The Lippmann–Schwinger form of (4.18a) reads

$$|\Psi_{\mathbf{k}}^{0(+)}\rangle = \frac{i\eta}{E_k - (H - \mathscr{E}_0^{(A)}) + i\eta}\, a_{\mathbf{k}}^{\dagger}\,|\Psi_0^{(A)}\rangle. \tag{4.19}$$

4.4.3. *Elastic Overlap*

We introduce the elastic overlap

$$\chi_{\mathbf{k}}^{0(+)}(\mathbf{r}) = \langle \Psi_0^{(A)}|\, a_{\mathbf{r}}\,|\Psi_{\mathbf{k}}^{0(+)}\rangle. \tag{4.20}$$

Equation (D.14) gives the relationship between this quantity and the spherical overlap $\chi_E^{c(+)}(\mathbf{r})$ that we had defined in (2.5b) and (4.1). By inserting (4.19) in (4.20), we obtain

$$\chi_{\mathbf{k}}^{0(+)}(\mathbf{r}) = i\eta\,\langle \Psi_0^{(A)}|\, a_{\mathbf{r}}\,\frac{1}{E_k - (H - \mathscr{E}_0^{(A)}) + i\eta}\, a_{\mathbf{k}}^{\dagger}\,|\Psi_0^{(A)}\rangle, \tag{4.21}$$

where

$$a_{\mathbf{k}}^{\dagger} = \int d\mathbf{r} \, \langle \mathbf{r} \, | \, \mathbf{k} \rangle \, a_{\mathbf{r}}^{\dagger}; \tag{4.22}$$

see (2.9). The matrix element which appears in (4.21) is the Fourier transform $G^{(p)}(\mathbf{r}, \mathbf{k}; E_k + i\eta)$ of the particle Green's function $G^{(p)}(\mathbf{r}, \mathbf{r}'; E_k + i\eta)$ defined by (4.5a). Therefore, one finds successively

$$\langle \mathbf{r} \, | \, \chi_{\mathbf{k}}^{0(+)} \rangle = i\eta \, \langle \mathbf{r} | \, G^{(p)}(E_k + i\eta) \, | \mathbf{k} \rangle \tag{4.23a}$$

$$= \langle \mathbf{r} | \, (E_k - h^{(p)}(E_k) + i\eta)^{-1} \, (i\eta + E_k - h^{(p)}(E_k) - T + h^{(p)}(E_k)) \, | \mathbf{k} \rangle \tag{4.23b}$$

$$= \langle \mathbf{r} \, | \, \mathbf{k} \rangle + \langle \mathbf{r} | \, (E_k - h^{(p)}(E_k) + i\eta)^{-1} \, M^{(p)}(E_k) \, | \mathbf{k} \rangle, \tag{4.23c}$$

where one uses the definition (4.14) of the particle mass operator. By comparing (4.16c) and (4.23c), we conclude that

$$| \chi_{\mathbf{k}}^{0(+)} \rangle = | \varphi_{\mathbf{k}} \rangle. \tag{4.24a}$$

Therefore, $| \chi_{\mathbf{k}}^{0(+)} \rangle$ is an eigenstate of the particle Hamiltonian:

$$h^{(p)}(E_k) \, | \chi_{\mathbf{k}}^{0(+)} \rangle = E_k \, | \chi_{\mathbf{k}}^{0(+)} \rangle. \tag{4.24b}$$

Equivalently, one may use Eq. (D.14) to write

$$h^{(p)}(E) \, | \chi_E^{0(+)} \rangle = E \, | \chi_E^{0(+)} \rangle, \tag{4.24c}$$

where E is the kinetic energy of the incoming nucleon and $| \chi_E^{0(+)} \rangle$ is the "spherical" elastic overlap. We have thus proved that the requirement (4.3b) is fulfilled by the particle Hamiltonian $h^{(p)}(E)$.

4.5. *Particle Projection Operator*

In order to establish later on a connection between $h^{(p)}(E)$ and Feshbach's optical-model Hamiltonian, let us decompose the vectors of the Hilbert space $\mathscr{H}^{(A+1)}$ into two orthogonal parts with the help of two hermitian projection operators $P^{(p)}$ and $Q^{(p)}$:

$$P^{(p)} + Q^{(p)} = \mathscr{I}^{(A+1)}, \qquad P^{(p)} Q^{(p)} = 0. \tag{4.25a}$$

Following Feshbach [3] we require the "particle projection operator" $P^{(p)}$ to have the property

$$P^{(p)} \, | \Psi^{(A+1)} \rangle = a_{u^{(+)}}^{\dagger} \, | \Psi_0^{(A)} \rangle, \qquad \text{for all} \quad | \Psi^{(A+1)} \rangle, \tag{4.25b}$$

where we have omitted the indices needed to fully characterize $|\Psi^{(A+1)}\rangle$. In keeping with (2.9),

$$a^{\dagger}_{u^{(+)}} = \int d\mathbf{r}\, a^{\dagger}_{\mathbf{r}} u^{(+)}(\mathbf{r}). \tag{4.25c}$$

In the coordinate space representation, (4.25b) reads

$$P^{(p)} |\Psi^{(A+1)}(\mathbf{r}, \xi)\rangle = \frac{1}{\sqrt{A+1}} \mathscr{A}\{u^{(+)}(\mathbf{r})\, \Psi_0^{(A)}(\xi)\}. \tag{4.25d}$$

This is the form which had been used by Feshbach in his pioneering paper [3]. In the present work, we shall rather deal with (4.25b), because this is the most convenient form for exhibiting the analogy with the hole case of Section 3, as well as with Green's function theory.

Let us first derive the relation between $|u^{(+)}\rangle$ and the overlap $|\chi^{(+)}\rangle$ associated with $|\Psi^{(A+1)}\rangle$. Using (4.25b), a sufficient condition for fulfilling (4.25a) is

$$\langle \Psi_0^{(A)}|\, a_{\mathbf{r}}(1 - P^{(p)})\, |\Psi^{(A+1)}\rangle = 0 \qquad \text{for all } \mathbf{r}. \tag{4.25e}$$

Equations (2.5b), (4.25b), (4.25c), and (4.25e) give

$$\chi^{(+)}(\mathbf{r}) = \langle \Psi_0^{(A)}|\, a_{\mathbf{r}} a^{\dagger}_{u^{(+)}}\, |\Psi_0^{(A)}\rangle \tag{4.26a}$$

$$= \int d\mathbf{r}' [\delta(\mathbf{r} - \mathbf{r}') - K(\mathbf{r}, \mathbf{r}')]\, u^{(+)}(\mathbf{r}'); \tag{4.26b}$$

i.e.,

$$|\chi^{(+)}\rangle = (1 - K)\, |u^{(+)}\rangle \tag{4.26c}$$

where $K(\mathbf{r}, \mathbf{r}')$ is the density matrix (2.8a). Since $|\chi^{(+)}\rangle$ is well-defined, (4.26c) fully determines $|u^{(+)}\rangle$, provided that $(1 - K)$ has an inverse. This inverse most probably exists when one uses the exact ground state $|\Psi_0^{(A)}\rangle$, since all the eigenvalues of K are expected to be smaller than unity; see (2.10c). However, some eigenvalues of K may be equal to unity when one adopts an approximation for $|\Psi_0^{(A)}\rangle$. Indeed, there may then exist natural orbitals $|\omega_{\nu(1)}\rangle$ whose occupancy is equal to unity. In that case, the inverse of $(1 - K)$ is ill-defined. The origin of this problem lies in the relation

$$a^{\dagger}_{\nu(1)}\, |\Psi_0^{(A)}\rangle = 0, \tag{4.27a}$$

which shows that any amount of the natural orbital $|\omega_{\nu(1)}\rangle$ can be added to $|u^{(+)}\rangle$ without influencing the requirement (4.25b). A condition must then be added to

(4.25a) and (4.25b) in order to fully specify $|u^{(+)}\rangle$ and $P^{(p)}$. Feshbach [3, 10] proposed that this condition be the following:

$$\langle \omega_{\nu(1)} \,|\, u^{(+)} \rangle = 0. \tag{4.27b}$$

This additional requirement is quite natural in view of the fact that we are most directly interested in the overlaps and that these are contained within the Hilbert space $\mathscr{H}^{(1)}_{(\neq 1)}$; see (2.11) and (2.13a). Thus, we replace (4.26c) by

$$|\chi^{(+)}\rangle = (\mathscr{I}^{(1)}_{(\neq 1)} - K^{(\neq 1)})\, |u^{(+)}\rangle; \tag{4.27c}$$

see (2.14). This has the unique solution

$$|u^{(+)}\rangle = \left(\mathscr{I}^{(1)}_{(\neq 1)} + \frac{K^{(\neq 1)}}{1 - K^{(\neq 1)}} \right) |\chi^{(+)}\rangle. \tag{4.27d}$$

Equations (4.25b) and (4.27d) give successively

$$P^{(p)}\,|\Psi^{(+)}\rangle = \int d\mathbf{r}\; a^{\dagger}_{\mathbf{r}}\,|\Psi^{(A)}_0\rangle\, u^{(+)}(\mathbf{r}) \tag{4.28a}$$

$$= \int d\mathbf{r}\; a^{\dagger}_{\mathbf{r}}\,|\Psi^{(A)}_0\rangle \int d\mathbf{r}' \left[\mathscr{I}^{(1)}_{(\neq 1)} + \frac{K^{(\neq 1)}}{1 - K^{(\neq 1)}} \right]_{\mathbf{r}\mathbf{r}'} \chi^{(+)}(\mathbf{r}') \tag{4.28b}$$

$$= \int d\mathbf{r}\; d\mathbf{r}'\; a^{\dagger}_{\mathbf{r}}\,|\Psi^{(A)}_0\rangle \left[\mathscr{I}^{(1)}_{(\neq 1)} + \frac{K^{(\neq 1)}}{1 - K^{(\neq 1)}} \right]_{\mathbf{r}\mathbf{r}'} \langle \Psi^{(A)}_0 |\, a_{\mathbf{r}'}\,|\Psi^{(+)}\rangle. \tag{4.28c}$$

One thereby obtains the following expression for the particle projection operator:

$$P^{(p)} = \int d\mathbf{r}\; d\mathbf{r}'\; a^{\dagger}_{\mathbf{r}}\,|\Psi^{(A)}_0\rangle \left[\mathscr{I}^{(1)}_{(\neq 1)} + \frac{K^{(\neq 1)}}{1 - K^{(\neq 1)}} \right]_{\mathbf{r}\mathbf{r}'} \langle \Psi^{(A)}_0 |\, a_{\mathbf{r}'}\,. \tag{4.29a}$$

This is the "second quantized" form of the projection operator which had originally been introduced by Feshbach [3]. In the natural orbital basis, it reads [41]

$$P^{(p)} = \sum_{n_\nu \neq 1} a^{\dagger}_{\nu}\,|\Psi^{(A)}_0\rangle \left(1 + \frac{n_\nu}{1 - n_\nu} \right) \langle \Psi^{(A)}_0 |\, a_\nu. \tag{4.29b}$$

We shall usually write (4.27d) in the simplified form

$$|u^{(+)}\rangle = \left(1 + \frac{K}{1 - K} \right) |\chi^{(+)}\rangle. \tag{4.30a}$$

In the coordinate space representation, this becomes

$$u^{(+)}(\mathbf{r}) = \chi^{(+)}(\mathbf{r}) + \sum_{\nu} \omega_{\nu}(\mathbf{r}) \frac{n_{\nu}}{1-n_{\nu}} \langle \omega_{\nu} | \chi^{(+)} \rangle. \tag{4.30b}$$

Since the natural orbitals are normalizable, $u^{(+)}(\mathbf{r})$ and $\chi^{(+)}(\mathbf{r})$ only differ at finite distance. It is in order to keep track of this property that, above, we did not write the right-hand side of (4.30a) as $(1-K)^{-1} |\chi^{(+)}\rangle$. The latter simplified notation will be used below, with the understanding that $(1-K)^{-1}$ stands for

$$(1-K)^{-1} = \left(1 + \frac{K}{1-K}\right). \tag{4.30c}$$

Thus, we shall often write (4.29a) in the form

$$P^{(p)} = \int d\mathbf{r}\, d\mathbf{r}'\, a_{\mathbf{r}}^{\dagger} |\Psi_0^{(A)}\rangle (1-K)^{-1}_{\mathbf{r}\mathbf{r}'} \langle \Psi_0^{(A)}| a_{\mathbf{r}'}. \tag{4.30d}$$

The functions $u^{(+)}(\mathbf{r})$ and $\chi^{(+)}(\mathbf{r})$ yield the same elastic scattering phase shift since they have the same asymptotic behaviour at large distance. Thus, either one of them could be chosen as the "elastic single-particle wave function." Here, we identify the latter with the overlap $\chi^{(+)}(\mathbf{r})$, mainly because this is the quantity which appears most naturally in the theory of one-nucleon transfer reactions [9, 14]. Moreover, $\chi^{(+)}(\mathbf{r})$ is always uniquely defined, while one has to introduce the condition (4.27b) in order to fully specify the value of $u^{(+)}(\mathbf{r})$.

4.6. *Particle Hamiltonian in Terms of Projection Operators*

In order to construct an expression for the particle Hamiltonian $h^{(p)}(E)$ in terms of the projection operators $P^{(p)}$ and $Q^{(p)}$, we replace by $(P^{(p)} + Q^{(p)})$ the unit operator $\mathscr{I}^{(A+1)}$ which appears as the middle factor in the identity

$$(z-H)\, \mathscr{I}^{(A+1)} (z-H)^{-1} = \mathscr{I}^{(A+1)}, \tag{4.31a}$$

where z is a complex energy. We multiply the resulting relation from the right by $P^{(p)}$ and from the left by, successively, $P^{(p)}$ and $Q^{(p)}$. This yields

$$(z - P^{(p)}HP^{(p)})\, P^{(p)}(z-H)^{-1}\, P^{(p)} - P^{(p)}HQ^{(p)}(z-H)^{-1}\, P^{(p)} = P^{(p)}, \tag{4.31b}$$

$$(z - Q^{(p)}HQ^{(p)})\, Q^{(p)}(z-H)^{-1}\, P^{(p)} - Q^{(p)}HP^{(p)}(z-H)^{-1}\, P^{(p)} = 0. \tag{4.31c}$$

We extract $Q^{(p)}(z-H)^{-1}\, P^{(p)}$ from (4.31c) and insert the result in (4.31b). This gives

$$P^{(p)}\mathscr{O}^{(p)}(z)\, P^{(p)}(z-H)^{-1}\, P^{(p)} = P^{(p)}, \tag{4.32a}$$

where

$$\mathcal{O}^{(p)}(z) = z - P^{(p)}HP^{(p)} - P^{(p)}HQ^{(p)}(z - Q^{(p)}HQ^{(p)})^{-1}\, Q^{(p)}HP^{(p)}. \quad (4.32b)$$

In order to obtain a relation between one-body operators, we multiply (4.32a) from the left by $\langle \Psi_0^{(A)}|\, a_{\mathbf{r}}$ and from the right by $a_{\mathbf{r}'}^{\dagger}\,|\Psi_0^{(A)}\rangle$. Noting that

$$P^{(p)}a_{\mathbf{r}}^{\dagger}\,|\Psi_0^{(A)}\rangle = a_{\mathbf{r}}^{\dagger}\,|\Psi_0^{(A)}\rangle, \qquad \langle \Psi_0^{(A)}|\, a_{\mathbf{r}}P^{(p)}a_{\mathbf{r}'}^{\dagger}\,|\Psi_0^{(A)}\rangle = (1-K)^{-1}_{\mathbf{r}\mathbf{r}'}, \quad (4.32c)$$

we find that

$$\int d\mathbf{s}\, d\mathbf{s}'\, \langle \Psi_0^{(A)}|\, a_{\mathbf{r}}\mathcal{O}^{(p)}(z)\, a_{\mathbf{s}}^{\dagger}\,|\Psi_0^{(A)}\rangle(1-K)_{\mathbf{s}\mathbf{s}'}\, G^{(p)}(\mathbf{s}', \mathbf{r}'; z - \mathscr{E}_0^{(A)}) = (1-K)^{-1}_{\mathbf{r}\mathbf{r}'}. \quad (4.32d)$$

With the help of the one-body operator

$$\langle \mathbf{r}|\, O^{(p)}(z)\,|\mathbf{r}'\rangle = \langle \Psi_0^{(A)}|\, a_{\mathbf{r}}\mathcal{O}^{(p)}(z)\, a_{\mathbf{r}'}^{\dagger}\,|\Psi_0^{(A)})\rangle, \quad (4.32e)$$

(4.32d) can then be written as

$$(1-K)\, O(z)(1-K)\, G^{(p)}(z - \mathscr{E}_0^{(A)}) = 1. \quad (4.32f)$$

This relation has the same form as (4.13). By setting $z = E + \mathscr{E}_0^{(a)} + i\eta$, it yields the expression that we were searching for the particle Hamiltonian, namely,

$$h^{(p)}(E + i\eta) = -\frac{K}{1-K}(E + i\eta) + (1-K)^{-1}\,[R^{(p)} + D^{(p)}(E + i\eta)\,](1-K)^{-1}, \quad (4.33)$$

where, in the coordinate space representation,

$$R^{(p)}_{\mathbf{r}\mathbf{r}'} = \langle \Psi_0^{(A)}|\,[a_{\mathbf{r}}, H]\, a_{\mathbf{r}'}^{\dagger}\,|\Psi_0^{(A)}\rangle, \quad (4.34)$$

$$D^{(p)}_{\mathbf{r}\mathbf{r}'}(E + i\eta) = \langle \Psi_0^{(A)}|\, a_{\mathbf{r}}HQ^{(p)}(E - Q^{(p)}HQ^{(p)} + \mathscr{E}_0^{(A)} + i\eta)^{-1}\, Q^{(p)}Ha_{\mathbf{r}'}^{\dagger}\,|\Psi_0^{(A)}\rangle. \quad (4.35)$$

In (4.10b) we introduced the simplified notation $h^{(p)}(E) = h^{(p)}(E + i\eta)$. We shall thus also write

$$D^{(p)}(E) = \lim_{\eta \to +0} D^{(p)}(E + i\eta). \quad (4.36a)$$

If one uses for $|\Psi_0^{(A)}\rangle$ a model in which some natural orbitals are fully occupied, (4.33) should be written in the more explicit form

$$h^{(p)}(E) = -\frac{K^{(\neq 1)}}{1-K^{(\neq 1)}}E + \left(\mathscr{I}^{(1)}_{(\neq 1)} + \frac{K^{(\neq 1)}}{1-K^{(\neq 1)}}\right) \times [R^{(p)} + D^{(p)}(E)] \left(\mathscr{I}^{(1)}_{(\neq 1)} + \frac{K^{(\neq 1)}}{1-K^{(\neq 1)}}\right). \tag{4.36b}$$

We shall henceforth no longer refer to this complication, which now raises no basic difficulty.

4.7. *Spectroscopic Factor*

Let us introduce the following "normalized overlap,"

$$|\lambda^{(+)}\rangle = [\mathscr{S}_\lambda^{(+)}]^{-1/2} |\chi_\lambda^{(+)}\rangle, \qquad \langle \lambda^{(+)}|\lambda^{(+)}\rangle = 1, \tag{4.37a}$$

where

$$\mathscr{S}_\lambda^{(+)} = \langle \chi_\lambda^{(+)} | \chi_\lambda^{(+)}\rangle. \tag{4.37b}$$

The latter quantity can be written as

$$\mathscr{S}_\lambda^{(+)} = \langle \Psi_0^{(A)}| a_\lambda |\Psi_\lambda^{(+)}\rangle\langle \Psi_\lambda^{(+)}| a_\lambda^\dagger |\Psi_0^{(A)}\rangle, \tag{4.37c}$$

where $a_\lambda^\dagger$ and a_λ are creation and annihilation operators. Equation (4.37c) shows that $\mathscr{S}_\lambda^{(+)}$ is the probability of exciting the bound level $|\Psi_\lambda^{(+)}\rangle$ when one adds to the ground state $|\Psi_0^{(A)}\rangle$ one nucleon with wave function $\lambda^{(+)}(\mathbf{r})$. Therefore, $\mathscr{S}_\lambda^{(+)}$ is the spectroscopic factor of the level $|\Psi_\lambda^{(+)}\rangle$. We now prove in two different ways that $\mathscr{S}_\lambda^{(+)}$ can be calculated from the particle Hamiltonian $h^{(p)}(E)$:

(a) By introducing the operators $P^{(p)}$ and $Q^{(p)}$ in (2.2a), one readily finds

$$(\mathscr{E}_\lambda^{(+)} - P^{(p)}HP^{(p)})\, P^{(p)} |\Psi_\lambda^{(+)}\rangle = P^{(p)}HQ^{(p)} |\Psi_\lambda^{(+)}\rangle \tag{4.38a}$$

$$(\mathscr{E}_\lambda^{(+)} - Q^{(p)}HQ^{(p)})\, Q^{(p)} |\Psi_\lambda^{(+)}\rangle = Q^{(p)}HP^{(p)} |\Psi_\lambda^{(+)}\rangle. \tag{4.38b}$$

The solution of (4.38b) is given by

$$Q^{(p)} |\Psi_\lambda^{(+)}\rangle = (\mathscr{E}_\lambda^{(+)} - Q^{(p)}HQ^{(p)})^{-1}\, Q^{(p)}HP^{(p)} |\Psi_\lambda^{(+)}\rangle. \tag{4.38c}$$

By substituting (4.38c) in the normalization condition

$$\langle \Psi_\lambda^{(+)}|\, P^{(p)} + Q^{(p)} |\Psi_\lambda^{(+)}\rangle = 1, \tag{4.39a}$$

one finds that

$$\langle \Psi_\lambda^{(+)} |\, P^{(p)} + P^{(p)} H Q^{(p)} (\mathscr{E}_\lambda^{(+)} - Q^{(p)} H Q^{(p)})^{-2}\, Q^{(p)} H P^{(p)} \,|\, \Psi_\lambda^{(+)} \rangle = 1. \tag{4.39b}$$

By using (4.29a) and (4.35), this gives

$$\mathscr{S}_\lambda^{(+)} \langle \lambda^{(+)} |\, (1-K)^{-1} \left\{ 1 - \left[\frac{d}{dE} D^{(p)}(E) \right]_{E = E_\lambda^{(+)}} (1-K)^{-1} \right\} |\lambda^{(+)}\rangle = 1. \tag{4.39c}$$

In view of (4.33), this yields the expression that we are looking for, namely,

$$\mathscr{S}_\lambda^{(+)} = \left[1 - \langle \lambda^{(+)} | \frac{d}{dE} h^{(p)}(E) \,|\lambda^{(+)}\rangle \right]^{-1}_{E = E_\lambda^{(+)}}. \tag{4.40}$$

(b) The other derivation of (4.40) is based on the Hellmann–Feynman theorem. We use the same notation as in (A.1a)–(A.1d) of Appendix A. The bilinear expansion of the particle Green's function reads

$$G^{(p)}(E + i\eta) = \sum_\alpha \frac{|\varphi_\alpha^{(p)}(E)\rangle \langle \tilde{\varphi}_\alpha^{(p)}(E)|}{E - e_\alpha^{(p)}(E) + i\eta} + \int_0^\infty de\, \frac{|\varphi_e^{(p)}(E)\rangle \langle \tilde{\varphi}_e^{(p)}(E)|}{E - e + i\eta}, \tag{4.41a}$$

where $e_\alpha^{(p)}(E)$ denotes a discrete eigenvalue of $h^{(p)}(E)$ for fixed E:

$$e_\alpha^{(p)}(E) = \langle \varphi_\alpha^{(p)}(E)|\ \mathrm{Re}\, h^{(p)}(E)\, |\varphi_\alpha^{(p)}(E)\rangle + i \langle \varphi_\alpha^{(p)}(E)|\ W^{(p)}(E)\, |\varphi_\alpha^{(p)}(E)\rangle. \tag{4.41b}$$

Below, it will be shown that $W^{(p)}(E)$ vanishes for $E < 0$, in keeping with (4.38c). Thus, (4.41b) implies that $e_\alpha(E)$ is real for $E < 0$. In that domain, there exists a one-to-one correspondence between the discrete index α and the index λ which characterizes a bound level of the $(A+1)$-system. The poles $E_\lambda^{(+)}$ of $G^{(p)}(E)$ are located at the roots of

$$E_\lambda^{(+)} = e_\lambda^{(p)}(E_\lambda^{(+)}) \qquad \text{with} \quad E_\lambda^{(+)} < 0. \tag{4.41c}$$

Equation (4.41a) shows that

$$\lim_{E \to E_\lambda^{(+)}} (E - E_\lambda^{(+)})\, G^{(p)}(E) = s_\lambda^{(+)}\, |\varphi_\lambda^{(p)}\rangle \langle \tilde{\varphi}_\lambda^{(p)}|, \tag{4.41d}$$

where $|\varphi_\lambda^{(p)}\rangle = |\varphi_\lambda^{(p)}(E_\lambda^{(+)})\rangle$, $|\tilde{\varphi}_\lambda^{(p)}\rangle = |\tilde{\varphi}_\lambda^{(p)}(E_\lambda^{(+)})\rangle$, and

$$s_\lambda^{(+)} = \left[1 - \frac{d}{dE} e_\lambda^{(p)}(E) \right]^{-1}_{E = E_\lambda^{(+)}}. \tag{4.41e}$$

Since $h^{(p)}(E_\lambda^{(+)})$ is hermitian, one has $|\varphi_\lambda^{(p)}\rangle = |\lambda^{(+)}\rangle = |\tilde{\varphi}_\lambda^{(p)}\rangle$. The Hellmann–Feynman theorem (A.3b) states that

$$\frac{d}{dE} e_\lambda^{(p)}(E) = \langle \tilde{\varphi}_\lambda^{(p)}(E)| \frac{d}{dE} h^{(p)}(E) \, |\varphi_\lambda^{(p)}(E)\rangle. \tag{4.41f}$$

The expression (4.40) of the spectroscopic factor results from (4.9e) and (4.41d)–(4.41f).

4.8. *Centroid Single-Particle Energy*

The operator $R^{(p)}$ is independent of energy and is hermitian. By writing explicitly the commutator in (4.34) and by inserting the expression (2.3c) of the unit operator $\mathscr{I}^{(A+1)}$, we obtain

$$R_{\mathbf{r}\mathbf{r}'}^{(p)} = \sum_\lambda^{\infty} \langle \Psi_0^{(A)}| \, a_{\mathbf{r}} \, |\Psi_\lambda^{(+)}\rangle [\mathscr{E}_\lambda^{(+)} - \mathscr{E}_0^{(A)}] \langle \Psi_\lambda^{(+)}| \, a_{\mathbf{r}'}^\dagger \, |\Psi_0^{(A)}\rangle. \tag{4.42a}$$

The middle factor is the single-particle energy $E_\lambda^{(+)}$. Thus, (4.6a) gives the sum rule

$$R^{(p)} = \int_{E_0^{(+)}}^{\infty} E S^{(p)}(E) \, dE. \tag{4.42b}$$

This has the following interpretation. Let $\{\psi_\alpha\}$ be some arbitrary real single-particle basis. According to (4.5a) and (4.6a) the diagonal element $S_{\alpha\alpha}^{(p)}(E)$ measures the probability per unit energy interval of finding the $(A+1)$-system with the excitation energy $E^* = E - E_0^{(+)}$, after having added one nucleon with wave function $\psi_\alpha(\mathbf{r})$ to the ground state $|\Psi_0^{(A)}\rangle$. Therefore, $R_{\alpha\alpha}^{(p)}$ is the centroid of the single-particle energies of the states of the $(A+1)$-system which are fed when one nucleon with wave function $\psi_\alpha(\mathbf{r})$ is added to $|\Psi_0^{(A)}\rangle$. Only little attention has been paid to the operator $R^{(p)}$. The main reason for this lack of interest is twofold. First, $R^{(p)}$ is not related to the ground state energy $\mathscr{E}_0^{(A)}$ by a sum rule, in contrast to $R^{(h)}$ (see (3.29)). Second, $R^{(p)}$ cannot be extracted from the experimental data, because this would require the measurement of stripping reactions which leave the residual nucleus in very highly excited states. High excitation energies have a large influence on the value of $R^{(p)}$ because of the short-range interactions. As a matter of fact, it will be shown in Section 5 that $R^{(p)}$ diverges when the nucleon–nucleon interaction contains a hard core. The physical origin of this divergence is that $R_{\mathbf{r}\mathbf{r}'}^{(p)}$ involves the creation of a nucleon at a location $\mathbf{r}'$, where its presence may be forbidden by the hard core.

The full many-body Hamiltonian $H = \mathscr{T} + \mathscr{V}$ is the sum of kinetic and interaction contributions. By inserting this in (4.34), one finds

$$R^{(p)} = T^{(p)} + \mathscr{V}^{(p)}, \tag{4.42c}$$

where

$$T^{(p)} = T(1-K), \qquad \mathscr{V}^{(p)}_{\mathbf{r}\mathbf{r}'} = \langle \Psi_0^{(A)} | \, [\, a_{\mathbf{r}}, \mathscr{V} \,] \, a^{\dagger}_{\mathbf{r}'} \, | \Psi_0^{(A)} \rangle. \tag{4.42d}$$

Note that the two terms on the right-hand side of (4.42c) are not hermitian, although their sum $R^{(p)}$ is hermitian.

4.9. *Particle Mass Operator*

In (4.14), we defined the particle mass operator as the difference

$$M^{(p)}(E) = h^{(p)}(E) - T. \tag{4.43a}$$

The real and imaginary parts of $M^{(p)}(E)$ are hermitian. Hence, they are symmetric in the coordinate space representation. By using (4.33) and (4.43a), one finds that

$$M^{(p)}(E) = -K(1-K)^{-1}\,(E-T) + (1-K)^{-1}\,[\,\mathscr{V}^{(p)} + D^{(p)}(E)\,](1-K)^{-1}. \tag{4.43b}$$

This expression is rather inconvenient because the operators $K(1-K)^{-1}\,T$ and $\mathscr{V}^{(p)}$ are not hermitian, although they are real. In particular, they are not symmetric in the coordinate space representation. It is thus preferable to leave $M^{(p)}(E)$ in the form (4.43a), where $h^{(p)}(E)$ is given by (4.33) and (4.10b).

4.10. *High Energy Behaviour of the Particle Hamiltonian and Sum Rules*

Because of the first term on the right-hand side of (4.33), the particle Hamiltonian diverges at large energy. We now show that this behaviour can be derived on general grounds, without making use of projection operators. According to (4.5b), (4.7a) and (4.42b) one has, at large E,

$$G^{(p)}(E) \sim E^{-1}(1 - K + E^{-1}R^{(p)}). \tag{4.44a}$$

By inserting this in

$$h^{(p)}(E) = E - [\,G^{(p)}(E)\,]^{-1}, \tag{4.44b}$$

one finds that

$$h^{(p)}(E) \sim -\frac{K}{1-K}\,E + \left(1 + \frac{K}{1-K}\right) R^{(p)} \left(1 + \frac{K}{1-K}\right). \tag{4.44c}$$

This is in keeping with (4.33), since $D^{(p)} \sim E^{-1}$.

According to (4.44a), the contour integral of $G^{(p)}(z)$ over a large closed circle in the complex z-plane is equal to

$$\int_{\text{circle}} dz\, G^{(p)}(z) = 2i\pi(1-K). \tag{4.44d}$$

By indenting the integration contour around the poles and the branch cut of $G^{(p)}(z)$, one finds that

$$(2i\pi)^{-1} \int_{E_0^{(+)}}^{\infty} dE \{ G^{(p)}(E-i\eta) - G^{(p)}(E+i\eta) \} = 1-K. \tag{4.44e}$$

This is compatible with the sum rule (4.7a), as it should be. According to (2.5b), (2.6a), and (2.8a), one has

$$1-K = K_{dt}^{(p)} + K_{ct}^{(p)}, \tag{4.45a}$$

where the indices refer to discrete and continuum:

$$K_{dt}^{(p)} = \sum_{\lambda} |\chi_{\lambda}^{(+)}\rangle\langle\chi_{\lambda}^{(+)}|, \tag{4.45b}$$

$$K_{ct}^{(p)} = \sum_{c} \int_{T_c^{(+)}}^{\infty} dE'\, |\chi_{E'}^{c(+)}\rangle\langle\chi_{E'}^{c(+)}|. \tag{4.45c}$$

4.11. *Independent Particle Model*

In the independent particle model outlined in Section 3.7, the particle Green's function reduces to

$$G_U^{(p)}(E) = \sum_{\alpha \notin F} \frac{|\varphi_\alpha\rangle\langle\varphi_\alpha|}{E-e(\alpha)+i\eta} + \int_0^{\infty} dE' \frac{|\varphi_{E'}\rangle\langle\varphi_{E'}|}{E-E'+i\eta}, \tag{4.46a}$$

where the single-particle wave functions $|\varphi_\alpha\rangle$ and $|\varphi_{E'}\rangle$ are defined by (3.33c) and (3.33d). The sum over α runs over the bound states which lie outside the Fermi sea. At large energy, $G_U^{(p)}(E)$ approaches $(1-K_U)/E$, where K_U is given by (3.34b). The particle spectral function

$$S_U^{(p)}(E) = \sum_{\alpha \notin F} |\varphi_\alpha\rangle\langle\varphi_\alpha|\, \delta(E-e(\alpha)) + |\varphi_E\rangle\langle\varphi_E| \tag{4.46b}$$

fulfills the sum rule

$$\int_{E_0^{(+)}}^{\infty} dE\, S_U^{(p)}(E) = 1-K_U. \tag{4.46c}$$

The matrix elements $\langle \varphi_\alpha | \, G_U^{(p)} \, | \varphi_\beta \rangle$ vanish for states φ_α or φ_β which lie within the Fermi sea. Hence, the inverse of $G_U^{(p)}$ is not defined on the full Hilbert space, likewise for the particle Hamiltonian, which reduces to the following energy independent operator:

$$h_U^{(p)} = R_U^{(p)} = \sum_{\alpha \notin F} |\varphi_\alpha\rangle\langle\varphi_\alpha| \, e(\alpha) + \int_0^\infty dE' \, |\varphi_{E'}\rangle\langle\varphi_{E'}| \, E'. \tag{4.46d}$$

In the sense discussed in connection with (2.13a), $G_U^{(p)}$ and $h_U^{(p)}$ are contained in the restricted Hilbert space $\mathscr{H}^{(1)}_{\notin F}$ spanned by the single-particle orbits which do not belong to the Fermi sea. This is the reason why $h_U^{(p)}$ differs from the single-particle Hamiltonian h_U.

The independent particle model illustrates some of the differences which exist between the particle Green's function $G_U^{(p)}(E)$ and the familiar Green's function

$$g_U^{(+)}(E) = [\, g_U^{(-)}(E)\,]^\dagger = (E - h_U + i\eta)^{-1} \tag{4.47a}$$

of potential scattering theory. These differences reflect the incomplete nature of the Hilbert space $\mathscr{H}^{(1)}_{\notin F}$:

(i) The spectral expansion of $g_U^{(+)}(E)$ reads

$$g_U^{(+)}(E) = \sum_\alpha \frac{|\varphi_\alpha\rangle\langle\varphi_\alpha|}{E - e(\alpha) + i\eta} + \int_0^\infty dE' \, \frac{|\varphi_{E'}\rangle\langle\varphi_{E'}|}{E - E' + i\eta}, \tag{4.47b}$$

where the sum over α extends over all bound eigenstates of h_U. Compare with (4.46a).

(ii) The high energy behaviour

$$g_U^{(+)}(E) \sim E^{-1} \tag{4.47c}$$

is to be contrasted with $G_U^{(p)}(E) \sim (1 - K_U)/E$.

4.12. *Discrete, Elastic, and Nonelastic Contributions to the Particle Spectral Function*

According to (4.6b) and (4.10a), the particle spectral function can be expressed in terms of the particle Hamiltonian:

$$S^{(p)}(E) = (2i\pi)^{-1} \{ [\, E - (h^{(p)}(E))^\dagger - i\eta \,]^{-1} - [\, E - h^{(p)}(E) + i\eta \,]^{-1} \}. \tag{4.48}$$

Let us write $h^{(p)}$ as the sum of its real and imaginary parts:

$$h^{(p)}(E) = \mathrm{Re}\, h^{(p)}(E) + iW^{(p)}(E), \tag{4.49a}$$

$$W^{(p)}(E) = \mathrm{Im}\, h^{(p)}(E) = (2i)^{-1} \, [h^{(p)}(E) - h^{(p)}(E)^\dagger]. \tag{4.49b}$$

We used the property that $h^{(p)}$ is hermitian-analytic, namely that

$$h^{(p)}(E-i\eta)=h^{(p)}(E+i\eta)^{\dagger} \qquad \text{for any} \quad \eta\neq 0. \tag{4.49c}$$

By introducing (4.49a) in (4.48), we find that

$$S^{(p)}(E)=S^{(p)}_{\mathrm{de}}(E)+S^{(p)}_{\mathrm{in}}(E), \tag{4.50a}$$

$$S^{(p)}_{\mathrm{de}}(E)=G^{(p)}(E+i\eta)\,\frac{\eta}{\pi}\,[\,G^{(p)}(E+i\eta)\,]^{\dagger}, \tag{4.50b}$$

$$S^{(p)}_{\mathrm{in}}(E)=-\frac{1}{\pi}\,G^{(p)}(E+i\eta)\;W^{(p)}(E)[\,G^{(p)}(E+i\eta)\,]^{\dagger}. \tag{4.50c}$$

The decomposition (4.50a)–(4.50c) is formally analogous to the one that we encountered in (3.10a)–(3.10c) in the case of the hole spectral function. However, this similarity masks an important difference due to the fact that the particle Hamiltonian $h^{(p)}(E)$ has scattering in addition to bound eigenstates. We shall see that these scattering eigenstates contribute to (4.50b) rather than to (4.50c).

(a) We first discuss the value of $S^{(p)}_{\mathrm{de}}(E)$ at negative energies. In that domain, there exists a one-to-one correspondence between the discrete indices α which appear in (4.41a) and the indices λ which characterize the bound levels of the $(A+1)$-system. According to (4.41a) and (4.50b) the contribution of the real eigenvalues $e^{(p)}_{\lambda}(E)$ to the quantity $S^{(p)}_{\mathrm{de}}(E)$ is equal to

$$\lim_{\eta\to+0}\frac{\eta}{\pi}\sum_{\lambda}|\varphi^{(p)}_{\lambda}(E)\rangle\{[\,E-e^{(p)}_{\lambda}(E)\,]^2+\eta^2\}^{-1}\langle\tilde{\varphi}^{(p)}_{\lambda}(E)|. \tag{4.51a}$$

By using (4.41e), we can write this expression as

$$\sum_{\lambda}\delta[\,E-e^{(p)}_{\lambda}(E)\,]\;|\varphi^{(p)}_{\lambda}(E)\rangle\langle\varphi^{(p)}_{\lambda}(E)|$$

$$=\sum_{\lambda}\frac{|\lambda^{(+)}\rangle\langle\lambda^{(+)}|}{1-(d/dE)\,e^{(p)}_{\lambda}(E)}\,\delta(E-E^{(+)}_{\lambda}). \tag{4.51b}$$

According to (4.40) and to the Hellmann–Feynman theorem (A.3b), this is equal to the discrete contribution (4.9b), namely to

$$S^{(p)}_{dt}(E)=\sum_{\lambda}\mathscr{S}^{(+)}_{\lambda}\;|\lambda^{(+)}\rangle\langle\lambda^{(+)}|\;\delta(E-E^{(+)}_{\lambda}). \tag{4.52a}$$

We conclude that

$$S^{(p)}_{\mathrm{de}}(E)=S^{(p)}_{dt}(E) \qquad \text{for} \quad E<0. \tag{4.52b}$$

(b) We now show that $S_{de}^{(p)}(E)$ is different from zero at positive energy because of the contribution of the scattering states to (4.50b); see also [48–50]. For this purpose, it is convenient to use the overlaps $\chi_{\mathbf{k}}^{t(+)}\rangle$ defined by Eq. (D.13) of Appendix D, rather than the spherical overlap functions $|\chi_E^{c(+)}\rangle$. We thus write (4.9c) in the form

$$S_{ct}^{(p)}(E) = \sum_t \int d\mathbf{k}\, \delta(E - E'_k)\, |\chi_{\mathbf{k}}^{t(+)}\rangle\langle\chi_{\mathbf{k}}^{t(+)}|, \tag{4.53a}$$

where, according to (D.3) and (4.2),

$$E_k^t = \frac{k_t^2}{2m} + (\mathscr{E}_t^{(A)} - \mathscr{E}_0^{(A)}). \tag{4.53b}$$

Let us first consider the value that the right-hand side of (4.50b) takes when $h^{(p)}(E)$ is replaced by the kinetic energy operator T, i.e., when $G^{(p)}(E)$ is replaced by

$$g_0^{(+)}(E) = g_0(E + i\eta) = (E - T + i\eta)^{-1}. \tag{4.54a}$$

Since T is hermitian, one has

$$\frac{\eta}{\pi}\, g_0(E+i\eta)\, g_0^\dagger(E+i\eta) = \frac{1}{2i\pi}\, g_0(E+i\eta)[(E-T+i\eta) - (E-T-i\eta)]\, g_0^\dagger(E+i\eta) \tag{4.54b}$$

$$= (2i\pi)^{-1}\, [\, g_0^\dagger(E+i\eta) - g_0(E+i\eta)\,] \tag{4.54c}$$

$$= \int d\mathbf{k}\, \delta(E - E_k)\, |\mathbf{k}\rangle\langle\mathbf{k}|, \tag{4.54d}$$

where (see (4.15b) and (4.53b))

$$E_k = k^2/2m = E_k^0. \tag{4.54e}$$

From (4.10c) and (4.14), one derives the Dyson-type equation

$$G^{(p)}(E+i\eta) = [\,1 + G^{(p)}(E+i\eta)\, M^{(p)}(E)\,] \times g_0(E+i\eta). \tag{4.55a}$$

The right-hand side of (4.50b) can thus be written in the form

$$[\,1 + G^{(p)}(E)\, M^{(p)}(E)\,] \left[\frac{\eta}{\pi}\, g_0(E+i\eta)\, g_0(E+i\eta)^\dagger\right]$$

$$\times [\,1 + M^{(p)}(E)^\dagger\, G^{(p)}(E)^\dagger], \tag{4.55b}$$

where we applied (4.8). When one replaces the middle factor of (4.55b) by (4.54d), this expression becomes

$$\int d\mathbf{k}\, \delta(E-E_k)[1+G^{(p)}(E)\, M^{(p)}(E)]\, |\mathbf{k}\rangle\langle\mathbf{k}|\, [1+M^{(p)}(E)^{\dagger}\, G^{(p)}(E)^{\dagger}]. \tag{4.55c}$$

Equations (4.16c) and (4.24a) yield the Lippmann–Schwinger equation

$$|\chi_{\mathbf{k}}^{0(+)}\rangle = \{1+G^{(p)}(E_k)\, M^{(p)}(E_k)\}\ |\mathbf{k}\rangle. \tag{4.56a}$$

By introducing this expression in (4.55c), we find that (4.55c) is equal to the elastic contribution to the particle spectral function, namely to

$$S_{\mathrm{el}}^{(p)}(E) = \int d\mathbf{k}\, \delta(E-E_k)\, |\chi_{\mathbf{k}}^{0(+)}\rangle\langle\chi_{\mathbf{k}}^{0(+)}|. \tag{4.56b}$$

Hence,

$$S_{\mathrm{de}}^{(p)}(E) = S_{\mathrm{el}}^{(p)}(E) \qquad \text{for} \quad E>0. \tag{4.56c}$$

From (4.52b) and (4.56c), we conclude that the quantity $S_{\mathrm{de}}^{(p)}(E)$ defined by (4.50b) is the sum of the discrete and elastic contributions to the particle spectral function,

$$S_{\mathrm{de}}^{(p)}(E) = S_{dt}^{(p)}(E) + S_{\mathrm{el}}^{(p)}(E), \tag{4.57}$$

where the first term differs from zero only for $E<0$ and the second term only for $E>0$. This accounts for our notation: the index "de" refers to "discrete + elastic." Equations (4.6a) and (4.57) imply that the quantity (4.50c) is the "inelastic" contribution to the particle spectral function, namely,

$$S_{\mathrm{in}}^{(p)}(E) = \sum_{t\neq 0} \int d\mathbf{k}_t\, \delta(E-E_k^t)\, |\chi_{\mathbf{k}}^{t(+)}\rangle\langle\chi_{\mathbf{k}}^{t(+)}|. \tag{4.58}$$

By making use of (D.14) and (D.19) these results can be written in terms of spherical overlaps:

$$S_{\mathrm{el}}^{(p)}(E) = \sum_{L_0\,\mu_0} |\chi_E^{0(+)}\rangle\langle\chi_E^{0(+)}|, \tag{4.59a}$$

$$S_{\mathrm{in}}^{(p)}(E) = \sum_{c(t\neq 0)} |\chi_E^{c(+)}\rangle\langle\chi_E^{c(+)}|. \tag{4.59b}$$

For simplicity, we shall write (4.59a) in the form

$$S_{\rm el}^{(p)}(E) = |\chi_E^{0(+)}\rangle\langle\chi_E^{0(+)}|, \tag{4.59c}$$

where a summation over the repeated indices L_0 and μ_0 is implicit; see (D.20).

Equations (4.50c) and (4.59b) entail the important result that $W^{(p)}(E)$ vanishes for energies smaller than the lowest nonelastic threshold:

$$W^{(p)}(E) = 0 \qquad \text{for} \quad E < T_{\rm in}^{(+)}. \tag{4.60}$$

An explicit algebraic proof of this property will be given below, in connection with Eq. (4.64c).

4.13. *Dispersion Relation for the Particle Hamiltonian*

Let us first derive an expression for $W^{(p)}(E)$ in terms of the eigenstates of $Q^{(p)}HQ^{(p)}$. These belong either to the discrete or the continuous spectrum,

$$Q^{(p)}HQ^{(p)}\,|\Phi_q^{(p)}\rangle = (\mathscr{E}_0^{(A)} + \varepsilon_q^{(p)})\,|\Phi_q^{(p)}\rangle, \tag{4.61a}$$

$$Q^{(p)}HQ^{(p)}\,|\Phi_{\mathscr{E}}^{c(+)}\rangle = (\mathscr{E}_0^{(A)} + \varepsilon^{(p)})\,|\Phi_{\mathscr{E}}^{c(+)}\rangle, \tag{4.61b}$$

where $\mathscr{E} = \mathscr{E}_0^{(A)} + \varepsilon^{(p)}$. The quantities $\varepsilon^{(p)}$ and $\varepsilon_q^{(p)}$ correspond to single-particle energies. These eigenstates are normalized as in (2.2c). The set of the nonvanishing expectation values of $Q^{(p)}HQ^{(p)}$ with respect to all the configurations of $(A+1)$ nucleons is contained in the set of the expectation values of H. Therefore, the smallest eigenvalue of $Q^{(p)}HQ^{(p)}$ must be larger than the smallest eigenvalue of H. This implies that the inequalities

$$\varepsilon^{(p)} \geqslant T_{\rm in}^{(+)} > E_0^{(+)}, \qquad \varepsilon_q^{(p)} > E_0^{(+)}, \tag{4.61c}$$

hold, where $E_0^{(+)}$ and $T_{\rm in}^{(+)}$ correspond to the ground state of the $(A+1)$-nucleon system and to its threshold for nucleon emission, respectively. By introducing the operator $\sum\!\!\!\!\!\!\int |\Phi^{(p)}\rangle\langle\Phi^{(p)}|$ in (4.35) we find that, in any single-particle representation $\{\psi_\alpha\}$,

$$\begin{aligned}\operatorname{Im} D_{\alpha\alpha'}^{(p)}(E) = -\pi \sum_c \int_{T_c^{(+)}}^{\infty} d\varepsilon^{(p)} [\mathscr{J}_{\alpha'}^{c(+)}(\varepsilon^{(p)})]^* \\ \times \mathscr{J}_{\alpha}^{c(+)}(\varepsilon^{(p)})\,\delta(E-\varepsilon^{(p)}),\end{aligned} \tag{4.62a}$$

with

$$\begin{aligned}\langle \psi_\alpha \,|\, \mathscr{J}^{c(+)}(\varepsilon^{(p)})\rangle &= \mathscr{J}_{\alpha}^{c(+)}(\varepsilon^{(p)}) \\ &= \langle \Psi_0^{(A)} |\, a_\alpha H Q^{(p)}\, |\Phi_{\mathscr{E}}^{c(+)}\rangle.\end{aligned} \tag{4.62b}$$

Above, we used the same degeneracy index $c(+)$ for labelling the continuum eigenstates $|\Phi_{\mathscr{E}}^{c(+)}\rangle$ of $Q^{(p)}HQ^{(p)}$ as for the entrance channels which characterize

the eigenstates $|\Psi_{\mathscr{E}}^{c(+)}\rangle$ of the full Hamiltonian. This is justified because we show in Appendix E that there exists a one-to-one correspondence between

$$|\Psi_{\mathbf{k}_t}^{(t+)}\rangle = \frac{i\eta}{\mathscr{E}_k^t - H + i\eta}\, a_{\mathbf{k}_t}^\dagger\, |\Psi_t^{(A)}\rangle \tag{4.63a}$$

and

$$|\Phi_{\mathbf{k}}^{t(+)}\rangle = \frac{i\eta}{\mathscr{E}_k^t - Q^{(p)}HQ^{(p)} + i\eta}\, a_{k_t}^\dagger\, |\Psi_t^{(A)}\rangle \qquad \text{for} \quad t \neq 0. \tag{4.63b}$$

The energy $\mathscr{E}_k^t$ is defined by (D.3). The restriction $t \neq 0$ means that (4.63b) only holds for channels associated with excited target states, as discussed at the end of Section E.2. Here, we note that (4.25a) and (4.25b) give

$$Q^{(p)} a_{\mathbf{k}}^\dagger\, |\Psi_0^{(A)}\rangle = 0. \tag{4.64a}$$

If (4.63b) were taken as a definition of $|\Phi_{\mathbf{k}}^{0(+)}\rangle$, (4.64a) would imply that

$$|\Phi_{\mathbf{k}}^{0(+)}\rangle = 0, \tag{4.64b}$$

except for the impulse κ_0, for which $\mathscr{E}_0^{(A)} = -\kappa_0^2/2m$. This exception can be disregarded, since κ_0 is a set of measure zero, and therefore it does not contribute to the completeness $\sum\!\!\!\!\!\!\int |\Phi^{(p)}\rangle\langle\Phi^{(p)}|$. Equation (4.64b) reflects the property that $Q^{(p)}HQ^{(p)}$ does not have eigenstates which would correspond to elastic scattering boundary conditions. Accordingly, the sum on the right-hand side of (4.62a) only runs over inelastic channels:

$$\operatorname{Im} D_{\alpha\alpha'}^{(p)}(E) = -\pi \sum_{c(t\neq 0)} \int_{T_{\text{in}}^{(+)}}^{\infty} d\varepsilon^{(p)} [\mathscr{J}_{\alpha'}^{c(+)}(\varepsilon^{(p)})]^* \mathscr{J}_{\alpha}^{c(+)}(\varepsilon^{(p)})\, \delta(E - \varepsilon^{(p)}). \tag{4.64c}$$

In other words,

$$W^{(p)}(E) = 0 \qquad \text{for} \quad E < T_{\text{in}}^{(+)}, \tag{4.64d}$$

$$W^{(p)}(E) < 0 \qquad \text{for} \quad E > T_{\text{in}}^{(+)}, \tag{4.64e}$$

where $T_{\text{in}}^{(+)}$ is the smallest inelastic threshold. This is the algebraic proof of (4.60) in the projection operator approach.

The dispersion relation between the real and imaginary parts of the particle Hamiltonian is readily obtained from (4.35). With the notation

$$\mathscr{J}_{q\alpha}^{(p)} = \langle \Psi_0^{(A)}|\, a_\alpha H Q^{(p)}\, |\Phi_q^{(p)}\rangle, \tag{4.64f}$$

it reads

$$\begin{aligned}\operatorname{Re} h^{(p)}(E) = &-\frac{K}{1-K} E + (1-K)^{-1} R^{(p)} (1-K)^{-1} \\ &+ \sum_q (1-K)^{-1} \frac{|\mathscr{I}_q^{(p)}\rangle\langle \mathscr{I}_q^{(p)}|}{E-\varepsilon_q^{(p)}} (1-K)^{-1} \\ &+ \frac{\mathscr{P}}{\pi} \int_{T_{\text{in}}^{(+)}}^{\infty} dE' \frac{\operatorname{Im} h^{(p)}(E')}{E'-E}. \end{aligned} \tag{4.64g}$$

This exhibits that, besides real poles at $\varepsilon_q^{(p)}$, the particle Hamiltonian $h^{(p)}(E)$ has a branch cut which runs below the real axis and extends from the inelastic threshold $T_{\text{in}}^{(+)}$ up to $+\infty$. We recall that we had shown in Section 4.2 that the branch cut of the particle Green's function extends from 0 to $+\infty$. These analytic properties are sketched in Fig. 2.

4.14. *Feshbach's Hamiltonian*

In the present section, we derive the relationship between the particle Hamiltonian $h^{(p)}(E)$ and the optical-model Hamiltonian which had been introduced by Feshbach in his pioneering paper [3]. Let us consider the Schrödinger equation

$$h^{(p)}(E)\, |\chi_E^{(+)}\rangle = E\, |\chi_E^{(+)}\rangle, \tag{4.65a}$$

where $|\chi_E^{(+)}\rangle$ denotes a bound or an elastic scattering overlap. We multiply (4.65a) from the left by any energy-independent operator $\mathscr{N}$. The result can be written in the form

$$h_{\mathscr{N}}^{(p)}(E)\, |\chi_E^{(+)}\rangle = E\, |\chi_E^{(+)}\rangle, \tag{4.65b}$$

where

$$h_{\mathscr{N}}^{(p)}(E) = E[1 - \mathscr{N}(1-K)^{-1}] + \mathscr{N}(1-K)^{-1}\, [R^{(p)} + D^{(p)}(E)](1-K)^{-1}. \tag{4.65c}$$

The resolvent $G_{\mathscr{N}}^{(p)}(E)$ defined by

$$[E - h_{\mathscr{N}}^{(p)}(E)]\, G_{\mathscr{N}}^{(p)}(E) = 1 \tag{4.65d}$$

and the particle Green's function $G^{(p)}$ are related by

$$G_{\mathscr{N}}^{(p)}(E) = G^{(p)}(E)\, \mathscr{N}^{-1}. \tag{4.65e}$$

The particle Hamiltonian proper corresponds to $\mathcal{N} = 1$. It diverges at large E, as discussed in Section 4.10. This divergence can be eliminated by setting

$$\mathcal{N} = 1 - K \tag{4.66a}$$

in (4.65c). The corresponding Hamiltonian reads

$$h_{\mathcal{F}}^{(p)}(E) = (1 - K)\, h^{(p)}(E) + KE \tag{4.66b}$$

$$= [\, R^{(p)} + D^{(p)}(E)\,](1 - K)^{-1} \tag{4.66c}$$

By using (4.42d), one gets

$$h_{\mathcal{F}}^{(p)}(E) = T + (\mathcal{V}^{(p)} + D^{(p)})(1 - K)^{-1}. \tag{4.66d}$$

The lower index $\mathcal{F}$ refers to Feshbach. This notation is justified because we shall now show explicitly that $h_{\mathcal{F}}^{(p)}(E)$ is identical to the optical-model Hamiltonian which had originally been constructed by Feshbach [3]. In order to exhibit this, we express the wave equation

$$E\, |\chi_E^{(+)}\rangle = h_{\mathcal{F}}^{(p)}(E)\, |\chi_E^{(+)}\rangle \tag{4.67a}$$

in the coordinate space representation. Let us introduce the notation

$$\mathcal{H}(E) = H + HQ^{(p)}(E - Q^{(p)}HQ^{(p)} + \mathcal{E}_0^{(A)} + i\eta)^{-1}\, Q^{(p)}H. \tag{4.67b}$$

By making use of (4.27c), (4.34), and (4.35), the wave equation (4.67a) reads, in the coordinate space representation,

$$(E + \mathcal{E}_0^{(A)})\, \chi_E^{(+)}(\mathbf{r}) = \int d\mathbf{r}'\, \mathcal{H}(\mathbf{r}, \mathbf{r}'; E)\, u_E^{(+)}(\mathbf{r}') \tag{4.67c}$$

where

$$\mathcal{H}(\mathbf{r}, \mathbf{r}'; E) = \langle\, \Psi_0^{(A)} |\, a_{\mathbf{r}}\, \mathcal{H}(E)\, a_{\mathbf{r}'}^{\dagger}\, |\Psi_0^{(A)}\rangle. \tag{4.67d}$$

The explicit form of the latter quantity is

$$\mathcal{H}(\mathbf{r}, \mathbf{r}'; E) = (A + 1) \int d\xi\, d\xi'\, \Psi_0^{(A)}(\xi)^*$$

$$\times \langle\, \mathbf{r}, \xi |\, \mathcal{H}(E)\, |\mathbf{r}', \xi'\rangle\, \Psi_0^{(A)}(\xi'). \tag{4.67e}$$

We recall that ξ generically denotes the coordinates of the target nucleons. Since the matrix element which appears on the right-hand side of (4.67e) is antisymmetric

by exchange of $\mathbf{r}'$ with any of the variables generically represented by ξ', one has

$$\int d\mathbf{r}'\ \mathscr{H}(\mathbf{r}, \mathbf{r}'; E)\, u_e^{(+)}(\mathbf{r}') = \int d\mathbf{r}'\ d\xi\ d\xi'\ \Psi_0^{(A)}(\xi)^* \times \langle \mathbf{r}, \xi |\ \mathscr{H}(E)\ |\mathbf{r}', \xi' \rangle\ \mathscr{A}\{u_E^{(+)}(\mathbf{r}')\ \Psi_0^{(A)}(\xi')\}, \quad (4.68a)$$

where $\mathscr{A}$ is the antisymmetrization operator. This expression is conventionally written as

$$\int d\mathbf{r}'\ \mathscr{H}(\mathbf{r}, \mathbf{r}'; E)\, u_E^{(+)}(\mathbf{r}') = (\Psi_0^{(A)} |\ \mathscr{H}(E)\ \mathscr{A}\{u_E^{(+)}(\mathbf{r})\ \Psi_0^{(A)}(\xi)\}\ \rangle. \quad (4.68b)$$

As in (2.4b), the symbol $(|\ \rangle$ denotes an integral over the target coordinates generically denoted by ξ. By introducing the eigenvalues n_ν and the eigenvectors $|\omega_\nu\rangle$ of the density matrix in the relation (4.30a) between $|u_E^{(+)}\rangle$ and $|\chi_E^{(+)}\rangle$, Eqs. (4.67b), (4.67c), and (4.68b) yield

$$(E + \mathscr{E}_0^{(A)})\ \chi_E^{(+)}(\mathbf{r}) = (\Psi_0^{(A)} |\ H + HQ^{(p)}(E - Q^{(p)}HQ^{(p)} + \mathscr{E}_0^{(a)} + i\eta)^{-1}\ Q^{(p)}H\ |\mathscr{A}\left\{\chi_E^{(+)}(\mathbf{r})\ \Psi_0^{(A)}(\xi) + \sum_{n_\nu \neq 1}\left[\frac{n_\nu}{1-n_\nu}\,\omega_\nu(\mathbf{r})\ \Psi_0^{(A)}(\xi)\langle \omega_\nu |\chi_E^{(+)}\rangle\right]\right\}\Big\rangle. \quad (4.68c)$$

This relation is identical to Eq. (3.37) of [3], in which Feshbach had denoted the overlap by $U(\mathbf{r})$ (instead of $\chi_E^{(+)}(\mathbf{r})$), the total energy by E (instead of $\mathscr{E}^{(+)} = E + \mathscr{E}_0^{(A)}$), and the eigenvectors and eigenvalues of the density matrix by $|u_\nu\rangle$ and $1/\lambda_\nu$ (instead of $|\omega_\nu\rangle$ and n_ν).

The following properties of $h_{\mathscr{F}}^{(p)}(E)$ are noticeable:

(a) The operator $h_{\mathscr{F}}^{(p)}(E)$ is not hermitian-analytic; i.e., it does not fulfill the property (4.49c). This is due to the factor $(1-K)^{-1}$ on the right-hand side of (4.66c). Accordingly, the real and imaginary parts of $h_{\mathscr{F}}^{(p)}(E)$ are not symmetric in the coordinate space representation.

(b) The normalized left-hand eigenstate of $h_{\mathscr{F}}^{(p)}(E_\lambda^{(+)})$ is given by

$$\langle \tilde{\lambda}_{\mathscr{F}}^{(+)}| = c_{\mathscr{F}}^{\lambda(+)} \langle \lambda^{(+)}|\ (1-K)^{-1}, \quad (4.69a)$$

where the normalization coefficient

$$c_{\mathscr{F}}^{\lambda(+)} = \langle \lambda^{(+)}|\ (1-K)^{-1}\ |\lambda^{(+)}\rangle^{-1} \quad (4.69b)$$

is determined by Eqs. (A.1c) and (A.1e) of Appendix A.

(c) The resolvent of Feshbach's Hamiltonian is equal to

$$G^{(p)}_{\mathscr{F}}(E) = G^{(p)}(E)(1-K)^{-1}. \tag{4.69c}$$

(d) The particle spectral function and the spectroscopic factor of the bound level $|\Psi^{(+)}_{\lambda}\rangle$ can be written in the form

$$S^{(p)}(E) = (2i\pi)^{-1}\left\{(1-K)\, G^{(p)}_{\mathscr{F}}(E+i\eta)^{\dagger} - G^{(p)}_{\mathscr{F}}(E+i\eta)(1-K)\right\}, \tag{4.69d}$$

$$\mathscr{S}^{(+)}_{\lambda} = \left\{ \langle \lambda^{(+)}| \frac{1}{1-K}\left[1 - \frac{d}{dE} h^{(p)}_{\mathscr{F}}(E)\right] |\lambda^{(+)}\rangle \right\}^{-1}_{E=E^{(+)}_{\lambda}}. \tag{4.69e}$$

The difference between the latter expression of $\mathscr{S}^{(+)}_{\lambda}$ and the simpler one given in [39, 40] is due to the fact that, in these papers, the effects of antisymmetrization and of ground state correlations were not fully taken into account.

(e) The real and imaginary parts of $h^{(p)}_{\mathscr{F}}(E)$ are connected by the dispersion relation

$$\begin{aligned} \mathrm{Re}\, h^{(p)}_{\mathscr{F}}(E) = R^{(p)}(1-K)^{-1} + \sum_{q} \frac{|\mathscr{J}^{(p)}_{q}\rangle\langle \mathscr{J}^{(p)}_{q}|}{E-\varepsilon^{(p)}_{q}}(1-K)^{-1} \\ + \frac{\mathscr{P}}{\pi}\int_{T^{(+)}_{\mathrm{in}}}^{\infty} dE' \frac{\mathrm{Im}\, h^{(p)}_{\mathscr{F}}(E')}{E'-E}. \end{aligned} \tag{4.69f}$$

Since the real and imaginary parts of $h^{(p)}_{\mathscr{F}}(E)$ are not hermitian, it is not justified to approximate the quantity $\mathrm{Im}\, h^{(p)}_{\mathscr{F}}(E)$ by the imaginary part of a phenomenological optical-model potential, as was implicitly done in [6, 51], for instance.

4.15. *Choice of the Single-Particle Wave Function*

We could have chosen to identify the optical-model wave function with $|u^{0(+)}_{E}\rangle$ instead of $|\chi^{0(+)}_{E}\rangle$. These two quantities are related by (4.27c). One readily derives an equation for $|u^{0(+)}_{E}\rangle$ once an equation for $|\chi^{0(+)}_{E}\rangle$ has been found. Indeed,

$$\bar{h}^{(p)}_{\chi}(E)\, |\chi^{0(+)}_{E}\rangle = E\, |\chi^{0(+)}_{E}\rangle \tag{4.70a}$$

amounts to

$$\bar{h}^{(p)}_{u}(E)\, |u^{0(+)}_{E}\rangle = E\, |u^{0(+)}_{E}\rangle, \tag{4.70b}$$

where

$$\bar{h}^{(p)}_{u}(E) = \bar{h}^{(p)}_{\chi}(E)(1-K) + EK. \tag{4.70c}$$

Let us consider two examples:

(a) According to (4.33) and (4.70c), the $u^{(+)}$-Hamiltonian associated with the particle Hamiltonian $h^{(p)}$ is equal to

$$h_u^{(p)}(E) = (1-K)^{-1}\,[R^{(p)} + D^{(p)}(E)]. \tag{4.71a}$$

This operator is not symmetric in the coordinate space representation and remains finite at large energy. It is the transpose of Feshbach's optical-model Hamiltonian:

$$h_u^{(p)}(E) = [h_{\mathscr{F}}^{(p)}(E)]^{\mathrm{T}}. \tag{4.71b}$$

(b) According to (4.66c) and (4.70c), the $u^{(+)}$-Hamiltonian associated with $h_{\mathscr{F}}^{(p)}$ is given by

$$h_{\mathscr{F},u}^{(p)} = R^{(p)} + D^{(p)}(E) + EK. \tag{4.72}$$

This operator is symmetric in the coordinate space representation and diverges at large energy.

Therefore, the mathematical properties of the particle Hamiltonian and of the Feshbach's Hamiltonian are interchanged when one describes the optical-model wave function by $|u_E^{0(+)}\rangle$ instead of $|\chi_E^{0(+)}\rangle$. In the present paper, we ascribe a privileged role to the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$ for the following three main reasons. First, these are the single-particle wave functions which most naturally appear in the description of one-nucleon transfer processes [9, 14]. Second and relatedly, it is in terms of these overlaps that the spectroscopic factors and the particle spectral function are most directly expressed. Third, $|\chi_\lambda^{(-)}\rangle$, $|\chi_\lambda^{(+)}\rangle$, and $|\chi_E^{0(+)}\rangle$ are eigenvectors of the mass operator (plus kinetic energy) which provides a unified description of the single-particle properties of the $(A-1)$- and $(A+1)$-systems (Section 5).

4.16. *Kerman's Hamiltonian*

The feature that Feshbach's Hamiltonian (4.66c) is not hermitian-analytic has led some authors to modify the elastic scattering overlap $\chi_E^{0(+)}(\mathbf{r})$ at finite distance, in such a way that the new scattering function is an eigenstate of an hermitian-analytic Hamiltonian [10, 41–44]. In particular, Kerman [41] introduced the following modified bound and elastic scattering single-particle wave functions

$$\begin{aligned} |\mathscr{K}_\lambda^{(+)}\rangle &= [c_{\mathscr{F}}^{\lambda(+)}]^{-1/2}\,(1-K)^{-1/2}\,|\lambda^{(+)}\rangle, \\ |\mathscr{K}_E^{0(+)}\rangle &= (1-K)^{-1/2}\,|\chi_E^{O(+)}\rangle, \end{aligned} \tag{4.73a}$$

where $c_{\mathscr{F}}^{\lambda(+)}$ is given by (4.69b). It can readily be checked from (4.66c) that these modified functions are eigenstates of

$$h_{\mathscr{K}}^{(p)}(E) = (1-K)^{1/2}\, h^{(p)}(E)(1-K)^{1/2} + KE \tag{4.73b}$$

$$= (1-K)^{-1/2}\, h_{\mathscr{F}}^{(p)}(E)(1-K)^{1/2} \tag{4.73c}$$

$$= (1-K)^{-1/2}\, [\, R^{(p)} + D^{(p)}(E)\,](1-K)^{-1/2}. \tag{4.73d}$$

This Kerman Hamiltonian has the following three main advantages: (a) It approaches a constant at large E. (b) Its real and imaginary parts are symmetric in the coordinate space representation. (c) These real and imaginary parts are connected by a simple dispersion relation.

It has the following two main drawbacks: (i) The radial dependence of its bound and scattering eigenstates $\mathscr{K}_{\lambda}^{(+)}(\mathbf{r})$ and $\mathscr{K}_{E}^{0(+)}(\mathbf{r})$ differs from that of the overlaps $\lambda^{(+)}(\mathbf{r})$ and $\chi_{E}^{0(+)}(\mathbf{r})$ at finite distance; this may be relevant for analyses of direct one-nucleon transfer reactions. (ii) The connection of $h_{\mathscr{K}}^{(p)}(E)$ to the spectroscopic factors and to the spectral function is not as direct as in the case of the particle Hamiltonian $h^{(p)}$. The spectroscopic factor reads

$$\mathscr{S}_{\lambda}^{(+)} = \langle \mathscr{K}_{\lambda}^{(+)} |\, (1-K)\, | \mathscr{K}_{\lambda}^{(+)} \rangle \langle \mathscr{K}_{\lambda}^{(+)} |\, 1 - \frac{d}{dE} h_{\mathscr{K}}^{(p)}(E)\, | \mathscr{K}_{\lambda}^{(+)} \rangle^{-1}, \tag{4.74a}$$

in which the first factor is due to the normalization coefficient $c_{\mathscr{F}}^{\lambda(+)}$. The particle spectral function is given by

$$S^{(p)}(E) = (2i\pi)^{-1}\, (1-K)^{1/2}\, \{ G_{\mathscr{K}}^{(p)}(E+i\eta)^{\dagger} - G_{\mathscr{K}}^{(p)}(E+i\eta) \} (1-K)^{1/2}, \tag{4.74b}$$

where $G_{\mathscr{K}}^{(p)}(E)$ is the resolvent of $h_{\mathscr{K}}^{(p)}(E)$:

$$[\, E - h_{\mathscr{K}}^{(p)}(E)\,]\, G_{\mathscr{K}}^{(p)}(E) = 1, \tag{4.74c}$$

$$G_{\mathscr{K}}^{(p)}(E) = (1-K)^{-1/2}\, G^{(p)}(E)(1-K)^{-1/2}. \tag{4.74d}$$

4.17. *A New Particle-type Hamiltonian*

The particle Hamiltonian $h^{(p)}$ diverges at large E. In contrast, Feshbach's Hamiltonian remains finite at large energy. However, its real and imaginary parts are not symmetric in the coordinate space representation. Kerman's Hamiltonian does not suffer from the latter drawback, but its bound and scattering eigenstates differ from the overlaps at finite distance. In the present section, we shall construct a particle-type Hamiltonian $\tilde{h}^{(p)}(E)$ which remains finite at large E, whose real and imaginary parts are symmetric in the coordinate space representation and which has the bound and elastic scattering overlaps as eigenstates. We shall exhibit the nature of the price which has to be paid for fulfilling simpler properties. This operator $\tilde{h}^{(p)}(E)$ will be derived by means of a variant of Feshbach's method, in which every vector of the Hilbert space $\mathscr{H}^{(A+1)}$ will be decomposed into two parts which are not orthogonal to one another.

4.17.1. *Operators $\tilde{P}^{(p)}$ and $\tilde{Q}^{(p)}$*

Since

$$\tilde{P}^{(p)} = \int d\mathbf{r}\, a_{\mathbf{r}}^{\dagger} |\Psi_0^{(A)}\rangle\langle \Psi_0^{(A)}|\, a_{\mathbf{r}}, \qquad \tilde{q}^{(p)} = \mathscr{I}^{(A+1)} - \tilde{P}^{(p)} \tag{4.75a}$$

are both positive definite,

$$\tilde{Q}^{(p)} = \sqrt{\tilde{q}^{(p)}} \tag{4.75b}$$

exists. The operators $\tilde{P}^{(p)}$ and $\tilde{Q}^{(p)}$ are hermitian. However, in contrast to $P^{(p)}$ and $Q^{(p)}$, they are not projection operators since

$$\tilde{P}^{(p)}\tilde{Q}^{(p)} \neq 0, \qquad [\tilde{P}^{(p)}]^2 \neq \tilde{P}^{(p)}, \qquad [\tilde{Q}^{(p)}]^2 \neq \tilde{Q}^{(p)}. \tag{4.75c}$$

One has

$$\tilde{P}^{(p)} + \tilde{Q}^{(p)}\tilde{Q}^{(p)} = \mathscr{I}^{(A+1)}. \tag{4.75d}$$

An explicit expression for $\tilde{Q}^{(p)}$ is readily obtained from (4.75a) and (4.75d),

$$\tilde{Q}^{(p)} = 1 - L^{(p)}, \tag{4.76a}$$

where

$$L^{(p)} = \int d\mathbf{r}\, d\mathbf{r}'\, |a_{\mathbf{r}}^{\dagger}\Psi_0^{(A)}\rangle\langle \mathbf{r}|\, \beta^{(p)}\, |\mathbf{r}'\rangle\langle \Psi_0^{(A)}|\, a_{\mathbf{r}'}, \tag{4.76b}$$

with

$$\beta^{(p)} = (1 - \sqrt{K})/(1 - K) = (1 + \sqrt{K})^{-1}. \tag{4.76c}$$

One has

$$\tilde{Q}^{(p)} + \tilde{P}^{(p)} = 1 - \int d\mathbf{r}\, d\mathbf{r}'\, a_{\mathbf{r}}^{\dagger}\, |\Psi_0^{(A)}\rangle\langle \mathbf{r}|\, (\beta^{(p)} - 1)\, |\mathbf{r}'\rangle\langle \Psi_0^{(A)}|\, a_{\mathbf{r}'}. \tag{4.76d}$$

4.17.2. *Definition of the Particle-type Hamiltonian*

Let us successively apply $\tilde{P}^{(p)}$ and $\tilde{Q}^{(p)}$ to

$$\mathscr{E}^{(+)}\, |\Psi_{\mathscr{E}}^{(+)}\rangle = H\, |\Psi_{\mathscr{E}}^{(+)}\rangle, \tag{4.77a}$$

where $|\Psi_{\mathscr{E}}^{(+)}\rangle$ is a bound or a scattering eigenstate of the $(A+1)$-nucleon Hamiltonian. Using (4.75d), one finds that

$$\mathscr{E}^{(+)}\tilde{P}^{(p)}\, |\Psi_{\mathscr{E}}^{(+)}\rangle = \tilde{P}^{(p)}H\tilde{P}^{(p)}\, |\Psi_{\mathscr{E}}^{(+)}\rangle + \tilde{P}^{(p)}H\tilde{Q}^{(p)}\tilde{Q}^{(p)}\, |\Psi_{\mathscr{E}}^{(+)}\rangle, \tag{4.77b}$$

$$\mathscr{E}^{(+)}\tilde{Q}^{(p)}\, |\Psi_{\mathscr{E}}^{(+)}\rangle = \tilde{Q}^{(p)}H\tilde{P}^{(p)}\, |\Psi_{\mathscr{E}}^{(+)}\rangle + \tilde{Q}^{(p)}H\tilde{Q}^{(p)}\tilde{Q}^{(p)}\, |\Psi_{\mathscr{E}}^{(+)}\rangle. \tag{4.77c}$$

We first use these equations in the case of a bound eigenstate $|\Psi_\lambda^{(+)}\rangle$. When solving (4.77c) for $\tilde{Q}^{(p)}|\Psi_\lambda^{(+)}\rangle$, two situations can occur: (a) The energy $\mathscr{E}_\lambda^{(+)}$ is embedded in the continuous spectrum of $\tilde{Q}^{(p)}H\tilde{Q}^{(p)}$. (b) The energy $\mathscr{E}_\lambda^{(+)}$ lies outside the continuous spectrum of $\tilde{Q}^{(p)}H\tilde{Q}^{(p)}$. By following the same procedure as in [32], it can be shown that both cases lead to the same solution. For simplicity, here we shall only consider case (b). Equation (4.77c) gives

$$\tilde{Q}^{(p)}|\Psi_\lambda^{(+)}\rangle = (\mathscr{E}_\lambda^{(+)} - \tilde{Q}^{(p)}H\tilde{Q}^{(p)})^{-1}\,\tilde{Q}^{(p)}H\tilde{P}^{(p)}|\Psi_\lambda^{(+)}\rangle. \tag{4.77d}$$

The right-hand side does not change if one replaces $\mathscr{E}_\lambda^{(+)}$ by either one of the two limiting prescriptions $\mathscr{E}_\lambda^{(+)} \to \mathscr{E}_\lambda^{(+)} \mp i\eta$. We shall choose the limit $(+i\eta)$ in such a way that the particle-type Hamiltonian $\tilde{h}^{(p)}(E)$ defined below will have analytic properties similar to those of $h^{(p)}(E)$. By introducing (4.77d) in (4.77b), one obtains

$$[\mathscr{E}_\lambda^{(+)} - \tilde{P}^{(p)}H - \tilde{P}^{(p)}H\tilde{Q}^{(p)}(\mathscr{E}_\lambda^{(+)} - \tilde{Q}^{(p)}H\tilde{Q}^{(p)} + i\eta)^{-1}\,\tilde{Q}^{(p)}H] \times \tilde{P}^{(p)}|\Psi_\lambda^{(+)}\rangle = 0. \tag{4.77e}$$

We now derive a one-body wave equation for the bound overlap $|\chi_\lambda^{(+)}\rangle$. According to (4.75a) and to the definition (2.8a) of the density matrix, one has

$$\langle \Psi_0^{(A)}|\, a_{\mathbf{r}}\tilde{P}^{(p)} = \int d\mathbf{r}'[\delta(\mathbf{r}-\mathbf{r}') - K_{\mathbf{r}\mathbf{r}'}]\langle \Psi_0^{(A)}|\, a_{\mathbf{r}'}, \tag{4.78}$$

$$\langle \Psi_0^{(A)}|\, a_{\mathbf{r}}\tilde{P}^{(p)}|\Psi_\lambda^{(+)}\rangle = \langle \mathbf{r}|\chi_\lambda^{(+)}\rangle - \int d\mathbf{r}'\, K_{\mathbf{r}\mathbf{r}'}\langle \mathbf{r}'|\chi_\lambda^{(+)}\rangle. \tag{4.79}$$

This suggests to multiply (4.77e) from the left successively by $\langle \Psi_0^{(A)}|\, a_{\mathbf{r}}$ and $(1-K)^{-1}$. This yields

$$E_\lambda^{(+)}\chi_\lambda^{(+)}(\mathbf{r}) = \int d\mathbf{r}'\,\tilde{h}^{(p)}(\mathbf{r},\mathbf{r}';E_\lambda^{(+)}+i\eta)\,\chi_\lambda^{(+)}(\mathbf{r}'), \tag{4.80}$$

where the particle-type Hamiltonian $\tilde{h}^{(p)}(E+i\eta)$ is defined as

$$\tilde{h}^{(p)}(E+i\eta) = -\mathscr{E}_0^{(A)}K + R^{(p)} + \tilde{D}^{(p)}(E+i\eta). \tag{4.81}$$

Here, $R^{(p)}$ is the energy-independent operator given by (4.34), while

$$\tilde{D}_{\mathbf{r}\mathbf{r}'}^{(p)}(E+i\eta) = \langle \Psi_0^{(A)}|\, a_{\mathbf{r}}H\tilde{Q}^{(p)}(E-\tilde{Q}^{(p)}H\tilde{Q}^{(p)}+\mathscr{E}_0^{(A)}+i\eta)^{-1}\,\tilde{Q}^{(p)}Ha_{\mathbf{r}'}^{\dagger}|\Psi_0^{(A)}\rangle. \tag{4.82}$$

Unless confusion might arise, we shall write, for E real,

$$\tilde{h}^{(p)}(E) = \tilde{h}^{(p)}(E+i\eta), \quad \tilde{D}^{(p)}(E) = \tilde{D}^{(p)}(E+i\eta). \tag{4.83}$$

Equation (4.80) shows that $\tilde{h}^{(p)}(E)$ is equivalent to $h^{(p)}(E)$ in the sense that both operators have the bound overlaps $|\lambda^{(+)}\rangle$ as eigenstates, with eigenvalues $E_\lambda^{(+)}$. They also share the property that their real and imaginary parts are hermitian, in particular are symmetric in the coordinate space representation. Below, we shall prove that $\tilde{h}^{(p)}(E)$ also has as eigenstate the elastic scattering overlap $|\chi_E^{0(+)}\rangle$:

$$\tilde{h}^{(p)}(E)\,|\chi_E^{0(+)}\rangle = E\,|\chi_E^{0(+)}\rangle. \tag{4.84}$$

Unlike $h^{(p)}$, however, the hole-type Hamiltonian $\tilde{h}^{(p)}(E)$ approaches a constant at large energy.

4.17.3. *Resolvent of the Particle-type Hamiltonian*

For z complex, the resolvent $\tilde{G}^{(p)}(z)$ of $\tilde{h}^{(p)}(z)$ is defined by

$$[\,z-\tilde{h}^{(p)}(z)\,]\;\tilde{G}^{(p)}(z)=1. \tag{4.85}$$

We now derive the relationship between $\tilde{G}^{(p)}(E+i\eta)$ and the particle Green's function $G^{(p)}(E+i\eta)$, for $\eta\neq 0$. Let us insert the unit operator $\mathscr{I}^{(A+1)}$ from (4.75d) in the following identity (z complex)

$$(z-H)^{-1}\,\mathscr{I}^{(A+1)}(z-H)=1. \tag{4.86a}$$

We get

$$(z-H)^{-1}\,(z-\tilde{P}^{(p)}H-\tilde{Q}^{(p)}\tilde{Q}^{(p)}H)=1. \tag{4.86b}$$

By multiplying this relation by $\tilde{Q}^{(p)}$ from the right, we obtain

$$(z-H)^{-1}\;\tilde{Q}^{(p)}(z-\tilde{Q}^{(p)}H\tilde{Q}^{(p)})=[\,1+(z-H)^{-1}\tilde{P}^{(p)}H\,]\;\tilde{Q}^{(p)}, \tag{4.86c}$$

which yields

$$(z-H)^{-1}\;\tilde{Q}^{(p)}=[\,1+(z-H)^{-1}\;\tilde{P}^{(p)}H\,]\;\tilde{Q}^{(p)}(z-\tilde{Q}^{(p)}H\tilde{Q}^{(p)})^{-1}. \tag{4.86d}$$

By introducing the latter result in (4.86b), we find

$$\begin{aligned}(z-H)^{-1}\,[\,z-\tilde{P}^{(p)}H-\tilde{P}^{(p)}H\tilde{Q}^{(p)}(z-\tilde{Q}^{(p)}H\tilde{Q}^{(p)})^{-1}\;\tilde{Q}^{(p)}H\,]\\ =1+\tilde{Q}^{(p)}(z-\tilde{Q}^{(p)}H\tilde{Q}^{(p)})^{-1}\;\tilde{Q}^{(p)}H.\end{aligned} \tag{4.87}$$

In order to derive a relation between one-body operators, we multiply (4.87) from the left by $\langle\,\Psi_0^{(A)}|\,a_{\mathbf{r}}$ and from the right by $a_{\mathbf{r}'}^{\dagger}\,|\Psi_0^{(A)}\rangle$. We set $z=E+\mathscr{E}_0^{(A)}+i\eta$, with $\eta\neq 0$. With the help of the expressions (4.75a) and (4.81) of $\tilde{P}^{(p)}$ and $\tilde{h}^{(p)}(E+i\eta)$, this leads to

$$G^{(p)}(E+i\eta)(E-\tilde{h}^{(p)}(E+i\eta)+i\eta)=1-K+\hat{F}^{(p)}(E+i\eta), \tag{4.88}$$

where

$$\hat{F}^{(p)}(\mathbf{r}, \mathbf{r}'; E+i\eta) = \langle \Psi_0^{(A)} |\, a_{\mathbf{r}} \tilde{Q}^{(p)} (E - \tilde{Q}^{(p)} H \tilde{Q}^{(p)} + \mathscr{E}_0^{(A)} + i\eta)^{-1}\, \tilde{Q}^{(p)} H a_{\mathbf{r}'}^{\dagger} \,|\Psi_0^{(A)}\rangle. \tag{4.89}$$

Equations (4.85) and (4.88) yield

$$G^{(p)}(E+i\eta) = [\,1 - K + \hat{F}^{(p)}(E+i\eta)\,]\, \tilde{G}^{(p)}(E+i\eta). \tag{4.90}$$

We now show that the relationship between the particle Green's function $G^{(p)}(E+i\eta)$ and the particle-type Green's function $\tilde{G}^{(p)}(E+i\eta)$ is much simpler than (4.90) appears to indicate. First note that, according to (4.81) and (4.34),

$$\tilde{D}_{\mathbf{r}\mathbf{r}'}^{(p)}(E+i\eta) = \tilde{h}_{\mathbf{r}\mathbf{r}'}^{(p)}(E+i\eta) + \mathscr{E}_0^{(A)} \delta(\mathbf{r}-\mathbf{r}') - \langle \Psi_0^{(A)} |\, a_{\mathbf{r}} H a_{\mathbf{r}'}^{\dagger} \,|\Psi_0^{(A)}\rangle. \tag{4.91a}$$

By inserting the unit operator (4.75d) between the operators $a_{\mathbf{r}}$ and H inside the matrix element on the right-hand side of (4.82), one readily finds that

$$\begin{aligned} \tilde{D}_{\mathbf{r}\mathbf{r}'}^{(p)}(E+i\eta) = & -\langle \Psi_0^{(A)} |\, a_{\mathbf{r}} (1 - \tilde{P}^{(p)})\, H a_{\mathbf{r}'}^{\dagger} \,|\Psi_0^{(A)}\rangle \\ & + \langle \Psi_0^{(A)} |\, a_{\mathbf{r}} [\, \tilde{P}^{(p)} H \tilde{Q}^{(p)} + \tilde{Q}^{(p)} (E + \mathscr{E}_0^{(A)} + i\eta)\,] \\ & \times \frac{1}{E - \tilde{Q}^{(p)} H \tilde{Q}^{(p)} + \mathscr{E}_0^{(A)} + i\eta}\, \tilde{Q}^{(p)} H a_{\mathbf{r}'}^{\dagger} \,|\Psi_0^{(A)}\rangle. \end{aligned} \tag{4.91b}$$

Equations (4.78), (4.89), (4.91a), and (4.91b) yield

$$K[\,\tilde{h}^{(p)}(E+i\eta) + \mathscr{E}_0^{(A)}\,] = (E + \mathscr{E}_0^{(A)} + i\eta)\, \hat{F}(E+i\eta). \tag{4.92}$$

We multiply this relation from the right by $\tilde{G}^{(p)}(E+i\eta)$ and obtain, with the use of (4.85),

$$[\,K - \hat{F}(E+i\eta)\,]\, \tilde{G}(E+i\eta) = (E + \mathscr{E}_0^{(A)} + i\eta)^{-1}\, K. \tag{4.93}$$

By inserting this result in (4.90), we obtain the simple relationship that we were looking for, namely,

$$\tilde{G}^{(p)}(E+i\eta) = G^{(p)}(E+i\eta) + (E + \mathscr{E}_0^{(A)} + i\eta)^{-1}\, K. \tag{4.94a}$$

Explicitly, this reads

$$\tilde{G}^{(p)}(E+i\eta) = G^{(p)}(E+i\eta) + \sum_{n_\nu \neq 1} \frac{|\omega_\nu\rangle\, n_\nu\, \langle \omega_\nu|}{E + \mathscr{E}_0^{(A)} + i\eta}, \tag{4.94b}$$

where we expressed K in terms of the natural orbitals; see (2.12b). Hence, $\tilde{G}^{(p)}(E+i\eta)$ has the same singularities as $G^{(p)}(E+i\eta)$, except for an additional pole

with infinite degeneracy located at $E = -\mathscr{E}_0^{(A)} - i\eta$. As specified in (2.2b), the energy $(-\mathscr{E}_0^{(A)})$ is large and positive: it is typically on the order of $+1000$ MeV.

4.17.4. *High Energy Behaviour and Sum Rules*

Equations (4.81) and (4.82) show that, at large E,

$$\tilde{h}^{(p)}(E) \sim -\mathscr{E}_0^{(A)} K + R^{(p)}. \tag{4.95}$$

According to (4.85), the resolvent $\tilde{G}^{(p)}(z)$ thus behaves as

$$\tilde{G}^{(p)}(z) \sim z^{-1}[\,1 - z^{-1}(\mathscr{E}_0^{(A)} K - R^{(p)})\,]. \tag{4.96a}$$

This result can also be obtained from (4.44a) and (4.94a). Indeed, these yield

$$\tilde{G}^{(p)}(z) \sim z^{-1}(1 - K + z^{-1}R^{(p)}) + z^{-1}(1 - z^{-1}\mathscr{E}_0^{(A)})\, K. \tag{4.96a}$$

The behaviour $\tilde{G}^{(p)}(z) \sim z^{-1}$ is in striking contrast with the asymptotic behaviour $G^{(p)}(z) \sim (1-K)/z$ of the particle Green's function; see (4.44a). We now derive sum rules by performing contour integrals, as we did in (4.44d) and (4.44e). Since $\tilde{G}^{(p)}(z)$ behaves as $1/z$ at large z, its contour integral over a large closed circle in the complex z-plane is equal to

$$\int_{\text{circle}} dz\ \tilde{G}^{(p)}(z) = 2i\pi. \tag{4.97a}$$

By indenting the contour around the singularities of $\tilde{G}(z)$, which are all located on the real axis, (4.97a) yields

$$(2i\pi)^{-1} \int_{E_0^{(+)}}^{\infty} dE[\,\tilde{G}^{(p)}(E + i\eta)^{\dagger} - \tilde{G}^{(p)}(E + i\eta)\,] = 1. \tag{4.97b}$$

In order to discuss the striking difference between this result and (4.44e), let us define a particle-type spectral function as

$$\tilde{S}^{(p)}(E) = (2i\pi)^{-1}\{\tilde{G}^{(p)}(E + i\eta)^{\dagger} - \tilde{G}^{(p)}(E + i\eta)\}; \tag{4.98}$$

compare with (4.6b). According to (4.94a), one has

$$\tilde{S}^{(p)}(E) = S^{(p)}(E) + \pi^{-1} \lim_{\eta \to +0} \frac{\eta}{[\,(E + \mathscr{E}_0^{(A)})^2 + \eta^2\,]}\, K \tag{4.99a}$$

$$= S^{(p)}(E) + K\delta(E + \mathscr{E}_0^{(A)}). \tag{4.99b}$$

Hence, the particle-type spectral function is equal to the particle spectral function at all energies except at $E = -\mathscr{E}_0^{(A)}$. Equation (4.97b) yields

$$\int_{E_0^{(+)}}^{\infty} dE\, \tilde{S}^{(p)}(E) = 1. \tag{4.100}$$

4.17.5. *Spectroscopic Factor in Terms of the Particle-type Hamiltonian*

Equation (4.94a) implies that $\tilde{G}^{(p)}(E)$ and $G^{(p)}(E)$ both have poles at the single-particle energies $E_\lambda^{(+)}$ of the bound states $|\Psi_\lambda^{(+)}\rangle$ of the $(A+1)$-system. By multiplying (4.94a) by $(E - E_\lambda^{(+)} + i\eta)$ and then taking the limit $E \to E_\lambda^{(+)} - i\eta$, one obtains

$$|\lambda^{(+)}\rangle\, \mathscr{S}_\lambda^{(+)}\, \langle \lambda^{(+)}| = |\lambda^{(+)}\rangle\, \tilde{\mathscr{S}}_\lambda^{(+)}\, \langle \lambda^{(+)}|, \tag{4.101a}$$

where $\mathscr{S}_\lambda^{(+)}$ is defined by (4.41e) while, according to the Hellmann–Feynman theorem (A.3a),

$$\tilde{\mathscr{S}}_\lambda^{(+)} = \left[\langle \lambda^{(+)}|\, 1 - \frac{d}{dE}\, \tilde{h}^{(p)}(E)\, |\lambda^{(+)}\rangle \right]^{-1}_{E = E_\lambda^{(+)}}. \tag{4.101b}$$

Equation (4.101a) and the equality $\mathscr{S}_\lambda^{(+)} = \tilde{\mathscr{S}}_\lambda^{(+)}$ imply that

$$\left[\langle \lambda^{(+)}|\, \frac{d}{dE}\, \tilde{h}^{(p)}(E)\, |\lambda^{(+)}\rangle \right]_{E = E_\lambda^{(+)}} = \left[\langle \lambda^{(+)}|\, \frac{d}{dE}\, h^{(p)}(E)\, |\lambda^{(+)}\rangle \right]_{E = E_\lambda^{(+)}}. \tag{4.101c}$$

4.17.6. *Elastic Overlap Functions*

In Appendix E, we use the time-dependent formulation of scattering theory to prove that the elastic overlap functions are eigenstates of the particle-type Hamiltonian, i.e., that

$$\tilde{h}^{(p)}(E_k)\, |\chi_{\mathbf{k}}^{0(+)}\rangle = E_k\, |\chi_{\mathbf{k}}^{0(+)}\rangle, \qquad \tilde{h}^{(p)}(E)\, |\chi_E^{0(+)}\rangle = E\, |\chi_E^{0(+)}\rangle; \tag{4.102}$$

see (E.9a) and (E.9b). We recall that $E_k = k^2/2m$. The particle-type Hamiltonian $\tilde{h}^{(p)}$ thus fulfills the requirement (4.3b). We now show that the result (4.102) can also be derived in the framework of stationary collision theory that we had used to obtain (4.24b). We showed that

$$|\chi_{\mathbf{k}}^{0(+)}\rangle = \lim_{\eta \to +0}\, i\eta G^{(p)}(E_k + i\eta)\, |\mathbf{k}\rangle; \tag{4.103}$$

see (4.23a). Since

$$\lim_{\eta \to +0}\, i\eta (E_k + \mathscr{E}_0^{(A)} + i\eta)^{-1}\, |\mathbf{k}\rangle = 0 \qquad \text{for} \quad E_k \neq -\mathscr{E}_0^{(A)}, \tag{4.104a}$$

(4.94a) shows that

$$\lim_{\eta \to +0} i\eta \tilde{G}^{(p)}(E_k + i\eta)\,|\mathbf{k}\rangle = |\chi_{\mathbf{k}}^{0(+)}\rangle \qquad \text{for} \quad E_k \neq -\mathscr{E}_0^{(A)}. \tag{4.104b}$$

The same reasoning as that followed for going from (4.23a) to (4.24a) then yields

$$\tilde{h}^{(p)}(E_k)\,|\chi_{\mathbf{k}}^{0(+)}\rangle = E_k\,|\chi_{\mathbf{k}}^{0(+)}\rangle \qquad \text{for} \quad E_k \neq -\mathscr{E}_0^{(A)}. \tag{4.105}$$

However, caution should be taken at $E_k = -\mathscr{E}_0^{(A)}$. Indeed, (4.94a) yields

$$\lim_{E \to -\mathscr{E}_0^{(A)}} \lim_{\eta \to +0} [E + \mathscr{E}_0^{(A)}]\,\tilde{G}^{(p)}(E + i\eta) = K. \tag{4.106a}$$

Correspondingly, (4.103) gives

$$\lim_{\eta \to +0} i\eta \tilde{G}^{(p)}(-\mathscr{E}_0^{(A)} + i\eta)\,|\mathbf{k}_0\rangle = |\chi_{\mathbf{k}_0}^{0(+)}\rangle + K\,|\mathbf{k}_0\rangle, \tag{4.106b}$$

where the momentum k_0 is related to $\mathscr{E}_0^{(A)}$ by

$$k_0^2/2m = -\mathscr{E}_0^{(A)}. \tag{4.106c}$$

The striking difference between (4.104b) and (4.106b) requires a careful examination of the limiting procedure $\eta \to +0$ when z is replaced by $(-\mathscr{E}_0^{(A)} + i\eta)$ in (4.85) and related equations.

4.17.7. *Limit towards the Real Axis*

We now define $\tilde{G}^{(p)}(E)$ for E real, and also we summarize (4.8), (4.10b), and (4.83):

$$\begin{aligned} \tilde{G}^{(p)}(E) &= \lim_{\eta \to +0} \tilde{G}^{(p)}(E + i\eta), \\ G^{(p)}(E) &= \lim_{\eta \to +0} G^{(p)}(E + i\eta), \end{aligned} \tag{4.107a}$$

$$\begin{aligned} \tilde{h}^{(p)}(E) &= \lim_{\eta \to +0} \tilde{h}^{(p)}(E + i\eta), \\ h^{(p)}(E) &= \lim_{\eta \to +0} h^{(p)}(E + i\eta). \end{aligned} \tag{4.107b}$$

The consistency of the results obtained in Sections 4.3–4.12 indicates that

$$G^{(p)}(E) = \lim_{\eta \to +0} \frac{1}{E - h^{(p)}(E + i\eta) + i\eta} = \lim_{\eta \to +0} \frac{1}{E - h^{(p)}(E) + i\eta}, \tag{4.108a}$$

$$\lim_{\eta \to +0} h^{(p)}(E + i\eta)\,G^{(p)}(E + i\eta) = h^{(p)}(E)\,G^{(p)}(E). \tag{4.108b}$$

Below, we argue that relations similar to (4.108a) and (4.108b) are not valid in the case of $\tilde{G}^{(p)}(E)$ and $\tilde{h}^{(p)}(E)$ at $E=-\mathscr{E}_0^{(A)}$, more specifically that

$$\tilde{G}^{(p)}(-\mathscr{E}_0^{(A)}) = \lim_{\eta \to +0} \frac{1}{-\mathscr{E}_0^{(A)} - \tilde{h}^{(p)}(-\mathscr{E}_0^{(A)} + i\eta) + i\eta}$$

$$\neq \lim_{\eta \to +0} \frac{1}{-\mathscr{E}_0^{(A)} - \tilde{h}^{(p)}(-\mathscr{E}_0^{(A)}) + i\eta}. \tag{4.109}$$

In other words, we shall show that $\tilde{G}^{(p)}(-\mathscr{E}_0^{(A)})$ is not the resolvent of $\tilde{h}^{(p)}(-\mathscr{E}_0^{(A)})$, namely that

$$\lim_{\eta \to +0} \tilde{G}^{(p)}(-\mathscr{E}_0^{(A)} + i\eta) \neq \lim_{\eta \to +0} [-\mathscr{E}_0^{(A)} - \tilde{h}^{(p)}(-\mathscr{E}_0^{(A)}) + i\eta]^{-1}. \tag{4.110}$$

We prove this feature *ab absurdo*, i.e., by reducing this opposite statement to the absurd. If $\tilde{G}^{(p)}(-\mathscr{E}_0^{(A)})$ would be the resolvent of $\tilde{h}^{(p)}(-\mathscr{E}_0^{(A)})$, then according to (4.94a) there would exist an operator

$$\tilde{\mathscr{C}}^{(p)} = -\mathscr{E}_0^{(A)} - \tilde{h}^{(p)}(-\mathscr{E}_0^{(A)}), \tag{4.111a}$$

which would fulfill the relation

$$\lim_{\eta \to +0} \left[\frac{1}{\tilde{\mathscr{C}}^{(p)} + i\eta} - \frac{1}{-\mathscr{E}_0^{(A)} - h^{(p)}(-\mathscr{E}_0^{(A)}) + i\eta} - \frac{K}{i\eta} \right] = 0 \tag{4.111b}$$

and would have a biorthogonal set of normalizable vectors belonging to the eigenvalue zero. Note the appearance of $\tilde{h}^{(p)}(-\mathscr{E}_0^{(A)})$ in $\tilde{\mathscr{C}}^{(p)}$ as opposed to that of $h^{(p)}(-\mathscr{E}_0^{(A)})$ in the second term of (4.111b). We now show that (4.111b) is not possible. Let $\{|\varphi_q^{(p)}\rangle, |\tilde{\varphi}_q^{(p)}\rangle\}$ be the biorthogonal set of normalizable vectors, belonging to the eigenvalue zero, of $\tilde{\mathscr{C}}^{(p)}$ and $\tilde{\mathscr{C}}^{(p)\dagger}$, respectively. Then,

$$\langle \tilde{\varphi}_q^{(p)} | \varphi_r^{(p)} \rangle = \delta_{qr}, \tag{4.112a}$$

$$\frac{1}{\tilde{\mathscr{C}}^{(p)} + i\eta} = \frac{1}{i\eta} \sum_q |\varphi_q^{(p)}\rangle \langle \tilde{\varphi}_0^{(p)}| + \rho^{(p)}(\eta), \tag{4.112b}$$

where $\rho^{(p)}$ has a finite limit when $\eta \to +0$. The second term within the square brackets in (4.111b) also has a finite limit when $\eta \to +0$, since $(-\mathscr{E}_0^{(A)})$ is not a discrete eigenvalue of $h^{(p)}(-\mathscr{E}_0^{(A)})$. By inserting (4.112b) into (4.111b), assumed to be correct, one would obtain

$$K = \sum_q |\varphi_q^{(p)}\rangle \langle \tilde{\varphi}_q^{(p)}|. \tag{4.113a}$$

Equations (4.112a) and (4.113a) would give

$$K\,|\varphi_q^{(p)}\rangle = |\varphi_q^{(p)}\rangle. \tag{4.113b}$$

This is an absurd relation since all quantities with which we deal are contained in the Hilbert space $\mathscr{H}^{(1)}_{(\neq 1)}$ spanned by the natural orbitals with eigenvalue different from unity; see (2.11). This confirms *ab absurdo* the validity of the statements (4.109)–(4.110). One of the consequences of this feature is that one may not derive expressions for $\tilde{S}^{(p)}(E)$ by means of the methods that we had used in connection with (4.50b) and (4.50c).

4.17.8. *Analytic Properties of the Particle-type Hamiltonian*

We now explicitly exhibit that $h^{(p)}$ and $\tilde{h}^{(p)}$ have similar analytical properties, and we derive a dispersion relation between the real and imaginary parts of $\tilde{h}^{(p)}(E)$. We assume that $\tilde{Q}^{(p)}H\tilde{Q}^{(p)}$ is self-adjoint. Let us introduce its scattering and bound eigenstates

$$\tilde{Q}^{(p)}H\tilde{Q}^{(p)}\,|\tilde{\Phi}_q^{(p)}\rangle = (\mathscr{E}_0^{(A)} + \tilde{\varepsilon}_q^{(p)})\,|\tilde{\Phi}_q^{(p)}\rangle, \tag{4.114a}$$

$$\tilde{Q}^{(p)}H\tilde{Q}^{(p)}\,|\Phi_{\mathscr{E}}^{c(+)}\rangle = (\mathscr{E}_0^{(A)} + \tilde{\varepsilon}^{(p)})\,|\Phi_{\mathscr{E}}^{c(+)}\rangle, \tag{4.114b}$$

where $\mathscr{E} = \mathscr{E}_0^{(A)} + \tilde{\varepsilon}_q^{(p)}$. The quantities $\tilde{\varepsilon}^{(p)}$ and $\tilde{\varepsilon}_q^{(p)}$ correspond to single-particle energies. We adopt the same normalization as in (2.2c). The upper degeneracy index c can be identified with the channel index. Indeed, it is shown in (E.8a) and (E.10b) that the scattering eigenstates of $\tilde{Q}^{(p)}H\tilde{Q}^{(p)}$ are given by $|\tilde{\Phi}_{\mathscr{E}}^{c(+)}\rangle = \Omega_{\tilde{Q}}^{(p)}\,|\Psi_{\mathscr{E}}^{c(+)}\rangle$, with $c \neq 0$. Here, $\Omega_{\tilde{Q}}^{(p)}$ is a generalized Møller operator while $|\Psi_{\mathscr{E}}^{c(+)}\rangle$ is a scattering eigenstate of H. The specification $c \neq 0$ indicates that the target is an excited state of the A-nucleon system; there exists no eigenstate of $\tilde{Q}^{(p)}H\tilde{Q}^{(p)}$ which would correspond to $c = 0$. By introducing the operator $\sum_q |\tilde{\Phi}^{(p)}\rangle\langle\tilde{\Phi}^{(p)}|$ in (4.82) we find that, in any real single-particle representation $\{\psi_\alpha\}$,

$$\operatorname{Im} \tilde{D}^{(p)}_{\alpha\alpha'}(E + i\eta) = -\pi \sum_{c(t\neq 0)} \int_{T_c^{(+)}}^{\infty} d\tilde{\varepsilon}^{(p)} [\,\tilde{\mathscr{J}}^{c(+)}_{\alpha'}(\tilde{\varepsilon}^{(p)})\,]^*\, \tilde{\mathscr{J}}^{c(+)}_{\alpha}(\tilde{\varepsilon}^{(p)})\, \delta(E - \tilde{\varepsilon}^{(p)}), \tag{4.115}$$

with

$$\langle\psi_\alpha|\,\tilde{\mathscr{J}}^{c(+)}(\tilde{\varepsilon}^{(p)})\rangle = \tilde{\mathscr{J}}^{c(+)}_{\alpha}(\tilde{\varepsilon}^{(p)}) = \langle\Psi_0^{(A)}|\,a_\alpha H\tilde{Q}^{(p)}\,|\tilde{\Phi}_{\mathscr{E}}^{c(+)}\rangle. \tag{4.116}$$

The imaginary part of the hole-type operator $\tilde{h}^{(p)}(E)$ defined by (4.81) is thus given by ($\mathscr{E} = \mathscr{E}_0^{(A)} + E$):

$$\tilde{W}^{(p)}(\mathbf{r}, \mathbf{r}'; E) = -\pi \sum_{c(t\neq 0)} [\,\tilde{\mathscr{J}}^{c(+)}_{\mathbf{r}'}(E)\,]^*\, [\,\tilde{\mathscr{J}}^{c(+)}_{\mathbf{r}}(E)\,]. \tag{4.117}$$

This quantity fulfills the same relations (4.64d) and (4.64e) as $W^{(p)}(E)$.

The resolvent $(z+\mathscr{E}_0^{(A)}-\tilde{Q}^{(p)}H\tilde{Q}^{(p)})^{-1}$ is an analytic function of z in the complementary set of the spectrum of $[\tilde{Q}^{(p)}H\tilde{Q}^{(p)}-\mathscr{E}_0^{(A)}]$. We thus conclude from (4.81) that, except for polar singularities at $\tilde{\varepsilon}_q^{(p)}$, the particle-type Hamiltonian $\tilde{h}^{(p)}(E)$ is analytic in the complex E-plane cut from $T_{\text{in}}^{(+)}$ to ∞. The real and imaginary parts of

$$\tilde{h}^{(p)}(E)=\operatorname{Re}\tilde{h}^{(p)}(E)+i\tilde{W}^{(p)}(E) \tag{4.118}$$

thus fulfill the dispersion relation,

$$\operatorname{Re}\tilde{h}^{(p)}(E)=-\mathscr{E}_0^{(A)}K+R^{(p)}+\sum_q \frac{|\tilde{\mathscr{J}}_q^{(p)}\rangle\langle\tilde{\mathscr{J}}_q^{(p)}|}{E-\tilde{\varepsilon}_q^{(p)}}+\frac{\mathscr{P}}{\pi}\int_{T_{\text{in}}^{(+)}}^{+\infty}dE'\,\frac{\tilde{W}^{(p)}(E')}{E'-E}, \tag{4.119}$$

where

$$\langle\mathbf{r}|\,\tilde{\mathscr{J}}_q^{(p)}\rangle=\langle\Psi_0^{(A)}|\,a_{\mathbf{r}}H\tilde{Q}^{(p)}\,|\tilde{\Phi}_q^{(p)}\rangle. \tag{4.120}$$

4.18. *A Wider Class of Particle Hamiltonians*

Let $\hat{C}^{(p)}(z)$ be an operator which, as a function of z, is analytic in a domain which includes the real energies $E>E_0^{(+)}$. Define

$$\hat{G}^{(p)}(E+i\eta)=G^{(p)}(E+i\eta)+\hat{C}^{(p)}(E+i\eta). \tag{4.121a}$$

It is readily checked from (4.16e) that, if it exits, the operator

$$\hat{h}^{(p)}(E)=E-[\,\hat{G}^{(p)}(E+i\eta)\,]^{-1} \tag{4.121b}$$

has the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$ as eigenstates:

$$\begin{aligned}\hat{h}^{(p)}(E_\lambda^{(+)})\,|\chi_\lambda^{(+)}\rangle&=E_\lambda^{(+)}\,|\chi_\lambda^{(+)}\rangle,\\ \hat{h}^{(p)}(E)\,|\chi_E^{0(+)}\rangle&=E\,|\chi_E^{0(+)}\rangle.\end{aligned} \tag{4.122}$$

Furthermore, the particle spectral function is given by an equation formally identical to (4.6b), namely,

$$S^{(p)}(E)=(2i\pi)^{-1}\{\hat{G}^{(p)}(E+i\eta)^\dagger-\hat{G}^{(p)}(E+i\eta)\}\qquad\text{for}\quad E>E_0^{(+)}. \tag{4.123}$$

A considerable freedom thus exists in the definition of the optical-model Hamiltonian. This encompasses $\tilde{h}^{(p)}(E)$. Indeed, the resolvent $\tilde{G}^{(p)}(z)$ as given by (4.94a) is of the form (4.121a), except at the isolated energy $E=-\mathscr{E}_0^{(A)}-i\eta$. In general, the modified Hamiltonians $\hat{h}^{(p)}$ will not have simple mathematical properties, unless additional conditions are imposed on $\hat{C}^{(p)}(z)$. This will be discussed in Section 5.7, in a broader context.

4.19. *Overview*

We have constructed and investigated various particle one-body Hamiltonians which all enable one to evaluate the single-particle properties of the $(A+1)$-system, i.e., those observables which can in principle be measured by means of stripping or elastic scattering reactions. We combined techniques and concepts of Feshbach's and Green's function theories. We identified the optical-model wave function with the elastic overlap $|\chi_E^{0(+)}\rangle$, for reasons given in Section 4.15.

We studied four main types of particle Hamiltonians, namely: (i) The particle Hamiltonian proper $\tilde{h}^{(p)}(E)$ (Sections 4.3–4.13); (ii) Feshbach's Hamiltonian $h_{\mathscr{F}}^{(p)}(E)$ (Section 4.14); (iii) Kerman's Hamiltonian $h_{\mathscr{K}}^{(p)}(E)$ (Section 4.16); (iv) a new particle-type Hamiltonian $\tilde{h}^{(p)}$ (Section 4.17).

All these operators were required to yield information on the following main observables: (a) the bound overlaps $|\chi_\lambda^{(+)}\rangle$, which are the projections of the bound levels $|\Psi_\lambda^{(+)}\rangle$ of the $(A+1)$-system on the ground state $|\Psi_0^{(A)}\rangle$; (b) the spectroscopic factors $\mathscr{S}_\lambda^{(+)}$ of these bound levels; (c) the elastic overlap $\chi_E^{0(+)}\rangle$; (d) the particle spectral function, which measures the amount of single-particle strength per unit energy interval in the $(A+1)$-system.

Let us generically denote these particle Hamiltonians by $h_{\mathscr{R}}^{(p)}(E)$. They are all nonlocal, energy-dependent and complex. They are analytic in the complex E-plane, except for poles located on the real axis and for a right-hand cut. This cut runs along the real axis and extends from the inelastic threshold $T_{\text{in}}^{(+)}$ up to $+\infty$. The particle Hamiltonians thus fulfill similar dispersion relations. In the case of Feshbach's Hamiltonian, this dispersion relation connects quantities which are not symmetric in the coordinate space representation. In contrast, the real and imaginary parts of $h^{(p)}(E)$, $h_{\mathscr{K}}^{(p)}(E)$ and $\tilde{h}^{(p)}$ are symmetric in that representation.

The particle Green's function is the resolvent of $h^{(p)}(E)$. It is intimately connected to the particle spectral function. The latter can readily be calculated from $h^{(p)}(E)$, $h_{\mathscr{F}}^{(p)}(E)$, $h_{\mathscr{K}}^{(p)}(E)$, and $\tilde{h}^{(p)}(E)$. In the latter case, however, one must leave out a spurious contribution to the spectral function, located at the large positive energy $E=-\mathscr{E}_0^{(A)}$, where $\mathscr{E}_0^{(A)}$ is the energy of the target ground state.

In Section 4.18, we pointed out that there exist many Hamiltonians, besides $h^{(p)}(E)$ and $\tilde{h}^{(p)}(E)$, which also have the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$ as eigenstates and, moreover, enable one to calculate the particle spectral function. We shall return to this freedom in Section 5.7.

5. HOLE, PARTICLE, AND TIME-ORDERED GREEN'S FUNCTION

In the Green's function theory of the optical-model potential developed by Bell and Squires [4] and others [46, 52, 53], this potential is identified with the "mass operator" $M(E)$. The latter is defined in terms of the "time-ordered" Green's function. The main purpose of the present section is to exhibit the relationship between these quantities and those that we studied in Sections 3 and 4. While the hole and

the particle Hamiltonians yield information on the single-particle properties of, respectively, the $(A-1)$- and $(A+1)$-systems, $M(E)$ contains information on both systems. More specifically, the one-body Hamiltonian $h(E)=T+M(E)$ has the overlaps $|\chi_\lambda^{(-)}\rangle$, $|\chi_\lambda^{(+)}\rangle$, and $|\chi_E^{0(+)}\rangle$ as eigenstates. In Section 5.7, we shall show that other Hamiltonians exist which share this property.

The single-particle energies provide a common energy scale for the $(A-1)$- and $(A+1)$-systems. It is convenient to define the "Fermi energy" as follows:

$$E_F=\tfrac{1}{2}\,(\mathscr{E}_0^{(A+1)}-\mathscr{E}_0^{(-1)}=\tfrac{1}{2}\,(E_0^{(-)}+E_0^{(+)}). \tag{5.1}$$

In keeping with (3.1a) and (4.2a), the single-particle energy E is related to the eigenvalues $\mathscr{E}^{(\pm)}$ of the Hamiltonians $H^{(A\pm1)}$ by

$$\begin{aligned} E&=\mathscr{E}_0^{(A)}-\mathscr{E}^{(-)} \qquad \text{if} \quad E<E_F,\\ E&=\mathscr{E}^{(+)}-\mathscr{E}_0^{(A)} \qquad \text{if} \quad E>E_F; \end{aligned} \tag{5.2}$$

see (3.1a) and (4.4a).

5.1. *Time-Ordered Green's Function and the Mass Operator*

The spectral function proper is the sum of the hole and particle spectral functions

$$S(E)=S^{(h)}(E)+S^{(p)}(E), \tag{5.3a}$$

$$\begin{aligned} S(E)&=S^{(h)}(E) \qquad \text{for} \quad E<E_F,\\ S(E)&=S^{(p)}(E) \qquad \text{for} \quad E>E_F. \end{aligned} \tag{5.3b}$$

The integral

$$G(z)=\int_{-\infty}^{\infty} dE'\,\frac{S(E')}{z-E'} \tag{5.4}$$

is analytic for all complex values of z. It has singularities on the real axis. In particular, it has a left-hand cut which runs along the real axis from $-\infty$ to $T_0^{(-)}$ and a right-hand cut which extends from 0 to $+\infty$. One has

$$\begin{aligned} S(E)&=(2i\pi)^{-1}\,[\,G(E-i\eta)-G(E+i\eta)\,]\\ &=(2i\pi)^{-1}\,[\,G^{\dagger}(E+i\eta)-G(E+i\eta). \end{aligned} \tag{5.5}$$

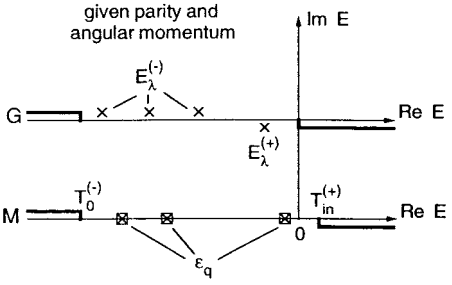

FIG. 3. Sketch of the analytic properties of the time-ordered Green's function and of the mass operator in the complex energy plane. The thick lines represent branch cuts. The crosses correspond to poles "on" the real axis. For given angular momentum and parity, only very few such poles exist.

In the second equality, we took into account that $G(z)$ is hermitian-analytic; see (5.40) below. For E real, the time-ordered (or "causal") Green's function $G(E)$ is obtained by taking the following limits:

$$\begin{aligned} G(E) &= G(E - i\eta) \qquad \text{when} \quad E < E_F, \\ G(E) &= G(E + i\eta) \qquad \text{when} \quad E > E_F. \end{aligned} \tag{5.6}$$

This amounts to drawing branch cuts as depicted in Fig. 3. The time-ordered Green's function is thus the sum of the hole and particle Green's functions:

$$G(E) = G^{(h)}(E) + G^{(p)}(E). \tag{5.7}$$

For z complex, the quantity $G(z)$ is the resolvent of an operator $h(z)$:

$$h(z) = z - [\,G(z)\,]^{-1}, \tag{5.8}$$

$$[\,z - h(z)\,]\,G(z) = 1. \tag{5.9}$$

For E real, we define $h(E)$ by taking limits similar to (5.6):

$$\begin{aligned} h(E) &= h(E - i\eta) \qquad \text{when} \quad E < E_F, \\ h(E) &= h(E + i\eta) \qquad \text{when} \quad E > E_F. \end{aligned} \tag{5.10}$$

We write "the one-body Hamiltonian" $h(E)$ as the sum of the kinetic energy operator T and of a potential-type operator:

$$h(E) = T + M(E). \tag{5.11}$$

The quantity $M(E)$ is called the mass operator (or "self energy"). It is, in general, complex:

$$M(E) = V(E) + iW(E). \tag{5.12}$$

The operators studied in Sections 3 and 4 were defined on Hilbert spaces $\mathscr{H}^{(1)}_{(\neq 0)}$ or $\mathscr{H}^{(1)}_{(\neq 1)}$, respectively. This was due to the fact that $G^{(h)}(z)$ and $G^{(p)}(z)$ yield zero when they act on natural orbitals whose occupation probability is equal to zero or unity, respectively. No similar restriction has to be imposed in the case of $G(z)$, because it does not annihilate any particular natural orbital. Therefore, in general there exists no limitation on the existence of $[G(z)]^{-1}$.

5.2. *Discrete and Continuum Eigenstates of the One-Body Hamiltonian*

5.2.1. *Spectroscopic Factors*

According to (3.5b) and (4.9d), the time-ordered Green's function is the sum of discrete and continuum contributions:

$$G(E) = G_{dt}(E) + G_{ct}(E), \tag{5.13a}$$

$$G_{dt}(E) = \sum_{\lambda} \frac{|\chi_\lambda^{(-)}\rangle\langle\chi_\lambda^{(-)}|}{E - E_\lambda^{(-)} - i\eta} + \sum_{\lambda} \frac{|\chi_\lambda^{(+)}\rangle\langle\chi_\lambda^{(+)}|}{E - E_\lambda^{(+)} + i\eta}, \tag{5.13b}$$

$$G_{ct}(E) = \sum_{c} \int_{-\infty}^{T_c^{(-)}} dE' \frac{|\chi_{E'}^{c(-)}\rangle\langle\chi_{E'}^{c(-)}|}{E - E' - i\eta} + \sum_{c} \int_{T_c^{(+)}}^{\infty} dE' \frac{|\chi_{E'}^{c(+)}\rangle\langle\chi_{E'}^{c(+)}|}{E - E' + i\eta}. \tag{5.14}$$

In the vicinity of a real pole $E_\lambda^{(\pm)}$ of $G(E)$, one can write

$$\begin{aligned} M(E) &\approx M(E_\lambda^{(\pm)}) + (E - E_\lambda^{(+)}) \left[\frac{d}{dE} M(E) \right]_{E - E_\lambda^{(\pm)}}, \\ G(E) &\approx \mathscr{S}_\lambda^{(\pm)} \frac{|\lambda^{(\pm)}\rangle\langle\lambda^{(\pm)}|}{E - E_\lambda^{(\pm)}}, \end{aligned} \tag{5.15}$$

where $\mathscr{S}_\lambda^{(\pm)}$ is the spectroscopic factor of the bound state $|\Psi_\lambda^{(\pm)}\rangle$. By inserting (5.15) in (5.9), one finds that

$$\{T + M(E_\lambda^{(\pm)})\}\ |\chi_\lambda^{(\pm)}\rangle = E_\lambda^{(\pm)}\ |\chi_\lambda^{(\pm)}\rangle, \tag{5.16}$$

$$\mathscr{S}_\lambda^{(\pm)} = \left[1 - \langle \lambda^{(\pm)}|\ \frac{d}{dE} h(E)\ |\lambda^{(\pm)}\rangle \right]^{-1}_{E - E_\lambda^{(\pm)}}. \tag{5.17}$$

Hence, $h(E)$ has as bound eigenstates the overlaps associated with the bound levels $|\Psi_\lambda^{(\pm)}\rangle$,and this enables one to calculate the spectroscopic factors of these levels.

5.2.2. *Elastic Overlap*

In (4.20), we defined the elastic overlap as

$$\langle \mathbf{r}\,|\,\chi_{\mathbf{k}}^{0(+)}(\mathbf{r})\rangle = \chi_{\mathbf{k}}^{0(+)}(\mathbf{r}) = \langle \Psi_0^{(A)}|\ a_{\mathbf{r}}\ |\Psi_{\mathbf{k}}^{0(+)}\rangle. \tag{5.18}$$

Equations (4.16d) and (4.24a) show that

$$|\chi_{\mathbf{k}}^{0(+)}\rangle = i\eta G^{(p)}(E_k + i\eta)\,|\mathbf{k}\rangle, \tag{5.19}$$

where $E_k = k^2/2m$ is the kinetic energy of the incoming plane wave $|\mathbf{k}\rangle$. Since $G^{(h)}(z)$ is analytic in the neighborhood of the positive real axis, it belongs to the $\hat{C}^{(p)}(z)$ class defined in Section 4.18. Therefore, one can replace $G^{(p)}(E_k + i\eta)$ by $G(E_k + i\eta)$ in (5.19). This yields

$$|\chi_{\mathbf{k}}^{0(+)}\rangle = i\eta G(E_k + i\eta)\,|\mathbf{k}\rangle. \tag{5.20}$$

By following the same reasoning as in (4.23a)–(4.23c), one finds that (5.20) is equivalent to the Lippmann–Schwinger equation

$$\langle \mathbf{k}'\,|\,\chi_{\mathbf{k}}^{0(+)}\rangle = \langle \mathbf{k}'\,|\,\mathbf{k}\rangle + \langle \mathbf{k}'|\,\frac{1}{E_k - E_{k'} + i\eta}\,M(E_k)\,|\chi_{\mathbf{k}}^{0(+)}\rangle, \tag{5.21a}$$

$$= \langle \mathbf{k}'\,|\,\mathbf{k}\rangle + \langle \mathbf{k}'|\,\{E_k - T - M(E_k) + i\eta\}^{-1}\,M(E_k)\,|\mathbf{k}\rangle, \tag{5.21b}$$

which itself amounts to the Schrödinger equation

$$h(E_k)\,|\chi_{\mathbf{k}}^{0(+)}\rangle = E_k\,|\chi_{\mathbf{k}}^{0(+)}\rangle. \tag{5.21c}$$

Hence, the elastic overlap is an eigenstate of the one-body Hamiltonian $h(E)$. This property was first proved by Bell and Squires [4] and Namiki [52], in the framework of time-dependent scattering theory. Our proof has the merit of readily leading to the observation that there exist many other Hamiltonians which also have the elastic overlap as eigenstate. This will be discussed in Section 5.7.

5.2.3. *Transition Matrix*

The "half-on-shell" elements of the transition matrix $\boldsymbol{t}$ are given by

$$\langle \mathbf{k}'\,|\,\chi_{\mathbf{k}}^{0(+)}\rangle = \delta(\mathbf{k}' - \mathbf{k}) + \frac{\langle \mathbf{k}'|\,\boldsymbol{t}(E_k)\,|\mathbf{k}\rangle}{E_k - E_{k'} + i\eta}. \tag{5.22}$$

By comparing this with the Lippmann–Schwinger equation (5.21a), one gets

$$\langle \mathbf{k}'|\,\boldsymbol{t}(E_k)\,|\mathbf{k}\rangle = \langle \mathbf{k}'|\,M(E_k)\,|\chi_{\mathbf{k}}^{0(+)}\rangle. \tag{5.23a}$$

This result is equivalent to Eq. (16) of [54] and to Eq. (3.68) of [55]. By using the Lippmann–Schwinger equation (5.21b) for $|\chi_{\mathbf{k}}^{0(+)}\rangle$, it can be written as

$$\langle \mathbf{k}'|\,\boldsymbol{t}(E_k)\,|\mathbf{k}\rangle = \langle \mathbf{k}'|\,\{M(E_k) + M(E_k)[E_k - T - M(E_k) + i\eta]^{-1}\,M(E_k)\}\,|\mathbf{k}\rangle. \tag{5.23b}$$

On the basis of this expression, the off-shell element of the transition matrix is usually defined as

$$\boldsymbol{t}(E) = M(E) + M(E)[E - T - M(E) + i\eta]^{-1} M(E). \tag{5.24}$$

If we had used (4.23c) instead of (5.21b), we would have been led to define another off-shell transition matrix, namely,

$$\boldsymbol{t}^{(p)}(E) = M^{(p)}(E) + M^{(p)}(E)[E - T - M^{(p)}(E) + i\eta]^{-1} M^{(p)}(E). \tag{5.25}$$

The quantities $\boldsymbol{t}(E)$ and $\boldsymbol{t}^{(p)}(E)$ have the same on-shell matrix elements

$$\langle \mathbf{k}' | \boldsymbol{t}(E_k) | \mathbf{k} \rangle = \langle \mathbf{k}' | \boldsymbol{t}^{(p)}(E_k) | \mathbf{k} \rangle, \tag{5.26}$$

but they have different analytical properties in the complex E-plane.

The transition matrix can be expressed directly in terms of the time-ordered Green's function (Eq. (3.66) of [55], Eq. (14.119) of [11], or Eq. (8) of [56]). We now give a simple derivation of this property. According to (5.21b), (5.21c), and (5.23a), one can write successively

$$\langle \mathbf{k}' | \boldsymbol{t}(E_k) | \mathbf{k} \rangle = \langle \mathbf{k}' | (E_k - T)[1 + G(E_k) M(E_k)] | \mathbf{k} \rangle \tag{5.27a}$$

$$= \lim_{E \to E_k} \langle \mathbf{k}' | (E - T)[1 + G(E) M(E)] | \mathbf{k} \rangle. \tag{5.27b}$$

For E positive, $G(E)$ is the solution of the Lippmann–Schwinger equation

$$G(E) = g_0^{(+)}(E) + G(E) M(E) g_0^{(+)}(E), \tag{5.28a}$$

where $g_0^{(+)}$ is defined by (4.54a). We multiply (5.28a) by $(E - T)$ on the left- and right-hand sides:

$$(E - T) G(E)(E - T) = (E - T)[1 + G(E) M(E)]. \tag{5.28b}$$

By inserting this identity in (5.27b), one finds the announced result,

$$\langle \mathbf{k}' | \boldsymbol{t}(E_k) | \mathbf{k} \rangle = \lim_{E \to E_k} \lim_{E \to E_{k'}} (E - E_k)(E - E_{k'}) \langle \mathbf{k}' | G(E) | \mathbf{k} \rangle. \tag{5.29}$$

5.3. *High Energy Limit or "Static Part" of the Mass Operator*

The behaviour of $G(E)$ at large E is given by the sum of (3.31a) and (4.44a),

$$G(E) \sim E^{-1}(1 + E^{-1}R), \tag{5.30}$$

where, in some $\{\alpha\}$ representation, the hermitian and energy-independent operator R is given by

$$R_{\alpha\alpha'} = R^{(h)}_{\alpha\alpha'} + R^{(p)}_{\alpha\alpha'} = \langle \Psi_0^{(A)} | \{[a_\alpha, H], a^\dagger_{\alpha'}\} | \Psi_0^{(A)} \rangle. \tag{5.31}$$

Since $G(z)$ behaves as z^{-1} at large z, its integral over a large closed circle in the complex z-plane is equal to

$$(2i\pi)^{-1}\int_{\text{circle}} dz\, G(z) = 1. \tag{5.32}$$

By indenting the contour along the real axis, one finds that

$$(2i\pi)^{-1}\int_{-\infty}^{\infty} dE[\,G(E-i\eta) - G(E+i\eta)\,] = 1. \tag{5.33}$$

According to (5.3a), this amounts to the sum rule (2.6b), namely,

$$\int_{-\infty}^{\infty} dE[\,S^{(h)}(E) + S^{(p)}(E) = \int dE\, S(E) = 1. \tag{5.34}$$

Equations (5.8) and (5.30) show that, at large E,

$$h(E) \sim R. \tag{5.35}$$

If one writes the full many-body Hamiltonian as the sum $H = \mathscr{T} + \mathscr{V}$ of kinetic and interaction contributions as in (3.41a), one readily finds that

$$R = T + V^{(S)}, \tag{5.36}$$

where the real and hermitian operator

$$V^{(S)}_{\alpha\alpha'} = \mathscr{V}^{(h)}_{\alpha\alpha'} + \mathscr{V}^{(p)}_{\alpha\alpha'} = \langle\, \Psi^{(A)}_0 |\, \{[\,a_\alpha,\, \mathscr{V}\,],\, a^\dagger_{\alpha'}\}\, |\Psi^{(A)}_0\rangle \tag{5.37}$$

is the high-energy limit of $M(E)$. This result is compatible with (3.41b)–(3.41d) and (4.42d). Since $V^{(S)}$ is independent of energy, its Fourier transform is a delta-function in time; $V^{(S)}$ is thus the "static" part of the mass operator. In the case of two-body interactions, a closed form of R can readily be obtained from (5.36),

$$V^{(S)}_{\alpha\alpha'} = \sum_{\beta,\,\beta'} \langle \alpha\beta |\, v\, |\alpha'\beta' - \beta'\alpha'\rangle\, K_{\beta\beta'} = \sum_{\beta\beta'} \langle \alpha\beta |\, v\, |\alpha'\beta'\rangle_a\, K_{\beta\beta'}, \tag{5.38}$$

where v is the two-body interaction and the index a denotes an antisymmetrized ket. Equation (5.38) shows that $V^{(S)}$ is the expression which would be obtained for $M(E)$ in the "frozen approximation" in which the target is assumed to remain in its ground state throughout the scattering process. In the independent particle model, the density matrix is diagonal. Then, $V^{(S)}$ reduces to the "Hartree–Fock" potential

$$V^{HF}_{\alpha\alpha'} = \sum_{\beta,\,\beta' \in F} \langle \alpha\beta |\, v\, |\alpha'\beta'\rangle_a, \tag{5.39}$$

where $\in F$ indicates that the summation runs over orbits contained in the Fermi sea. The static potential (5.38) can be viewed as an "extended" Hartree–Fock approximation, in which the correlated nature of the ground state $|\Psi_0^{(A)}\rangle$ is partly taken into account through the one-body density matrix K. It has been suggested to identify $V^{(S)}$ with the empirical mean field [57]. This is not appropriate in nuclear physics, in which $V^{(S)}$ is extremely large and repulsive because of the short-range repulsion contained in the nucleon–nucleon interaction [58, 59]. In contrast, $V^{(S)}$ can be viewed as an approximation to $M(E)$ in atomic physics [60, 61].

5.4. *Analytic Properties*

The functions $G(z)$ and $h(z)$ are analytic outside the real axis. More precisely, they are hermitian-analytic:

$$\begin{aligned} &G(E-i\eta) = G(E+i\eta)^\dagger, \\ &h(E-i\eta) = h(E+i\eta)^\dagger \qquad \text{for } E \text{ real and } \eta \neq 0. \end{aligned} \tag{5.40}$$

In particular, the real and imaginary parts of $G(E)$ and $h(E)$ are symmetric in the coordinate space representation. It is convenient to introduce the following "retarded" quantities

$$\begin{aligned} &\mathscr{G}(E) = G(E+i\eta), \\ &\mathscr{M}(E) = M(E+i\eta) \qquad \text{for } E \text{ real;} \end{aligned} \tag{5.41}$$

see, e.g., [62–64]. Differently from $G(E)$ and $M(E)$, they present the interest of being boundary values of analytic functions. Setting

$$\mathscr{M}(E) = \mathscr{V}(E) + i\mathscr{W}(E), \tag{5.42}$$

one has

$$\mathscr{V}(E) = V(E) \qquad \text{for all } E, \tag{5.43}$$

$$\begin{aligned} &\mathscr{W}(E) = -W(E) \qquad \text{for} \quad E < E_F, \\ &\mathscr{W}(E) = W(E) \qquad \text{for} \quad E > E_F. \end{aligned} \tag{5.44}$$

Since $M(z)$ is analytic in the upper half-plane and approaches $V^{(S)}$ at large z, the following dispersion relation holds:

$$\mathscr{M}(E) - V^{(S)} = (2i\pi)^{-1} \int_{-\infty}^{\infty} dE' \, \frac{\mathscr{M}(E') - V^{(S)}}{E' - E - i\eta}. \tag{5.45}$$

The mass operator may have discrete poles on the real axis. We assume that these poles ε_q lie inside the interval $(T_0^{(-)}, T_{\text{in}}^{(+)})$; see Figs. 1 and 2. Taking (5.44) into account, the real part of (5.44) yields the following dispersion relation:

$$V(E) = V^{(S)} + \sum_q \frac{|\mathscr{J}_q\rangle\langle\mathscr{J}_q|}{E-\varepsilon_q} + \left[-\frac{\mathscr{P}}{\pi}\int_{-\infty}^{T_0^{(-)}} dE' + \frac{\mathscr{P}}{\pi}\int_{T_{\text{in}}^{(+)}}^{\infty} dE' \right] \frac{W(E')}{E'-E}. \tag{5.46}$$

5.5. *Spectral Function*

According to (5.5) and (5.9), the spectral function can be written as

$$S(E) = (2i\pi)^{-1} \{ [E - h^\dagger(E+i\eta) - i\eta]^{-1} - [E - h(E+i\eta) + i\eta]^{-1} \}. \tag{5.47a}$$

By using

$$\mathscr{W}(E) = (2i)^{-1} [h(E+i\eta) - h^\dagger(E+i\eta)], \tag{5.47b}$$

one finds

$$S(E) = S_\eta(E) + S_{\mathscr{W}}(E), \tag{5.48a}$$

$$S_\eta(E) = \mathscr{G}(E) \frac{\eta}{\pi} \mathscr{G}(E)^\dagger, \tag{5.48b}$$

$$S_{\mathscr{W}}(E) = -\frac{1}{\pi} \mathscr{G}(E)\, \mathscr{W}(E)\, \mathscr{G}(E)^\dagger. \tag{5.48c}$$

The hole Green's function $G^{(h)}(E)$ is regular for $E > E_{\text{F}}$, while the particle Green's function $G^{(p)}(E)$ is regular for $E < E_{\text{F}}$. Therefore, (5.48b) can be replaced by

$$S_\eta(E) = G^{(h)}(E) \frac{\eta}{\pi} G^{(h)}(E)^\dagger \qquad \text{for} \quad E < E_{\text{F}}, \tag{5.49a}$$

$$S_\eta(E) = G^{(p)}(E) \frac{\eta}{\pi} G^{(p)}(E)^\dagger \qquad \text{for} \quad E > E_{\text{F}}. \tag{5.49b}$$

By comparing (5.49a) with (3.10b) and (3.57c), one gets

$$S_\eta(E) = S_{dt}^{(h)}(E) = \sum_\lambda \mathscr{S}_\lambda^{(-)} |\chi_\lambda^{(+)}\rangle\langle\chi_\lambda^{(-)}|\, \delta(E - E_\lambda^{(-)}) \qquad \text{for} \quad E < E_{\text{F}}. \tag{5.50a}$$

Likewise, (5.49b), (4.50b), and (4.57) show that

$$\begin{aligned} S_\eta(E) &= S_{\text{de}}^{(p)}(E) \\ &= \sum_\lambda |\chi_\lambda^{(+)}\rangle\langle\chi_\lambda^{(+)}|\, \delta(E - E_\lambda^{(+)}) + S_{\text{el}}(E) \qquad \text{for} \quad E > E_{\text{F}}, \end{aligned} \tag{5.50b}$$

where $S_{\text{el}}(E)$ is the elastic scattering contribution (4.56b).

According to (5.3a),

$$S(E) = S^{(h)}(E) \qquad \text{for} \quad E < E_{\mathrm{F}}, \tag{5.51a}$$

$$S(E) = S^{(p)}(E) \qquad \text{for} \quad E > E_{\mathrm{F}}. \tag{5.51b}$$

Therefore, (5.50a), (5.51a), and (3.10a) entail that

$$S_{\mathscr{W}}(E) = S^{(h)}_{ct}(E) = \sum_{c} |\chi_E^{c(-)}\rangle\langle\chi_E^{c(-)}| \qquad \text{for} \quad E < E_{\mathrm{F}}, \tag{5.52}$$

while (5.50b), (5.51b), (4.50a), and (4.59b) yield

$$S_{\mathscr{W}}(E) = S^{(p)}_{\mathrm{in}}(E) = \sum_{c(t \neq 0)} |\chi_E^{c(+)}\rangle\langle\chi_E^{c(+)}| \qquad \text{for} \quad E > E_{\mathrm{F}}. \tag{5.53}$$

These results show that $S_{\mathscr{W}}(E)$ is a non-negative operator. Therefore, (5.48c) implies that $\mathscr{W}(E)$ is a non-positive operator. More precisely, one has

$$\mathscr{W}_{\alpha\alpha}(E) = -W_{\alpha\alpha}(E) < 0 \qquad \text{for} \quad E < T_0^{(-)}, \tag{5.54a}$$

$$\mathscr{W}_{\alpha\alpha}(E) = W_{\alpha\alpha}(E) = 0 \qquad \text{for} \quad T_0^{(-)} < E < T_{\mathrm{in}}^{(+)}, \tag{5.54b}$$

$$\mathscr{W}_{\alpha\alpha}(E) = W_{\alpha\alpha}(E) < 0 \qquad \text{for} \quad E > T_{\mathrm{in}}^{(+)}. \tag{5.54c}$$

5.6. *Dyson's Equation*

In coordinate space, (5.9) reads

$$\left(E + \frac{1}{2m}\nabla_{\mathbf{r}}^2\right) G(\mathbf{r}, \mathbf{r}'; E) = \delta(\mathbf{r} - \mathbf{r}') + \int d\mathbf{r}''\, M(\mathbf{r}, \mathbf{r}''; E)\, G(\mathbf{r}, \mathbf{r}''; E), \tag{5.55}$$

Since the vacuum is translationally invariant, all the quantities which appear in (5.55) depend only on coordinate differences. This symmetry is of little practical interest, because it is extremely difficult to isolate the center-of-mass coordinate [47]. In practice, one thus breaks translational symmetry by introducing an external potential U. The latter is called a "localizing" potential because it enables one to localize the target; see, e.g., [46, 65]. This leads to approximation schemes in which the recoil of the target is neglected. It appears that one does not know how to properly handle the center-of-mass motion in the case of the time-ordered Green's function; the existing methods apply to the particle Green's function [56, 66].

One thus usually writes the full Hamiltonian (3.41a) as

$$H = (\mathscr{T} + U) + (\mathscr{V} - U) = H_U + (\mathscr{V} - U), \tag{5.56}$$

where H_U is the independent particle Hamiltonian (3.33a). Here, all the operators should be understood as expressed in the second quantization formalism. Equation (5.55) becomes

$$(E-T-U)\,G(E)=1+[\,M(E)-U\,]\,G(E). \tag{5.57}$$

It is fulfilled by the solution of "Dyson's equation"

$$G(E)=G_U(E)+G_U(E)[\,M(E)-U\,]\,G(E), \tag{5.58}$$

where $G_U(E)$ is the time-ordered Green's function associated with the independent particle model; see (3.34a) and (4.46a):

$$G_U(E)=\sum_{\alpha\in F}\frac{|\varphi_\alpha\rangle\langle\varphi_\alpha|}{E-e(\alpha)-i\eta}+\sum_{\alpha\notin F}\frac{|\varphi_\alpha\rangle\langle\varphi_\alpha|}{E-e(\alpha)+i\eta}+\int_0^\infty dE'\,\frac{|\varphi_{E'}\rangle\langle\varphi_{E'}|}{E-E'+i\eta}. \tag{5.59}$$

In a "normal" system, (5.58) can be solved by iteration, at least formally. This leads to an expansion of the mass operator $M(E)$ in powers of the strength of the nucleon–nucleon interaction. Each term of this perturbation series can be represented by a "linked" diagram, whence the expression linked-cluster expansion; see, e.g., [12, 64, 67]. An algebraic form of the linked-cluster expansion of $M(E)$ is given on page 330 of [55]. We return to this point in Section 6.

5.7. *A Wider Class of Mass Operator-type Potentials*

5.7.1. *Sufficient Conditions*

Let $\hat{C}(z)$ be an operator which, as a function of z, is analytic in a domain which contains the whole real axis. If the "modified" Green's function

$$\hat{G}(z)=G(z)+\hat{C}(z) \tag{5.60a}$$

has an inverse, the operator

$$\hat{h}(z)=z-[\,\hat{G}(z)\,]^{-1} \tag{5.60b}$$

exists. We shall now prove that the Hamiltonian

$$\hat{h}(E)=E-[\,\hat{G}(E+i\eta)\,]^{-1} \tag{5.60c}$$

has the overlaps $|\chi_\lambda^{(-)}\rangle$, $|\chi_\lambda^{(+)}\rangle$, and $|\chi_E^{0(+)}\rangle$ as eigenstates and that it also enables one to calculate the spectral function $S(E)$. Since $\hat{C}(z)$ is analytic in the neighborhood of the real axis, the strong limit

$$\hat{C}(E)=\operatorname*{st.lim}_{z\to E}\hat{C}(z) \tag{5.61a}$$

exists. This implies that $\|\hat{C}(E \pm i\eta)\,|\psi\rangle\|$ tends to a finite limit when $\eta \to +0$ for any normalizable $|\psi\rangle$ and that

$$\lim_{\eta \to +0} i\eta \hat{C}(E+i\eta)\,|\mathbf{k}\rangle = 0, \qquad \lim_{E \to E_\lambda^{(\pm)}} (E - E_\lambda^{(\pm)})\,\hat{C}(E) = 0. \tag{5.61b}$$

From (5.15) and (5.20), it follows that

$$\hat{h}(E_\lambda^{(\pm)})\,|\chi_\lambda^{(\pm)}\rangle = E_\lambda^{(\pm)}\,|\chi_\lambda^{(\pm)}\rangle, \qquad \hat{h}(E)\,|\chi_E^{0(+)}\rangle = E\,|\chi_E^{0(+)}\rangle, \tag{5.62}$$

as we claimed. The spectroscopic factors are given by

$$\mathscr{I}_\lambda^{(\pm)} = \left[\, 1 - \langle \lambda^{(\pm)}|\, \frac{d}{dE}\, \hat{h}(E)\,|\lambda^{(\pm)}\rangle \,\right]^{-1}_{E = E_\lambda^{(\pm)}}. \tag{5.63}$$

The spectral function can be written as

$$S(E) = (2i\pi)^{-1}\,[\,\hat{G}(E - i\eta) - \hat{G}(E + i\eta)\,], \tag{5.64a}$$

where $\hat{G}(z)$ need not be hermitian-analytic. Equation (5.64a) can be cast in the form

$$S(E) = \hat{G}(E+i\eta)\,\frac{\eta}{\pi}\,\hat{G}(E-i\eta) + \frac{1}{\pi}\,\hat{G}(E+i\eta)\;\hat{W}(E)\;\hat{G}(E-i\eta), \tag{5.64b}$$

where

$$\hat{W}(E) = (2i)^{-1}\,[\,\hat{h}(E+i\eta) - \hat{h}(E-i\eta)\,]. \tag{5.65}$$

Using (5.60a), the first term on the right-hand side of (5.64b) is equal to

$$\begin{aligned} &G(E+i\eta)\,\frac{\eta}{\pi}\,G(E-i\eta) + G(E+i\eta)\,\frac{\eta}{\pi}\,\hat{C}(E-i\eta) \\ &\quad + \hat{C}(E+i\eta)\,\frac{\eta}{\pi}\,G(E-i\eta) + \hat{C}(E+i\eta)\,\frac{\eta}{\pi}\,\hat{C}(E-i\eta). \end{aligned} \tag{5.66a}$$

According to (5.61a), the last term of this expression vanishes, because of (5.61a). Equations (11.5)–(11.6) of [35] show that, on its branch cuts, $\|G(E \pm i\eta)\,|\psi\rangle\|$ diverges as $\eta^{-1/2}$. Therefore, the second and third terms of (5.66a) vanish on these branch cuts. Outside the cuts, they differ from zero only at $E = E_\lambda^{(\pm)} \pm i\eta$, where their limit is finite. Since the set $E_\lambda^{(\pm)}$ has measure zero, these finite contributions to (5.66a) are rigorously negligible. We conclude that (5.66a) reduces to its first term. The latter is identical to the "discrete + elastic" part of the spectral function; see (5.48a)–(5.50b):

$$\hat{G}(E+i\eta)\frac{\eta}{\pi}\hat{G}(E-i\eta)=G(E+i\eta)\frac{\eta}{\pi}G(E-i\eta)=S_{\mathrm{de}}(E) \qquad \text{for} \quad E>E_0^{(-)}, \tag{5.66b}$$

$$\hat{G}(E+i\eta)\frac{\eta}{\pi}\hat{G}(E-i\eta)=G(E+i\eta)\frac{\eta}{\pi}G(E-i\eta)=0 \qquad \text{for} \quad E<E_0^{(-)}. \tag{5.66c}$$

This implies that the second term on the right-hand side of (5.64b) is equal to the inelastic part of the particle spectral function for $E>T_{\mathrm{in}}^{(+)}$ and to the continuous part of the hole spectral function for $E<T_0^{(-)}$:

$$\frac{1}{\pi}\hat{G}(E+i\eta)\,\hat{W}(E)\,\hat{G}(E-i\eta)=S_{\mathrm{in}}^{(p)}(E) \qquad \text{for} \quad E>T_{\mathrm{in}}^{(+)}, \tag{5.67a}$$

$$\frac{1}{\pi}\hat{G}(E+i\eta)\,\hat{W}(E)\,\hat{G}(E-i\eta)=S_{ct}^{(h)}(E) \qquad \text{for} \quad E<T_0^{(-)}. \tag{5.67b}$$

5.7.2. *Useful Additional Requirements*

The mathematical structure of $\hat{h}(E)$ will be quite complicated unless one imposes additional conditions on $\hat{C}(z)$:

(a) In order to be able to construct the "local equivalent" of $\hat{h}(E)$, it is necessary that its coordinate space representation $\hat{h}(\mathbf{r},\mathbf{r}';E)$ be symmetric in $\mathbf{r}$ and $\mathbf{r}'$. This requires that

$$\hat{C}(\mathbf{r},\mathbf{r}';z)=\hat{C}(\mathbf{r}',\mathbf{r};z). \tag{5.68}$$

(b) It is desirable that $\hat{h}(E)$ be hermitian for values of E located outside the branch cuts of $G(z)$. This will be the case if $\hat{C}(E)$ is required to be hermitian in that energy domain:

$$\hat{C}(\mathbf{r},\mathbf{r}';E)^*=\hat{C}(\mathbf{r}',\mathbf{r};E) \qquad \text{for} \quad T_0^{(-)}<E<0. \tag{5.69}$$

(c) If (5.68) and (5.69) both hold,

$$\hat{C}(E) \qquad \text{is real for} \quad T_0^{(-)}<E<0. \tag{5.70}$$

Actually, $\hat{C}(E)$ is real for all real values of E even if (5.69) is imposed only outside the branch cuts of $G(z)$. Indeed, $\hat{C}(z^*)^*$ defines a continuation of $\hat{C}(z)$; the equality of these two quantities on a finite domain of the real axis is sufficient to render them equal for all values of z located in the domain of analyticity of $\hat{C}(z)$, in particular on the whole real axis. Hence, if (5.68) and (5.69) hold, $\hat{C}(E)$ is hermitian and real for all E:

$$\hat{C}(\mathbf{r},\mathbf{r}';E)^*=\hat{C}(\mathbf{r}',\mathbf{r};E) \qquad \text{for all real } E. \tag{5.71a}$$

In its domain of analyticity, $\hat{C}(z)$ is hermitian-analytic if (5.68) and (5.69) both hold:

$$\hat{C}(\mathbf{r}, \mathbf{r}'; z)^* = \hat{C}(\mathbf{r}, \mathbf{r}'; z^*) = \hat{C}(\mathbf{r}', \mathbf{r}; z^*). \tag{5.71b}$$

(d) Causality arguments make it desirable that $\hat{h}(z)$ be analytic in the upper-half plane [6, 68], so that its real and imaginary parts fulfill a dispersion relation. This suggests choosing

$$\hat{C}(z) \qquad \text{analytic for} \quad \text{lm } z > -\eta. \tag{5.72}$$

(e) If (5.68), (5.69), and (5.72) are all required,

$$\hat{C}(z) \qquad \text{is entire.} \tag{5.73}$$

Then, the integral of $\hat{C}(z)$ over a closed contour vanishes. In particular, it vanishes over a large closed circle even if $\hat{C}(z)$ does not tend to zero when $z \to \infty$.

(f) one wants to behave as $\hat{G}(z) \sim z^{-1}$ at large z, like $G(z)$, one must require that

$$\hat{C}(z) = O(z^{-2}) \qquad \text{at large } z. \tag{5.74a}$$

If this condition is added to (5.73), no freedom is left, since

$$\hat{C}(z) = 0. \tag{5.74b}$$

In that sense, it appears that the time-ordered Green's function $G(z)$ is the simplest among the $\hat{G}(z)$ family.

(g) Instead of (5.74a), one could only impose the less stringent condition

$$\hat{C}(E) \sim O(E^{-2}) \qquad \text{at large real } E. \tag{5.75}$$

Then, $\hat{C}(z)$ can be different from zero, but remains entire.

5.7.3. *Less Stringent Requirements*

In Section 5.7.1, we required $\hat{C}(z)$ to be analytic in the neighborhood of the whole real axis, because we wanted (5.64a) to give the spectral function for all energies. A less stringent requirement would enlarge the freedom on the choice of $\hat{C}(z)$.

Suppose, for instance, that one wants to construct "particle-like" Hamiltonians which have the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$ (but not $|\chi_\lambda^{(-)}\rangle$ as eigenstates. Let $\bar{C}^{(p)}(z)$ be an operator which, as a function of z, is analytic in a domain which contains the real energies $E \geqslant E_0^{(+)}$. If the modified Green's function

$$\bar{G}^{(p)}(z) = G(z) + \bar{C}^{(p)}(z) \tag{5.76}$$

as an inverse, then

$$\bar{h}^{(p)}(E) = E - [\,\bar{G}^{(p)}(E+i\eta)\,]^{-1} \tag{5.77}$$

has the overlaps $|\chi_\lambda^{(+)}\rangle$ and $|\chi_E^{0(+)}\rangle$ as eigenstates:

$$\bar{h}^{(p)}(E_\lambda^{(+)})\,|\chi_\lambda^{(+)}\rangle = E_\lambda^{(+)}\,|\chi_\lambda^{(+)}\rangle, \qquad \bar{h}^{(p)}(E)\,|\chi_E^{0(+)}\rangle = E\,|\chi_E^{0(+)}\rangle. \tag{5.78}$$

The spectroscopic factor is given by

$$\mathscr{S}_\lambda^{(+)} = \left[\,1 - \langle\lambda^{(+)}|\,\frac{d}{dE}\,\bar{h}^{(p)}(E)\,|\lambda^{(+)}\rangle\,\right]^{-1}_{E=E_\lambda^{(+)}}. \tag{5.79}$$

The particle spectral function reads

$$S^{(p)}(E) = (2i\pi)^{-1}\,[\,\bar{G}^{(p)}(E-i\eta) - \bar{G}^{(p)}(E+i\eta)\,] \qquad \text{for} \quad E \geqslant E_0^{(+)}. \tag{5.80a}$$

Its discrete + elastic and inelastic parts are given by

$$S_{\text{de}}^{(p)}(E) = \bar{G}^{(p)}(E+i\eta)\,\frac{\eta}{\pi}\,\bar{G}^{(p)}(E-i\eta) \qquad \text{for} \quad E \geqslant E_0^{(+)}, \tag{5.80b}$$

$$S_{\text{in}}^{(p)}(E) = \frac{1}{\pi}\,\bar{G}^{(p)}(E+i\eta)\;\bar{W}^{(p)}(E)\;\bar{G}^{(p)}(E-i\eta) \qquad \text{for} \quad E > T_{\text{in}}^{(+)}, \tag{5.80c}$$

where

$$\bar{W}^{(p)}(E) = (2i)^{-1}\,[\,\bar{h}^{(p)}(E+i\eta) - \bar{h}^{(p)}(E-i\eta)\,]. \tag{5.80d}$$

As in Section 5.7.2, additional requirements can be imposed on $\bar{C}^{(p)}(z)$ if one wants $\bar{h}^{(p)}(z)$ to have simple mathematical properties. In particular, it appears natural to choose $\bar{C}^{(p)}(z)$ in such a way that it is symmetric in the coordinate space representation,

$$\bar{C}^{(p)}(\mathbf{r}, \mathbf{r}'; z) = \bar{C}^{(p)}(\mathbf{r}', \mathbf{r}; z), \tag{5.81}$$

and that $\bar{C}^{(p)}(E)$ is hermitian for $0 > E \geqslant E_0^{(+)}$:

$$\bar{C}^{(p)}(\mathbf{r}, \mathbf{r}'; E)^* = \bar{C}^{(p)}(\mathbf{r}', \mathbf{r}; E) \qquad \text{for} \quad 0 > E \geqslant E_0^{(+)}. \tag{5.82}$$

Then, $\bar{C}^{(p)}(E)$ is real for $0 > E \geqslant E_0^{(+)}$.

The main difference between $\hat{C}(z)$ and $\bar{C}^{(p)}(z)$ is that the latter is not required to be analytic in a domain which contains the real energies $E < E_0^{(+)}$. In particular, one could choose

$$\bar{C}^{(p)}(z) = G^{(h)}(z), \tag{5.83a}$$

where $G^{(h)}(z)$ is the hole Green's function. For that particular choice,

$$\bar{G}(E+i\eta) = G^{(p)}(E+i\eta) \qquad \text{for} \quad E \geqslant E_0^{(+)}, \tag{5.83b}$$

$$\bar{h}(E) = h^{(p)}(E) \qquad \text{for} \quad E \geqslant E_0^{(+)}. \tag{5.83c}$$

Basically, the freedom that we just described is equivalent to the one that we pointed out in Section 4.18. Likewise, one can recover in the present context the freedom that we exhibited in Section 3.15 in the case of Hamiltonians required to yield the hole spectral function $S^{(h)}(E)$.

5.8. *Overview*

The time-ordered Green's function $G(E)$ is the sum of the hole Green's function $G^{(h)}(E)$ and of the particle Green's function $G^{(p)}(E)$. It is related to the mass operator $M(E)$ by Dyson's equation. The one-body Hamiltonian $h(E) = T + M(E)$ has as bound eigenstates the overlaps $|\chi_\lambda^{(\pm)}\rangle$ associated with the bound levels $|\Psi_\lambda^{(A\pm1)}\rangle$ of the $(A+1)$- and the $(A-1)$-systems. It also enables one to calculate the corresponding spectroscopic factors. Moreover, at positive energy its eigenstate is the elastic scattering overlap $|\chi_E^{0(+)}\rangle$. These properties make one expect that the mass operator is closely related to both the shell- and optical-model potentials.

We showed in Section 5.7 that, besides $h(E)$, many Hamiltonians $\hat{h}(E)$ exist which also have the overlaps $|\chi_\lambda^{(+)}\rangle$, $|\chi_\lambda^{(-)}\rangle$, and $|\chi_E^{0(+)}\rangle$ as eigenstates. They, moreover, enable one to calculate the spectral function at all energies. Among these many equivalent Hamiltonians, the one-body Hamiltonian $h(E) = T + M(E)$ has the important advantage that one knows the expansion of $M(E)$ in powers of the strength of the nucleon–nucleon interaction. This linked-cluster expansion leads to practical approximation schemes [69–71].

6. NUCLEAR MATTER

In the present section, we derive explicit expressions for the hole, particle, and time-ordered Green's function and related quantities, in the case of nuclear matter and in the framework of perturbation theory. Because of translational and rotational invariance, all equations are much simpler in nuclear matter than in a finite system. In momentum space, the relevant quantities are diagonal in $\mathbf{k}$ and only depend upon the modulus $k = |\mathbf{k}|$. For instance,

$$\langle \mathbf{k}|\ G(E)\ |\mathbf{k}'\rangle = G(k; E)\,\delta(\mathbf{k}-\mathbf{k}'), \tag{6.1}$$

where $G(k; E)$ is the Fourier transform of

$$\langle \mathbf{r}|\ G(E)\ |\mathbf{r}'\rangle = G(\mathbf{r}, \mathbf{r}'; E) \tag{6.2}$$

over $\mathbf{s} = \mathbf{r} - \mathbf{r}'$. Hence, the dependence upon k of $G(k; E)$ reflects the spatial nonlocality of the Green's function. The same interpretation holds for related quantities. For convenience, we shall retain an upper index (A) when referring to the ground state of nuclear matter, even though A is infinite.

6.1. *Green's Functions and Mass Operators in Nuclear Matter*

In the independent particle model, the energy of a nucleon with momentum k is equal to

$$e(k) = \frac{k^2}{2m} + U(k). \tag{6.3}$$

The corresponding "unperturbed" ground state wave function $|\Phi_U^{(A)}\rangle$ is a Slater determinant built with plane waves with momentum smaller than the "Fermi momentum" k_{F}. The time-ordered Green's function (5.59) reduces to

$$G_U(k; E) = \frac{\Theta(k_{\mathrm{F}} - k)}{E - e(k) - i\eta} + \frac{\Theta(k - k_{\mathrm{F}})}{E - e(k) + i\eta} = G_U^{(h)}(k; E) + G_U^{(p)}(k; E). \tag{6.4}$$

Note that

$$G_U^{(h)}(k > k_{\mathrm{F}}; E) = 0, \qquad G_U^{(p)}(k < k_{\mathrm{F}}; E) = 0. \tag{6.5a}$$

Hence, $G_U^{(h)}(k; E)$ has no inverse for $k > k_{\mathrm{F}}$, while $G_U^{(p)}(k; E)$ has no inverse for $k < k_{\mathrm{F}}$. In contrast, the inverse of $G_U(k; E)$ exists for all values of k:

$$[\, G_U(k; E)\,]^{-1} = E - e(k). \tag{6.5b}$$

Dyson's equation (5.58) reads

$$G(k; E) = G_U(k; E) + G_U(k; E)[\, M(k; E) - U(k)\,]\, G(k; E). \tag{6.6}$$

The mass operator is given by

$$M(k; E) = V(k; E) + iW(k; E) = E - k^2/2m - [\, G(k; E)\,]^{-1} \tag{6.7}$$

which amounts to (5.8). The spectral function is equal to

$$S(k; E) = \pm\frac{1}{\pi}\frac{W(k; E)}{[\, E - k^2/2m - V(k; e)\,]^2 + [\, W(k; E)\,]^2}, \tag{6.8}$$

where the $+$ sign should be taken for $E < E_{\mathrm{F}}$ and the $-$ sign for $E > E_{\mathrm{F}}$. The Fermi energy E_{F} is the root of

$$E_{\mathrm{F}} = k_{\mathrm{F}}^2/2m + V(k_{\mathrm{F}}; E_{\mathrm{F}}). \tag{6.9}$$

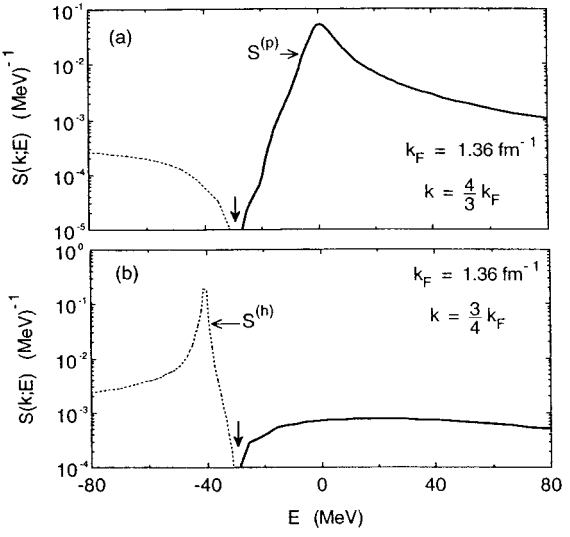

FIG. 4. Adapted from [58]. Dependence upon E of the particle spectral function $S^{(p)}(k; E)$ (solid curves) and of the hole spectral function $S^{(h)}(k; E)$ (dashed curves) spectral functions in nuclear matter, as evaluated in the framework of Brueckner's theory for the momenta $k = \frac{4}{3}k_F$, and $k = \frac{3}{4}k_F$. The vertical arrows point to the Fermi momentum $k_F = 1.36\ \text{fm}^{-1}$.

It is real since, near the Fermi energy, $W(k; E)$ vanishes like

$$W(k; E) \sim \pm c_k^2 (E - E_F)^2. \tag{6.10}$$

The spectral function has a peak centered near the "quasi-particle energy" $E_{qp}(k)$, that we define as the root of

$$E_{qp}(k) = \frac{k^2}{2m} + V(k; E_{qp}(k)). \tag{6.11}$$

This equation has the form of an energy-momentum relation. This is why one identifies $V(k; E_{qp}(k))$ with potential energy of a nucleon with momentum k. As illustrated in Fig. 4, in all realistic cases one has

$$E_{qp}(k) < E_F \quad \text{for } k < k_F, \qquad E_{qp}(k) > E_F \quad \text{for } k > k_F. \tag{6.12}$$

6.2. *Second-Order Approximation to the Mass Operator*

The mass operator can be expanded in powers of the strength of the interaction. We now discuss the second-order approximation. Below, each summation will run over all the numbered momenta. We adopt the convention [72]

$$h_1, h_2, \ldots < k_F, \qquad p_1, p_2, \ldots > k_F, \tag{6.13}$$

where h and p refer to hole and particle, respectively. Up to second order,

$$M(k; E) = M_1(k) + M_{2(+)}(k; E) + M_{2(-)}(k; E), \tag{6.14}$$

where the index refers to the order of the contribution. The first-order contribution is the Hartree–Fock potential. It is real:

$$M_1(k) = V_1(k) = \sum \langle \mathbf{k}\mathbf{h}_1 | \, v \, | \mathbf{k}\mathbf{h}_1 \rangle_a. \tag{6.15}$$

As in (5.38), the index a denotes an antisymmetrized ket. There exist two second-order contributions; they read

$$\begin{aligned} M_{2(+)}(k; E) &= V_{2(+)}(k; E) + iW_{2(+)}(k; E) \\ &= \frac{1}{2} \sum \frac{|\langle \mathbf{k}\mathbf{h}_1 | \, v \, | \mathbf{p}_2 \mathbf{p}_1 \rangle_a|^2}{E + e(h_1) - e(p_1) - e(p_2) + i\eta}, \end{aligned} \tag{6.16a}$$

$$\begin{aligned} M_{2(-)}(k; E) &= V_{2(-)}(k; E) + iW_{2(-)}(k; E) \\ &= \frac{1}{2} \sum \frac{|\langle \mathbf{k}\mathbf{p}_1 | \, v \, | \mathbf{h}_2 \mathbf{h}_1 \rangle_a|^2}{E + e(p_1) - e(h_1) - e(h_2) - i\eta}. \end{aligned} \tag{6.16b}$$

Equations (6.15)–(6.16b) retain the same form when one performs Brueckner-type rearrangements of the perturbation expansion [73, 74]. The nucleon–nucleon interaction v is then replaced by Brueckner's reaction matrix, and $M_1(k)$ is called the "Brueckner–Hartree–Fock potential." Much of our discussion remains valid in that case.

In second-order perturbation theory, the external potential is often chosen in such a way that

$$U(k) \approx M_1(k). \tag{6.17a}$$

Then, the potential energy of a nucleon with momentum k can be approximated by $V(k; e(k))$, since

$$V(k; E_{\mathrm{qp}}(k)) \approx V(k; e(k)). \tag{6.17b}$$

In view of (6.17a), we shall treat a term which is of first order in U on the same level as a term which is of first order in the strength of the nucleon–nucleon interaction. In second order, (6.11) reads

$$E_{\mathrm{qp}}(k) = \frac{k^2}{2m} + V_1(k) + V_{2(+)}(k; e(k)) + V_{2(-)}(k; e(k)). \tag{6.18a}$$

The "quasi-particle strength" is the integral strength of the quasi-particle peak of the spectral function over energy. It is given by

$$Z_{\rm qp}(k) = 1 + \left\{ \frac{d}{dE} [\, V_{2(+)}(k; E) + V_{2(-)}(k; E)] \right\}_{E = e(k)} . \tag{6.18b}$$

It plays the role of a spectroscopic factor; see (5.17).

6.3. *Goldstone's Theorem*

Goldstone's theorem enables one to write a "linked-cluster expansion" for the expectation value of an operator $\mathcal{O}$ with respect to the correlated ground state. For our present purpose, it is sufficient to express it in the following schematic form:

$$\langle \Psi_0^{(A)} | \, \mathcal{O} \, | \Psi_0^{(A)} \rangle = \langle \Phi_U^{(A)} | \sum_{s=0}^{\infty} [(\mathcal{V} - U)(\mathcal{E}_U^{(A)} - H_U)^{-1}]^s$$

$$\times \mathcal{O} \sum_{q=0}^{\infty} [(\mathcal{E}_U^{(A)} - H_U)^{-1} (\mathcal{V} - U)]^q \, | \Phi_U^{(A)} \rangle_{\mathcal{L}} . \tag{6.19a}$$

The index $\mathcal{L}$ means that the right-hand side only contains terms which can be represented by linked diagrams [75, 76]. The quantity $\mathcal{E}_U^{(A)}$ denotes the ground state energy in the independent particle approximation:

$$H_U^{(A)} \, | \Phi_U^{(A)} \rangle = \mathcal{E}_U^{(A)} \, | \Phi_U^{(A)} \rangle . \tag{6.19b}$$

6.4. *Density Matrix*

The momentum distribution $K(k)$ in the correlated ground state of nuclear matter is defined by

$$\langle \Psi_0^{(A)} | \, a_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}} \, | \Psi_0^{(A)} \rangle = K(k) \, \delta(\mathbf{k} - \mathbf{k}') . \tag{6.20}$$

One can use (6.19a) to derive its perturbation expansion [72]. The zero-order contribution results from setting $s = q = 0$,

$$K_0(k) = \Theta(k_{\rm F} - k), \tag{6.21a}$$

which is the momentum distribution of a free Fermi gas. Because of momentum conservation, there exists no first-order contribution to $K(k)$. The second-order contribution reads,

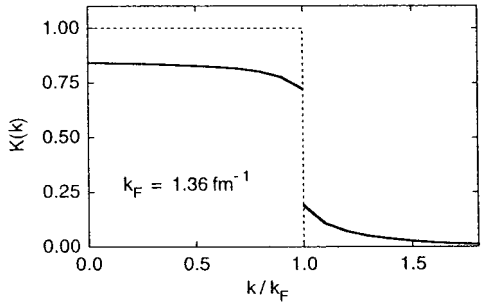

FIG. 5. Adapted from [18]. The solid curve represents the momentum distribution in nuclear matter, as evaluated from Brueckner's theory, for $k_F = 1.36\,\mathrm{fm}^{-1}$. The dashed line shows the momentum distribution of a free Fermi gas.

$$K_2(k) = -\frac{1}{2}\sum \frac{|\langle \mathbf{k}\mathbf{h}_1 |\, v\, |\mathbf{p}_2\mathbf{p}_1\rangle_a|^2}{[e(k)+e(h_1)-e(p_1)-e(p_2)]^2} \qquad \text{for} \quad k<k_F, \tag{6.21b}$$

$$K_2(k) = \frac{1}{2}\sum \frac{|\langle \mathbf{k}\mathbf{p}_1 |\, v\, |\mathbf{h}_2\mathbf{h}_1\rangle_a|^2}{[e(k)+e(p_1)-e(h_1)-e(h_2)]^2} \qquad \text{for} \quad k>k_F. \tag{6.21c}$$

Figure 5 shows a typical example. The discontinuity at $k=k_F$ persists to all orders.

6.5. *Second-Order Approximation to the Particle Mass Operator for $k>k_F$*

According to (4.33), the particle Hamiltonian $h^{(p)}(E)$ has the form

$$h^{(p)}(k;E) = -\frac{K(k)}{1-K(k)}\,E + [1-K(k)]^{-2}\,R^{(p)}(k) + [1-K(k)]^{-2}\,D^{(p)}(k;E). \tag{6.22}$$

It is not a continuous function of k, since $K(k)$ has a discontinuity at $k=k_F$. In contrast, $h^{(p)}(k;E)$ is a continuous function of E. The energy-independent quantity $R^{(p)}(k)$ is given by (4.42c) and (4.42d),

$$R^{(p)}(k) = \frac{k^2}{2m}[1-K(k)] + \mathscr{V}^{(p)}(k), \tag{6.23}$$

with

$$\mathscr{V}^{(p)}(k) = \mathscr{V}_\alpha^{(p)}(k) - \mathscr{V}_\beta^{(p)}(k), \tag{6.24a}$$

$$\mathscr{V}_\alpha^{(p)}(k)\,\delta(\mathbf{k}-\mathbf{k}') = \langle \Psi_0^{(A)} |\, a_{\mathbf{k}}\,\mathscr{V}\,a_{\mathbf{k}'}^\dagger\,|\Psi_0^{(A)}\rangle, \tag{6.24b}$$

$$\mathscr{V}_\beta^{(p)}(k)\,\delta(\mathbf{k}-\mathbf{k}') = \langle \Psi_0^{(A)} |\, \mathscr{V}\,a_{\mathbf{k}}\,a_{\mathbf{k}'}^\dagger\,|\Psi_0^{(A)}\rangle. \tag{6.24c}$$

Goldstone's theorem (6.19a) yields, up to second order,

$$\mathscr{V}_{\alpha}^{(p)}(k) = \Theta(k-k_{\mathrm{F}})[\,V_1(k) + 2V_{2(-)}(k; e(k))\,], \tag{6.25a}$$

$$\mathscr{V}_{\beta}^{(p)}(k) = \Theta(k-k_{\mathrm{F}})\; V_{2(-)}(k; e(k)) + \Theta(k_{\mathrm{F}}-k)\; V_{2(+)}(k; e(k)). \tag{6.25b}$$

Note that $\mathscr{V}^{(p)}(k)$ also has a discontinuity at $k = k_{\mathrm{F}}$. For $k > k_{\mathrm{F}}$, the factor $[\,1-K(k)\,]^{-1}$ which appears in the second factor of (6.22) can be replaced by $[\,1+K_2(k)\,]$. Instead, $[\,1-K(k)\,]^{-1} \approx [\,-K_2(k)\,]^{-1}$ is the inverse of a second-order quantity for $k < k_{\mathrm{F}}$. Thus, the second term of (6.22) reads

$$[\,1-K(k)\,]^{-2}\, R^{(p)}(k) \approx V_1(k) + V_{2(-)}(k; e(k)) \qquad \text{for} \quad k > k_{\mathrm{F}}, \tag{6.26a}$$

$$[\,1-K(k)\,]^{-2}\, R^{(p)}(k) \approx [\,K_2(k)\,]^{-2}\; V_{2(+)}(k; e(k)) \qquad \text{for} \quad k < k_{\mathrm{F}}. \tag{6.26b}$$

Let λ denote the strength of the nucleon–nucleon interaction. The quantity (6.26a) is a sum of terms of first and second order in λ. Instead, (6.26b) diverges in the weak coupling limit. Indeed, $V_{2(+)}(k; e(k))$ is of order λ^2, but $[\,K_2(k)\,]^{-2}$ is of order λ^{-4}. We shall discuss this type of divergence in Section 5.7.6.

In the remainder of the present section, we only consider the case $k > k_{\mathrm{F}}$. Since $K(k > k_{\mathrm{F}})$ is of second order, one may write (6.22) in the form

$$h^{(p)}(k > k_{\mathrm{F}}; E) = \frac{k^2}{2m} - \left[\, E - \frac{k^2}{2m} \right] K_2(k) + V_1(k) + V_{2(-)}(k; e(k)) + D^{(p)}(k; E). \tag{6.27a}$$

In lowest order,

$$D^{(p)}(k > k_{\mathrm{F}}; E)\, \delta(\mathbf{k}-\mathbf{k}') = \langle \Phi_U^{(A)} |\, a_{\mathbf{k}}\, \mathscr{V}\, Q_0^{(p)} (E - Q_0^{(p)} H_U^{(A+1)} Q_0^{(p)} + \mathscr{E}_U^{(A)} + i\eta)^{-1}\; Q_0^{(p)}\, \mathscr{V}\, a_{\mathbf{k}'}^{\dagger}\, | \Phi_U^{(A)} \rangle, \tag{6.27b}$$

where $Q_0^{(p)}$ projects on intermediate two particle-one hole excitations. Equation (6.27b) yields

$$D^{(p)}(k > k_{\mathrm{F}}; E) = M_{2(+)}(k > k_{\mathrm{F}}; E). \tag{6.27c}$$

Gathering these results, one finds that, up to second order and for $k > k_{\mathrm{F}}$, the particle mass operator is given by

$$M^{(p)}(k > k_{\mathrm{F}}; E) = -\left(E - \frac{k^2}{2m} \right) K_2(k) + V_1(k) + V_{2(-)}(k; e(k)) + M_{2(+)}(k; E). \tag{6.28a}$$

In keeping with (4.44c), it behaves as

$$M^{(p)}(k > k_F; E) \sim -EK_2(k > k_F) \tag{6.28b}$$

at high energy.

In the case $k < k_F$, it appears quite difficult to find the expression of $h^{(p)}(k; E)$ by means of the projection operator approach. Likewise, it seems quite difficult to use that approach to develop a systematic perturbation expansion. Thus, we shall calculate $h^{(p)}(k; E)$ from a "pure" Green's function method in the next section.

For all values of k, the particle spectral function is given by the identity

$$S^{(p)}(k; E) = -\frac{1}{\pi} \frac{W^{(p)}(k; E)}{[E - k^2/2m - V^{(p)}(k; E)]^2 + [W^{(p)}(k; E)]^2}. \tag{6.29a}$$

It vanishes for $E < E_F$. The identity

$$S^{(p)}(k; E) = S(k; E) \qquad \text{for} \quad E > E_F \tag{6.29b}$$

holds for all k, where $S(k; E)$ is given by (6.8). For k somewhat larger than k_F, the particle spectral function has a narrow peak near the quasi-particle energy. In conjunction with (6.29a), this peak energy is found to be the root of

$$E_{qp}^{(p)}(k) = \frac{k^2}{2m} + V^{(p)}(k; E_{qp}^{(p)}(k)); \tag{6.29c}$$

compare with (6.11).

Since the existence of that peak is at the origin of the success of the empirical optical model, we now exhibit that the identity (6.29b) is fulfilled near the peak energy. Equations (6.11) and (6.29c) both yield the same quasi-particle energy, namely,

$$E_{qp}(k > k_F) = E_{qp}^{(p)}(k > k_F) = \frac{k^2}{2m} + V_1(k) + V_{2(+)}(k; e(k)) + V_{2(+)}(k; e(k)). \tag{6.30}$$

According to (6.29a), the quasi-particle strength is equal to

$$Z_{qp}^{(p)}(k > k_F) = 1 + \left[\frac{d}{dE} M^{(p)}(k; E)\right]_{E = e(k)} = 1 - K_2(k) + \left[\frac{d}{dE} V_{2(+)}(k; E)\right]_{E = e(k)}. \tag{6.31a}$$

Equations (6.16b) and (6.21c) show that

$$K_2(k > k_F) = -\left[\frac{d}{dE} V_{2(-)}(k; E)\right]_{E = e(k)}. \tag{6.31b}$$

Therefore, (6.31a) is equal to the second-order approximation to (6.18b), namely to

$$Z_{\mathrm{qp}}(k) = 1 + \frac{d}{dE}\,[\,V_{2(-)}(k;E) + V_{2(+)}(k;E)\,]_{E=e(k)}\,, \tag{6.31c}$$

which completes our demonstration.

Equations (4.70c) and (4.66c) show that Feshbach's and Kerman's particle potentials are equal to one another in the case of nuclear matter. The case $k < k_{\mathrm{F}}$ will be discussed in the next section. For $k > k_{\mathrm{F}}$, one has

$$M^{(p)}_{\mathscr{F}}(k > k_{\mathrm{F}};E) = M^{(p)}_{\mathscr{K}}(k > k_{\mathrm{F}};E) = V_1(k) + V_{2(-)}(k;e(k)) + M_{2(+)}(k;E). \tag{6.32a}$$

For $k > k_{\mathrm{F}}$ and in second order, Feshbach's potential is thus obtained from the mass operator (6.14) by setting $E = e(k)$ in the contribution $M_{2(-)}(k;E)$. This type of simple recipe no longer holds true in higher order, or for $k < k_{\mathrm{F}}$. In keeping with (4.69c), one has, up to second order,

$$[\,1 - K_2(k)\,]\left[\,1 + \frac{d}{dE}\,V^{(p)}_{\mathscr{F}}(k;E)\right]_{E=e(k)} \approx \left[\,1 + \frac{d}{dE}\,V^{(p)}(k;E)\right]_{E=e(k)} \qquad \text{for} \quad k > k_{\mathrm{F}}\,. \tag{6.32b}$$

6.6. *Second-Order Approximation to the Particle Green's Function*

The problem of finding the particle mass operator $M^{(p)}(k;E)$ amounts to that of calculating the particle Green's function, since

$$M^{(p)}(k;E) = E - \frac{k^2}{2m} - [\,G^{(p)}(k;E)\,]^{-1}. \tag{6.33}$$

Two main methods exist for evaluating the particle Green's function.

(a) The first one consists in using the following linked-cluster expansion [56]:

$$\begin{aligned} G^{(p)}_{\mathbf{k}\mathbf{k}'}(E) = \sum_{s,q,t} \langle \Phi^{(A)}_U |\, [\,(\mathscr{V} - U)(\mathscr{E}^{(A)}_U - H^{(A)}_U)^{-1}\,]^s\, a_{\mathbf{k}}(E + \mathscr{E}^{(A)}_U - H^{(A+1)}_U + i\eta)^{-1} \\ \times [\,(\mathscr{V} - U)(E + \mathscr{E}^{(A)}_U - H^{(A+1)}_U + i\eta)^{-1}\,]^q \\ \times a^{\dagger}_{\mathbf{k}'}[\,(\mathscr{E}^{(A)}_U - H^{(A)}_U)^{-1}\,(\mathscr{V} - U)\,]^t\, |\Phi^{(A)}_U\rangle_{\mathscr{L}}. \end{aligned} \tag{6.34a}$$

This formula can be obtained by inserting

$$\mathscr{O} = a_{\mathbf{k}}[\,E + \mathscr{E}^{(A)}_0 - H^{(A+1)}_U - (\mathscr{V} - U) + i\eta\,]^{-1}\, a^{\dagger}_{\mathbf{k}'} \tag{6.34b}$$

in (6.19a), and by expanding the right-hand side of (6.34b) in powers of $(\mathscr{V} - U)$; the elimination of the unlinked clusters leads to the replacement of $\mathscr{E}^{(A)}_0$ by $\mathscr{E}^{(A)}_U$.

(b) The second method [5] consists in using the identity

$$G^{(p)}(E) = -\frac{1}{2i\pi}\int dE' \frac{G(E')}{E - E' + i\eta}. \tag{6.35}$$

The rules for constructing the second-order approximation to the time-ordered Green's function $G(k; E)$ are known; see, e.g., [12, 67]. The particle Green's function $G^{(p)}(k; E)$ can thus be obtained by means of (6.35), and then by using the particle mass operator from (6.33).

These two methods enable one to calculate $G^{(p)}(k; E)$ to all orders, for $k < k_F$ as well as for $k > k_F$. In the case $k > k_F$ and in second order, the particle Green's function $G^{(p)}(k; E)$ is the sum of six contributions. The first one is of order zero and reads

$$G_U^{(p)}(k > k_F; E) = [E - e(k) + i\eta]^{-1}. \tag{6.36a}$$

It corresponds to setting $(s, q, t) = (0, 0, 0)$ in (6.34a). The other five contributions to $G^{(p)}(k > k_F; E)$ are of first and second order. They can be obtained by setting $(s, q, t) = (0, 1, 0)$, $(0, 2, 0)$, $(0, 1, 1)$, $(1, 1, 0)$, and $(1, 0, 1)$ in (6.34a). Once $G^{(p)}(k > k_F; E)$ is known, $M^{(p)}(k > k_F; E)$ can be calculated from (6.33). This method reproduces (6.28a), as it should [5].

In the case $k < k_F$, one finds that $G^{(p)}(k < k_F; E)$ has no zero- or first-order contribution. This is in keeping with (6.5a). The leading term of the expansion of $G^{(p)}(k < k_F; E)$ is thus of second order. It can, for instance, be obtained by setting $(s, q, t) = (1, 0, 1)$ in (6.34a):

$$G_2^{(p)}(k < k_F; E) = \frac{1}{2}\sum \frac{|\langle \mathbf{p}_2\, \mathbf{p}_1 |\, v\, |\mathbf{k}\mathbf{h}_1\rangle_a|^2}{[E + e(h_1) - e(p_1) - e(p_2) + i\eta][e(k) + e(h_1) - e(p_1) - e(p_2)]^2}. \tag{6.36b}$$

This expression is in keeping with the high energy behaviour (4.44a), since

$$G^{(p)}(k < k_F; E) \sim -E^{-1}K_2(k < k_F). \tag{6.36c}$$

Equation (6.36b) shows that the inverse of $G_2^{(p)}(k < k_F; E)$ diverges as $1/\lambda^2$ when the strength λ of the interaction approaches zero. This is in keeping with (6.5a). According to (6.33), the quantity $M^{(p)}(k < k_F; E)$ also diverges like $1/\lambda^2$ in the weak coupling limit. We now argue that this divergence does not reflect any physical difficulty.

We recall that it is only for $E > E_F$ that $M^{(p)}(k; E)$ is meaningful and that it is only $V^{(p)}(k > k_F; E_{qp}(k))$ which has the physical meaning of a potential energy. According to (6.12), the quasiparticle energy $E_{qp}(k)$ is smaller than E_F for $k < k_F$.

Thus, $M^{(p)}(k<k_F; E>E_F)$ cannot be interpreted in terms of a potential energy to be introduced in a one-body wave equation.

In this domain ($k<k_F$ and $E>E_F$), the quantity of physical interest is the particle spectral function. The latter corresponds to adding one nucleon with momentum $k<k_F$ to the ground state; this is possible since momentum states $k<k_F$ are partly empty in the correlated ground state. In (6.8), the particle spectral function is expressed in terms of the mass operator $M(k; E)$, while in (6.29a) it is expressed in terms of the particle mass operator $M^{(p)}(k; E)$. In the weak coupling limit, expression (6.8) vanishes like λ^2 for all values of k since $M(k; E)$ correspondingly vanishes. In contrast, $M^{(p)}(k<k_F; E)$ diverges as λ^{-2} in the weak coupling limit. In view of this formal similarity between (6.8) and (6.29a), it may seem surprising that the vanishing of the particle spectral function in the weak coupling limit corresponds to two opposite asymptotic behaviours of $M(k; E)$ and $M^{(p)}(k; E)$, respectively. We now show that, actually, this feature is a natural consequence of the relations which connect $G^{(p)}(k; E)$ to the quantities $V^{(p)}(k; E)$, $W^{(p)}(k; E)$, and $S^{(p)}(k; E)$. According to (6.33),

$$V^{(p)}(k; E) = E - \frac{k^2}{2m} - \frac{\text{Re } G^{(p)}(k; E)}{|G^{(p)}(k; E)|^2}, \tag{6.37a}$$

$$W^{(p)}(k; E) = \frac{\text{Im } G^{(p)}(k; E)}{|G^{(p)}(k; E)|^2}. \tag{6.37b}$$

The divergence of $M^{(p)}(k<k_F; E)$ in the weak coupling limit is due to the fact that $G^{(p)}(k; E)$ is of order λ^2 while $|G^{(p)}(k; E)|^2$ is of order λ^4. Nevertheless, by substituting (6.37a) and (6.37b) in (6.29a) one recovers the identity

$$\text{Im } G^{(p)}(k; E) = -\pi S^{(p)}(k; E), \tag{6.38}$$

as it should be. The fact that $G^{(p)}(k<k_F; E)$ vanishes like λ^2 is thus the common origin of the divergence of $M^{(p)}(k<k_F; E)$ and of the vanishing of the particle spectral function in the weak coupling limit.

6.7. *Momentum Dependence of the Particle Green's Function*

As a function of k, the particle mass operator $M^{(p)}(k; E)$ has a discontinuity at $k=k_F$. This is illustrated by the appearance of the discontinuous function $K(k)$ in the expression (6.22) of the particle Hamiltonian. Equation (6.33) then implies that $G^{(p)}(k; E)$ also has a discontinuity at $k=k_F$. However, its imaginary part is a continuous function of k. Indeed, according to (6.38), this imaginary part is proportional to the particle spectral function, which is continuous. We conclude that it is the real part of $G^{(p)}(k; E)$ which is discontinuous at $k=k_F$.

At first sight, the fact that $\mathrm{Im}\, G^{(p)}(k; E)$ is continuous and $\mathrm{Re}\, G^{(p)}(k; E)$ is discontinuous appears to be at variance with the dispersion relation

$$\mathrm{Re}\, G^{(p)}(k; E) = \frac{\mathscr{P}}{\pi} \int_{E_F}^{\infty} dE' \, \frac{\mathrm{Im}\, G^{(p)}(k; E')}{E' - E}, \tag{6.39}$$

which derives from the analyticity of $G^{(p)}(k; z)$ in the upper half of the complex z-plane. Actually, no disagreement exists. Indeed, the integral which appears on the right-hand side of (6.39) is a discontinuous function of k even though its integrand is continuous. This is illustrated by the following identity (see (4.44e))

$$\int_{E_F}^{\infty} dE \, \mathrm{Im}\, G^{(p)}(k; E) = \pi[\, K(k) - 1\,], \tag{6.40}$$

which exhibits that the integral of $\mathrm{Im}\, G^{(p)}(k; E)$ is discontinuous at $k = k_F$, although $\mathrm{Im}\, G^{(p)}(k; E)$ is a continuous function of k.

6.8. *Second-Order Approximation to the Hole Mass Operator for $k < k_F$*

According to (3.27b), the hole Hamiltonian can be written in the form

$$h^{(h)}(k; E) = E - E[\, K(k)\,]^{-1} + [\, K(k)\,]^{-2} \, R^{(h)}(k) + [\, K(k)\,]^2 \, D^{(h)}(k; E). \tag{6.41}$$

It is not a continuous function of k since $K(k)$ has a discontinuity at $k = k_F$. In contrast, it is a continuous function of E. The energy-independent quantity $R^{(h)}(k)$ is given by (3.41c) and (3.41d),

$$R^{(h)}(k) = \frac{k^2}{2m} K(k) + \mathscr{V}^{(h)}(k), \tag{6.42a}$$

where

$$\mathscr{V}^{(h)}(k)\, \delta(\mathbf{k} - \mathbf{k}') \langle \Psi_0^{(A)} |\, a_{\mathbf{k}'}^{\dagger} [\, \mathscr{V}, a_{\mathbf{k}}\,] \,| \Psi_0^{(A)} \rangle. \tag{6.42b}$$

By applying Goldstone's theorem (6.19a) one finds that, up to second order,

$$\mathscr{V}^{(h)}(k) = V_1(k) + V_{2(+)}(k; e(k)) \qquad \text{for} \quad k < k_F, \tag{6.43a}$$

$$\mathscr{V}^{(h)}(k) = V_{2(-)}(k; e(k)) \qquad \text{for} \quad k > k_F\,. \tag{6.43b}$$

Note that $\mathscr{V}^{(h)}(k)$ is discontinuous at $k = k_F$. For $k < k_F$, the factor $[\, K(k)\,]^{-1}$ can be replaced by $[\, 1 - K_2(k)\,]$ in the second factor of (6.41). Instead, for $k > k_F$ one has $[\, K(k)\,]^{-1} \approx [\, K_2(k)\,]^{-1}$; this quantity diverges in the weak coupling limit. We return to this divergence below.

In the remainder of the present section, we only consider momenta $k < k_F$. Up to second order, one can write

$$[K(k)]^{-2}\, \mathscr{V}^{(h)}(k) = V_1(k) + V_{2(+)}(k; e(k)) \qquad \text{for} \quad k < k_F. \tag{6.43c}$$

Equation (6.41) then yields

$$M^{(h)}(k < k_F; E) = \left(E - \frac{k^2}{2m}\right) K_2(k) + V_1(k) + V_{2(+)}(k; e(k)) + D^{(h)}(k; E). \tag{6.44}$$

According to (3.26), the leading contribution to $D^{(h)}(k; E)$ is of second order for $k < k_F$. It reads

$$D^{(h)}(k < k_F; E)\, \delta(\mathbf{k} - \mathbf{k}') = \langle \Phi_U^{(A)} |\, a_{\mathbf{k}'}^\dagger \mathscr{V} Q_0^{(h)} (E + Q_0^{(h)} H_U^{(A-1)} Q_0^{(h)} - \mathscr{E}_U^{(A)} - i\eta)^{-1} \times Q_0^{(h)} \mathscr{V} a_{\mathbf{k}}\, | \Phi_U^{(A)} \rangle, \tag{6.45a}$$

where $Q_0^{(h)}$ projects on intermediate two hole-one particle excitations. Equation (6.45a) gives, in second order,

$$D^{(h)}(k < k_F; E) = M_{2(-)}(k < k_F; E). \tag{6.45b}$$

Gathering these results, one finds that, up to second order and for $k < k_F$, the hole mass operator is given by

$$M^{(h)}(k < k_F; E) = \left(E - \frac{k^2}{2m}\right) K_2(k) + V_1(k) + V_{2(+)}(k; e(k)) + M_{2(-)}(k; E). \tag{6.46}$$

In keeping with (3.31c), it behaves as

$$M^{(h)}(k < k_F; E) \sim E K_2(k) \sim E\left(1 - \frac{1}{1 + K_2(k)}\right) \tag{6.47}$$

at high energy.

It appears difficult to apply this projection operator approach to $h^{(h)}(k; E)$ in the case $k > k_F$ or to use it to develop a systematic perturbation expansion. Thus, we shall turn to a pure Green's function method in the next section.

In terms of the real and imaginary parts of the hole mass operator, the hole spectral function is given by

$$S^{(h)}(k; E) = \frac{1}{\pi} \frac{W^{(h)}(k; E)}{[E - k^2/2m - V^{(h)}(k; E)]^2 + [W^{(h)}(k; E)]^2}. \tag{6.48a}$$

It vanishes for $E > E_F$. The following identity must hold for all values of k,

$$S^{(h)}(k; E) = S(k; E) \qquad \text{for} \quad E < E_F, \tag{6.48b}$$

where $S(k; E)$ is given by (6.8). For k somewhat smaller than k_F, the hole spectral function has a narrow "quasi-hole" peak. In conjunction with (6.48a) the energy of the peak is close to the root of

$$E_{qp}^{(h)}(k) = \frac{k^2}{2m} + V^{(h)}(k; E_{qp}^{(h)}(k)); \tag{6.49a}$$

compare with (6.11).

Since the existence of that peak is at the origin of the success of the empirical shell model, we now exhibit that (6.48b) is fulfilled near the peak energy. Equations (6.11) and (6.49a) both yield the same quasi-hole energy, namely,

$$E_{qp}^{(h)}(k) = E_{qp}(k) \qquad \text{for} \quad k < k_F . \tag{6.49b}$$

The quasi-hole strength is the integral of the "quasi-hole" peak over energy. It is equal to

$$Z_{qp}^{(h)}(k < k_F) = 1 + \left[\frac{d}{dE} M^{(h)}(k; E) \right]_{E = e(k)} \tag{6.50a}$$

$$= 1 + K_2(k) + \left[\frac{d}{dE} V_{2(-)}(k; E) \right]_{E = e(k)} . \tag{6.50b}$$

In keeping with (3.55b) and (6.21b), this quantity is equal to $Z_{qp}(k < k_F)$, since

$$K_2(k < k_F) = \left[\frac{d}{dE} V_{2(+)}(k; E) \right]_{E = e(k)} . \tag{6.50c}$$

This completes our demonstration.

Equations (3.59b) and (3.67b) show that the Feshbach-type and Kerman-type hole Hamiltonians are equal to one another in the case of nuclear matter. For $k < k_F$, they read

$$M_{\mathscr{F}}^{(h)}(k < k_F; E) = M_{\mathscr{F}}^{(h)}(k < k_F; E) = V_1(k) + V_{2(+)}(k; e(k)) + M_{2(-)}(k; E). \tag{6.51}$$

In second order and for $k < k_F$, the "hole Feshbach-type" potential is thus obtained from the mass operator (6.14) by setting $E = e(k)$ in $M_{2(+)}(k; E)$. This type of simple recipe no longer holds true in higher order, or for momenta $k > k_F$. The case $k > k_F$ will be discussed in the next section. In keeping with (3.60c), one has, up to second order,

$$[1 - K_2(k)] \left[1 + \frac{d}{dE} V_{\mathscr{F}}^{(h)}(k; E) \right]_{E = e(k)} = \left[1 + \frac{d}{dE} V^{(h)}(k; E) \right]_{E = e(k)} \qquad \text{for} \quad k < k_F . \tag{6.52}$$

6.9. *Second-Order Approximation to the Hole Green's Function*

Instead of using the projection operator approach to derive an expression for the hole mass operator, one can calculate it from the hole Green's function by means of the Dyson-type equation

$$M^{(h)}(k; E) = E - \frac{k^2}{2m} - [G^{(h)}(k; E)]^{-1}. \tag{6.53}$$

Two main methods exist for evaluating the hole Green's function.

(a) The first one consists in using a linked-cluster expansion similar to (6.34a), namely,

$$\begin{aligned} G^{(h)}_{\mathbf{k}\mathbf{k}'}(E) = \sum_{s,\,q,\,t} \langle \Phi^{(A)}_U | [(\mathscr{V} - U)(\mathscr{E}^{(A)}_U - H^{(A)}_U)^{-1}]^s \, a^\dagger_{\mathbf{k}'} (E - \mathscr{E}^{(A)}_U + H^{(A-1)}_U - i\eta)^{-1} \\ \times [-(\mathscr{V} - U)(E - \mathscr{E}^{(A)}_U + H^{(A-1)}_U - i\eta)^{-1}]^q \\ \times a_{\mathbf{k}} [(\mathscr{E}^{(A)}_U - H^{(A)}_U)^{-1} (\mathscr{V} - U)]^t | \Phi^{(A)}_U \rangle_{\mathscr{L}}. \end{aligned} \tag{6.54a}$$

This expansion can be obtained by inserting

$$\mathscr{O} = a^\dagger_{\mathbf{k}'} [E - \mathscr{E}^{(A)}_0 + H^{(A-1)}_U + (\mathscr{V} - U) - i\eta]^{-1} \, a_{\mathbf{k}} \tag{6.54b}$$

in (6.19a) and by then expanding the right-hand side of (6.54b) in powers of $(\mathscr{V} - U)$; the elimination of the unlinked clusters leads to the replacement of $\mathscr{E}^{(A)}_0$ by $\mathscr{E}^{(A)}_U$.

(b) The second method consists in using the identity

$$G^{(h)}(E) = \frac{1}{2i\pi} \int dE' \, \frac{G(E')}{E - E' - i\eta}. \tag{6.55}$$

The rules for constructing the second-order approximation to the time-ordered Green's function $G(k; E)$ are known; see, e.g., [12, 67]. The hole Green's function can thus be obtained by means of (6.55) and, then, the hole mass operator from (6.53).

These two methods enable one to calculate $G^{(h)}(k; E)$ to all orders, for $k > k_F$ as well as for $k < k_F$. In the case $k < k_F$ and in second order, the hole Green's function $G^{(h)}(k < k_F; E)$ is the sum of six contributions. The zero-order term can be obtained by setting $(s, q, t) = (0, 0, 0)$ in (6.54a). It reads

$$G^{(h)}(k < k_F; E) = [E - e(k) - i\eta]^{-1}. \tag{6.56}$$

The other contributions to $G^{(h)}(k < k_F; E)$ are of first and second order. They correspond to $(s, q, t) = (0, 1, 0)$, $(0, 2, 0)$, $(0, 1, 1)$, $(1, 1, 0)$, and $(1, 0, 1)$. Once $G^{(h)}(k < k_F; E)$ is known, $M^{(h)}(k < k_F; E)$ can be calculated from (6.53). This method reproduces (6.46), as it should.

From method (a) or (b), one finds that $G^{(h)}(k > k_F; E)$ has no zero- or first-order contribution, in keeping with (6.5a). The leading term is of second order. It reads

$$G_2^{(h)}(k > k_F; E) = \frac{1}{2} \sum \frac{|\langle \mathbf{h}_2 \mathbf{h}_1 | \, v \, | \mathbf{k} \mathbf{p}_1 \rangle_a|^2}{[E + e(p_1) - e(h_1) - e(h_2) - i\eta][e(k) + e(p_1) - e(h_1) - e(h_2)]^2}. \tag{6.57}$$

This expression can for instance be obtained by setting $(s, q, t) = (1, 0, 1)$ in (6.54a). It is in keeping with the high energy behaviour (3.31a), since

$$G_2^{(h)}(k > k_F; E) \sim E^{-1} K_2(k > k_F). \tag{6.58}$$

Equation (6.57) shows that the inverse of $G_2^{(h)}(k > k_F; E)$ diverges as $1/\lambda^2$ when the strength λ of the interaction approaches zero. According to (6.53), the quantity $M^{(h)}(k > k_F; E)$ thus also diverges like $1/\lambda^2$ in the weak coupling limit. This divergence does not reflect any physical difficulty, for reasons similar to those that we described in Section 6.6 in the particle case.

6.10. *Momentum Dependence of the Hole Green's Function*

As a function of k, the hole mass operator has a discontinuity at $k = k_F$. This is illustrated by the appearance of the discontinuous function $K(k)$ in the expression (6.41) of the hole Hamiltonian. Equation (6.53) then implies that $G^{(h)}(k; E)$ also has a discontinuity at $k = k_F$. On the other hand, its imaginary part is a continuous function of k. Indeed, it is proportional to the hole spectral function, which is continuous,

$$\text{Im } G^{(h)}(k; E) = \pi S^{(h)}(k; E). \tag{6.59}$$

We conclude that it is the real part of $G^{(h)}(k; E)$ which is discontinuous at $k = k_F$.

At first sight, the fact that Im $G^{(h)}(k; E)$ is continuous and Re $G^{(h)}(k; E)$ is discontinuous appears to be at variance with the dispersion relation

$$\text{Re } G^{(h)}(k; E) = -\frac{\mathscr{P}}{\pi} \int_{-\infty}^{E_F} dE' \, \frac{\text{Im } G^{(h)}(k; E')}{E' - E}, \tag{6.60}$$

which derives from the analyticity of $G^{(h)}(k; z)$ in the lower half of the complex z-plane. Actually, no disagreement exists. Indeed, the integral which appears on the right-hand side of (6.60) is a discontinuous function of k, even though its integrand is continuous. This is illustrated by the identity (see (3.32b))

$$\int_{-\infty}^{E_F} dE \, \text{Im } G^{(h)}(k; E) = \pi K(k), \tag{6.61}$$

which shows that the integral of Im $G^{(h)}(k; E)$ is discontinuous at $k = k_F$, although Im $G^{(h)}(k; E)$ is a continuous function of k.

6.11. *Dispersion Relations*

We now adapt to nuclear matter dispersion relations which had been derived in Sections 3–5 in the case of finite systems. These relations are valid to all orders of perturbation theory and for all values of k and E.

(a) From (5.46) one readily finds that the real and imaginary parts of the mass operator are connected by

$$V(k; E) = V^{(S)}(k) + \left[-\frac{\mathscr{P}}{\pi} \int_{-\infty}^{E_F} dE' + \frac{\mathscr{P}}{\pi} \int_{E_F}^{+\infty} dE' \right] \frac{W(k; E')}{E' - E}, \tag{6.62a}$$

where the static part of the potential is

$$V^{(S)}(k) = \sum_{\mathbf{k}_1} \langle \mathbf{k}\mathbf{k}_1 | \, v \, | \mathbf{k}\mathbf{k}_1 \rangle_a \, K(k); \tag{6.62b}$$

note that the sum runs over all momenta $\mathbf{k}_1$, not only those located at the Fermi sea as in the Hartree–Fock potential (6.15).

(b) Equation (4.64g) yields

$$V^{(p)}(k; E) = -\frac{K(k)}{1 - K(k)} \left(E - \frac{k^2}{2m} \right) + [\, 1 + K(k) \,]^{-2} \, \mathscr{V}^{(p)}(k) + \frac{\mathscr{P}}{\pi} \int_{E_F}^{\infty} dE' \, \frac{W^{(p)}(k; E')}{E' - E}. \tag{6.63a}$$

where (see (6.24a))

$$\mathscr{V}^{(p)}(k) \, \delta(\mathbf{k} - \mathbf{k}') = \langle \Psi_0^{(A)} | \, [\, a_{\mathbf{k}}, \mathscr{V} \,] \, a_{\mathbf{k}'}^{\dagger} \, | \Psi_0^{(A)} \rangle. \tag{6.63b}$$

(c) Equation (3.39) becomes

$$V^{(h)}(k; E) = \frac{K(k) - 1}{K(k)} \left(E - \frac{k^2}{2m} \right) + [\, K(k) \,]^{-2} \, \mathscr{V}^{(h)}(k) - \frac{\mathscr{P}}{\pi} \int_{-\infty}^{E_F} dE' \, \frac{W^{(h)}(k; E')}{E' - E}, \tag{6.64}$$

where $\mathscr{V}^{(h)}(k)$ is defined by (6.42b).

(d) These dispersion relations take the following form in the case of Feshbach's particle and hole potentials:

$$V^{(p)}_{\mathscr{F}}(k;E)=\mathscr{V}^{(p)}(k)[1-K(k)]^{-1}+\frac{\mathscr{P}}{\pi}\int_{E_F}^{\infty}dE'\,\frac{W^{(p)}_{\mathscr{F}}(k;E')}{E'-E}, \tag{6.65a}$$

$$V^{(h)}_{\mathscr{F}}(k;E)=\mathscr{V}^{(h)}(k)[K(k)]^{-1}-\frac{\mathscr{P}}{\pi}\int_{-\infty}^{E_F}dE'\,\frac{W^{(h)}_{\mathscr{F}}(k;E')}{E'-E}. \tag{6.65b}$$

Feshbach's particle and hole Hamiltonians are related to the particle and hold spectral functions by

$$S^{(p)}(k;E)=-\frac{1}{\pi}\frac{W^{(p)}_{\mathscr{F}}(k;E)}{[E-k^2/2m-V^{(p)}_{\mathscr{F}}(k;E)]^2+[W^{(p)}_{\mathscr{F}}(k;E)]^2}[1-K(k)]$$
$$\text{for}\quad E>E_F, \tag{6.66a}$$

$$S^{(h)}(k;E)=\frac{1}{\pi}\frac{W^{(h)}_{\mathscr{F}}(k;E)}{[E-k^2/2m-V^{(h)}_{\mathscr{F}}(k;E)]^2+[W^{(h)}_{\mathscr{F}}(k;E)]^2}[K(k)]^{-1}$$
$$\text{for}\quad E<E_F; \tag{6.66b}$$

see (4.69d) and (3.60c).

6.12. *Overview*

In nuclear matter, the quantity which can be considered as an "observable" is the spectral function $S(k;E)$. Equation (6.8) expresses it in terms of the real and imaginary parts of the mass operator $M(k;E)$. The particle spectral function $S^{(p)}(k;E)$ is the value taken by $S(k;E)$ when E is larger than the Fermi energy E_F. Equations (6.29a) and (6.66a) express $S^{(p)}(k;E)$ in terms of the real and imaginary parts of the particle mass operator $M^{(p)}(k;E)$ and of Feshbach's particle potential $M^{(p)}_{\mathscr{F}}(k;E)$. Equations (6.8), (6.29a), and (6.66a) are valid for all values of k. Despite the formal similarity between these equations, the quantities $M(k;E)$, $M^{(p)}(k;E)$, and $M^{(p)}_{\mathscr{F}}(k;E)$ are quite different.

The "on-shell" value $V(k;E_{qp}(k))$ of the real part $V(k;E)$ of the mass operator can be interpreted as a potential energy for any value of k, larger or smaller than k_F. In contrast, it is only when $k>k_F$ that the particle spectral function has a peak and that the on-shell value $V^{(p)}_{\mathscr{F}}(k>k_F;E_{qp}(k))$ can be interpreted as the potential energy of a nucleon with momentum $k>k_F$. Similar comments hold for the hole mass operator $M^{(h)}(k;E)$.

We derived explicit expressions of $M(k;E)$, $M^{(p,h)}(k;E)$, and $M^{(p,h)}_{\mathscr{F}}(k;E)$ in the framework of second-order perturbation theory. For simplicity, let us only consider their real parts. That of $M(k;E)$ reads $V(k;E)=V_1(k)+V_{2(+)}(k;E)+V_{2(-)}(k;E)$, where $V_1(k)$ is the Hartree–Fock potential. For $k>k_F$ and in second order, Feshbach's particle potential is obtained by replacing E by $E_{qp}(k)$ in one of the two second-order contributions to $V(k;E)$, namely in $V_{2(-)}(k;E)$. Although this simple recipe is not valid in higher order, it illustrates that, in Feshbach's potential, part of the energy dependence of $V(k;E)$ is replaced by a momentum dependence.

As functions of k, the quantities $M^{(p)}(k; E)$, $M^{(p)}_{\mathscr{F}}(k; E)$, $M^{(h)}(k; E)$, and $M^{(h)}_{\mathscr{F}}(k; E)$ are discontinuous at $k = k_F$. In contrast, $M(k; E)$ is a continuous function of k. The k-dependence is associated to the spatial nonlocality via a Fourier transform. Hence, one expects that, in the finite case, the spatial nonlocalities of $M^{(p)}(E)$, $M^{(p)}_{\mathscr{F}}(E)$, $M^{(h)}(E)$, or $M^{(h)}_{\mathscr{F}}(E)$ are more complicated than that of the mass operator $M(E)$.

In this section, we used linked-cluster perturbation expansions of $G(k; E)$, $G^{(p)}(k; E)$, and $G^{(h)}(k; E)$ in powers of the strength of the nucleon–nucleon interaction. In finite systems too, one can expand the Green's functions $G(E)$, $G^{(p)}(E)$, and $G^{(h)}(E)$. The linked-cluster expansion of the mass operator $M(E)$ is also known. In contrast, it appears unlikely that linked-cluster expansions exist for the particle Hamiltonians $h^{(p)}(E)$ and $h^{(p)}_{\mathscr{F}}(E)$ or for the hole Hamiltonians $h^{(h)}(E)$ and $h^{(h)}_{\mathscr{F}}(E)$. Indeed, these operators involve the inverse of $G^{(p)}(E)$ or $G^{(h)}(E)$. Let us, for instance, consider $h^{(p)}(E) = E - [G^{(p)}(E)]^{-1}$. In the weak coupling limit, the matrix element $\langle \varphi_\alpha | G^{(p)}(E) | \varphi_\alpha \rangle$ approaches $\langle \varphi_\alpha | G^{(p)}_U(E) | \varphi_\alpha \rangle$. Equation (4.46a) shows that the latter quantity vanishes for single-particle states $|\varphi_\alpha\rangle$ which belong to the Fermi sea. Hence, the weak coupling limit $[G^{(p)}_U(E)]^{-1}$ of $[G^{(p)}(E)]^{-1}$ does not exist [77]. In the case of nuclear matter, this is exhibited by (6.5a) and is responsible for the fact that the particle Hamiltonian $h^{(p)}(k < k_F; E)$ diverges in the weak coupling limit.

7. SUMMARY AND DISCUSSION

Our initial motivation was to investigate whether a relationship exists between the microscopic theories of the optical-model potential which had been developed by Feshbach [3], on the one hand, and by Bell and Squires [4], on the other hand. These theories are both widely used, but their connection remains obscure because they are formulated in very different frameworks. Namely, Feshbach's approach is based on his projection operator theory of nuclear reactions [2], while Bell and Squires' approach uses Green's function theory. Moreover, the two theories lead to optical-model potentials which are basically different [6].

Our belief that a link could nevertheless be established between these two theories was mainly based on the following two main facts: (a) Feshbach's projection operator techniques have been combined with Green's function approach in a study of the spectroscopic amplitudes involved in direct nucleon removal reactions [25]. (b) It has been shown that there exist many Hamiltonians which all have the same optical-model wave function as eigenstate; one of these Hamiltonians is identical to that of Bell and Squires, while another one has properties similar to those of Feshbach's [5].

Feature (a) enticed us to first investigate single-particle quantities which are involved in nucleon removal processes. Thus, Section 3 is centered on the hole Green's function. The latter is that component of the time-ordered Green's, function which contains information on the $(A-1)$-nucleon system which is excited when one nucleon is taken away from the target ground state, for instance by

means of knockout or pickup processes. We study this hole Green's function by means of a combination of projection operator and Green's function techniques. In Section 4, we use similar methods to investigate the particle Green's function. The latter is that component of the time-ordered Green's function which contains information on the $(A+1)$-nucleon system which is excited when one nucleon is added to the target ground state, for instance by means of elastic scattering or stripping processes. Section 4 is self-contained. Its presentation partly paraphrases that of Section 3, in order to better exhibit the similarities and differences between the theoretical descriptions of the $(A-1)$- and $(A+1)$-systems. One of the outcomes of Section 4 is that there exists a family of equivalent optical-model Hamiltonians which is even larger than had been argued in [5]. One member of that family is shown to be identical to Feshbach's optical-model Hamiltonian (Section 4.14). Its relationship with Bell and Squires' optical-model potential is exhibited in Section 5. Section 6 deals with nuclear matter; we derive explicit expressions for quantities which had been introduced in Sections 3, 4, and 5.

As a prerequisite, one has to adopt a definition for the single-particle wave functions. Let us consider the example of the optical-model wave function. We denoted by $|\Psi_E^{0(A+1)}\rangle$ that antisymmetrized eigenstate of the $(A+1)$-nucleon Hamiltonian which corresponds to the asymptotic boundary condition that one nucleon is incident on the target ground state $|\Psi_0^{(A)}\rangle$.

(a) Bell and Squires [4] identified the "optical-model wave function" with the projection of $|\Psi_E^{0(A+1)}\rangle$ on $|\Psi_0^{(A)}\rangle$, namely with

$$\chi_E^{0(+)}(\mathbf{r}=\sqrt{A+1}\,(\Psi_0^{(A)}(\xi)\,|\,\Psi_E^{0(A+1)}(\mathbf{r};\xi)\rangle=\langle\,\Psi_0^{(A)}|\,a(\mathbf{r})\,|\,\Psi_E^{0(A+1)}\rangle. \tag{7.1}$$

Here, the symbol $(|\,\rangle$ means that the integration runs over the coordinates ξ of the target nucleons. The quantity $\chi_E^{0(+)}(\mathbf{r})$ is one of the overlap functions, whose relevant properties are surveye in Section 2.

(b) In Feshbach's approach, one decomposes $|\Psi_E^{0(A+1)}\rangle$ into two orthogonal parts by means of projection operators $P^{(p)}$ and $Q^{(p)}=1-P^{(p)}$. The operator $P^{(p)}$ is required to have the property that

$$P^{(p)}\,|\,\Psi_E^{0(A+1)}(\mathbf{r},\xi)\rangle=\frac{1}{\sqrt{A+1}}\,\mathscr{A}\{u_E^{0(+)}(\mathbf{r})\;\Psi_0^{(A)}(\xi)\}, \tag{7.2}$$

where $\mathscr{A}$ is the antisymmetrization operator (Section 4.5). In that approach, it may appear natural to identify the optical-model wave function with $u_E^{0(+)}(\mathbf{r})$.

These quantities are related by $|\chi_E^{0(+)}\rangle=(1-K)\,|u_E^{0(+)}\rangle$, where K denotes the density matrix. Since the elastic overlap $|\chi_E^{0(+)}\rangle$ is uniquely defined by (7.1), this relation fully determines $|u_E^{0(+)}\rangle$ provided that the inverse $(1-K)^{-1}$ exists. The latter condition is most probably fulfilled for the exact $|\Psi_0^{(A)}\rangle$, since the eigenvalues of K are expected to be all smaller than unity. However, when one uses a simplified model for $|\Psi_0^{(A)}\rangle$ some eigenvalues of K may be equal to unity. In that case, an additional condition must be imposed to determine $|u_E^{0(+)}\rangle$. Feshbach [3] thus

required $|u_E^{0(+)}\rangle$ to be orthogonal to those eigenvectors $|\omega_{v(1)}\rangle$ of K which correspond to the eigenvalue unity. This orthogonality condition is natural because (2.11) states that $\langle \omega_{v(1)} | \chi_E^{0(+)} \rangle = 0$. One can readily derive a wave equation for $|u_E^{0(+)}\rangle$ from an equation for $|\chi_E^{0(+)}\rangle$. Therefore, any basic difference between the microscopic optical-model potentials constructed by Feshbach and by Bell and Squires, respectively, should not be ascribed to a possible difference between the definitions adopted by these authors for the optical-model wave function.

The theory of Bell and Squires [4] is based on the time-ordered Green's function $G(E)$. The latter is the sum of the hole and particle components: $G(E) = G^{(h)}(E) + G^{(p)}(E)$. The particle Hamiltonian $h^{(p)}(E)$ is related to the particle Green's function $G^{(p)}(E)$ by $[E - h^{(p)}(E)]\, G^{(p)}(E) = 1$. We called $G^{(p)}(E)$ the resolvent of $h^{(p)}(E)$. The elastic overlap function is an eigenstate of $h^{(p)}(E)$:

$$h^{(p)}(E)\, |\chi_E^{0(+)}\rangle = E\, |\chi_E^{0(+)}\rangle. \tag{7.3}$$

We derived this property in two different ways, which are both of interest: (a) The derivation presented in Section 4.4 is formulated in the framework of stationary collision theory; it only involves the definition of the particle Green's function. (b) The proof given in Appendix E is based on time-dependent collision theory; that proof uses an explicit expression of $h^{(p)}(E)$ that we had derived in Section 4.6.

Indeed, in Section 4.6 we show that $h^{(p)}(E)$ can be expressed in terms of Feshbach's projection operators,

$$h^{(p)}(E) = -\frac{K}{1-K}\, E + (1-K)^{-1}\, R^{(p)} (1-K)^{-1} + (1-K)^{-1}\, D^{(p)}(E) (1-K)^{-1}, \tag{7.4}$$

where $R^{(p)}$ is hermitian and independent of energy. The projection operators $P^{(p)}$, and $Q^{(p)}$ appear only in the energy-dependent quantity $D^{(p)}(E)$. By transferring the first term of (7.4) from the left- to the right-hand side of the wave equation (7.3), the latter can readily be cast in the form

$$h_{\mathscr{F}}^{(p)}(E)\, |\chi_E^{0(+)}\rangle = E\, |\chi_E^{0(+)}\rangle, \tag{7.5a}$$

with

$$h_{\mathscr{F}}^{(p)}(E) = (1-K)\, h^{(p)}(E) + KE. \tag{7.5b}$$

In Section 4.14, we showed that $h_{\mathscr{F}}^{(p)}(E)$ is strictly identical to the optical-model Hamiltonian which had been introduced by Feshbach [3]. This result establishes contact between Feshbach's and Green's function theories of the optical-model potential. It thereby enables one to relate Feshbach's potential to quantities which had heretofore been discussed in the framework of Green's function theory, in particular the spectroscopic factors and the particle spectral function.

In the coordinate space representation, the real and imaginary parts of $h^{(p)}(\mathbf{r}, \mathbf{r}'; E)$ are symmetric in $\mathbf{r}$ and $\mathbf{r}'$. In contrast, $h_{\mathscr{F}}^{(p)}(\mathbf{r}, \mathbf{r}'; E)$ is not symmetric. Since no

approximation scheme is known for constructing the local-equivalent of an operator which is not symmetric in $\mathbf{r}$ and $\mathbf{r}'$, it appears difficult to relate $h_{\mathscr{F}}^{(p)}(\mathbf{r}, \mathbf{r}'; E)$ to phenomenological optical-model Hamiltonians. However, if (7.3) and (7.5) are transformed into wave equations for $|u_E^{0(+)}\rangle$,

$$h_u^{(p)}(E)\,|u_E^{0(+)}\rangle = E\,|u_E^{0(+)}\rangle, \qquad h_{\mathscr{F},u}^{(p)}(E)\,|u_E^{0(+)}\rangle = E\,|u_E^{0(+)}\rangle, \tag{7.6}$$

one finds that, in the coordinate space representation, the real and imaginary parts of $h_{\mathscr{F},u}^{(p)}(\mathbf{r}, \mathbf{r}'; E)$ are symmetric functions of $\mathbf{r}$ and $\mathbf{r}'$, while those of $h_u^{(p)}(\mathbf{r}, \mathbf{r}'; E)$ are not symmetric (Section 4.15).

We identified the optical-model wave function with $|\chi_E^{0(+)}\rangle$ rather than with $|u_E^{0(+)}\rangle$ because it is in terms of the overlap functions that the spectroscopic factors and the spectral function take the simple form assumed in the analysis of one-nucleon transfer reactions. Moreover, the relevant overlap functions are eigenvectors of the mass operator (plus kinetic energy), which leads to a unified description of the single-particle properties of the $(A-1)$- and $(A+1)$-systems as will be summarized below.

We also considered the overlap functions $\chi_E^{t(+)}(\mathbf{r}) = \langle \Psi_0^{(A)} |\, a(\mathbf{r})\, | \Psi_E^{t(A+1)}\rangle$, where the inelastic scattering state $|\Psi_E^{t(A+1)}\rangle$ is specified by the asymptotic boundary condition that one nucleon is incident on an excited state $|\Psi_t^{(A)}\rangle$ of the target. These continuum overlaps appear in the interpretation of stripping reactions which feed highly excited states of the $(A+1)$-system. We showed in Appendix E that $|\chi_E^{t(+)}\rangle$ is the solution of an inhomogeneous equation.

The overlap functions $\chi_\lambda^{(+)}(\mathbf{r}) = \langle \Psi_0^{(A)} |\, a(\mathbf{r})\, | \Psi_\lambda^{(A+1)}\rangle$ play a major role in the analysis of stripping reactions leading to the bound levels $|\Psi_\lambda^{(A+1)}\rangle$ of the $(A+1)$-system. They are eigenstates of $h^{(p)}(E)$ and $h_{\mathscr{F}}^{(p)}(E)$:

$$h^{(p)}(E_\lambda^{(+)})\,|\chi_\lambda^{(+)}\rangle = E_\lambda^{(+)}\,|\chi_\lambda^{(+)}\rangle, \qquad h_{\mathscr{F}}^{(p)}(E_\lambda^{(+)})\,|\chi_\lambda^{(+)}\rangle = E_\lambda^{(+)}\,|\chi_\lambda^{(+)}\rangle. \tag{7.7}$$

The discrete eigenvalues are equal to the difference $E_\lambda^{(+)} = \mathscr{E}_\lambda^{(A+1)} - \mathscr{E}_0^{(A)}$ between the energies of the levels $|\Psi_\lambda^{(A+1)}\rangle$ and $|\Psi_0^{(A)}\rangle$. The square of the norm of $|\chi_\lambda^{(+)}\rangle$ is the spectroscopic factor of the level $|\Psi_\lambda^{(+)}\rangle$. It can be calculated from the energy derivative of $h^{(p)}(E)$ or of $h_{\mathscr{F}}^{(p)}(E)$ at $E = E_\lambda^{(+)}$ (Section 4.7). One has $E_0^{(+)} \leqslant E_\lambda^{(+)} < 0$ where, except for a sign, $E_0^{(+)}$ is the separation energy of a nucleon from the ground state of the $(A+1)$-system. For instance, $E_0^{(+)} = -2.63$ MeV for the $(^{208}\mathrm{Pb} + n)$-system. *The fact that $h^{(p)}(E)$ and $h_{\mathscr{F}}^{(p)}(E)$ have no bound eigenstate with eigenvalue smaller than $E_0^{(+)}$ has the important physical consequence that their real parts are not closely related to the real part of phenomenological optical-model Hamiltonians, at least at low energy.* Indeed, the phenomenological optical-model potentials have bound single-particle eigenstates with energy smaller than $E_0^{(+)}$.

The particle spectral function $S^{(p)}(E)$ describes the energy distribution of the single-particle strength in the $(A+1)$-system. It is the sum of three contributions: $S^{(p)}(E) = S_{dt}^{(p)}(E) + S_{\mathrm{el}}^{(p)}(E) + S_{\mathrm{in}}^{(p)}(E)$. These are associated with the discrete, elastic and inelastic eigenstates of the $(A+1)$-nucleon Hamiltonian, namely with $|\Psi_\lambda^{(A+1)}\rangle$, $|\Psi_E^{0(A+1)}\rangle$, and $|\Psi_E^{t(A+1)}\rangle$. In Section 4.12, we show that one can evaluate each of these

three contributions from the particle Hamiltonian $h^{(p)}(E)$. Equation (4.69c) indicates that they can also be calculated from Feshbach's Hamiltonian $h^{(p)}_{\mathscr{F}}(E)$.

The integral of $S^{(p)}(E)$ over all energies is equal to $1-K$. This sum rule is responsible for the appearance of the first term on the right-hand side of the expression (7.4) of $h^{(p)}$. It reflects the fact that $G^{(p)}(E) \sim (1-K)/E$ at large E. This is strikingly different from the high energy behaviour ($\sim E^{-1}$) of the Green's function encountered in potential scattering theory. The resolvent $G^{(p)}_{\mathscr{F}}(E)$ of Feshbach's Hamiltonian approaches E^{-1} at large E, but $h^{(p)}_{\mathscr{F}}(\mathbf{r}, \mathbf{r}'; E)$ is not symmetric in $\mathbf{r}$ and $\mathbf{r}'$.

One may wonder whether it is possible to find a Hamiltonian $\tilde{h}^{(p)}(\mathbf{r}, \mathbf{r}'; E)$ which would be symmetric in $\mathbf{r}$ and $\mathbf{r}'$, remain finite at large energy, and have the elastic overlap $|\chi^{0(+)}_E\rangle$ as eigenstate. In Section 4.16, we showed that this question can be answered in the affirmative. For this purpose, we used an extension of Feshbach's method. Namely, we decomposed $|\Psi^{(A+1)}\rangle$ into two components which are not orthogonal to each other. Furthermore, $\tilde{h}^{(p)}(E)$ enables one to calculate the particle spectral function $S^{(p)}(E)$. However, the resolvent $\tilde{G}^{(p)}(z)$ of $\tilde{h}^{(p)}(z)$ has a spurious pole at $z = -\mathscr{E}^{(A)}_0 - i\eta$. This pole is spurious in the sense that it does not correspond to a bound state of $\tilde{h}^{(p)}(E)$ or of $h^{(p)}(E)$.

Section 3 is devoted to the investigation of hole Hamiltonians. These are required to have as eigenstates the overlap functions

$$\chi^{(-)}_\lambda(\mathbf{r}) = \sqrt{A}\,(\Psi^{(A-1)}_\lambda\,|\,\Psi^{(A)}_0\rangle = \langle\,\Psi^{(A-1)}_\lambda|\,a(\mathbf{r})\,|\,\Psi^{(A)}_0\rangle \tag{7.8}$$

associated with the bound levels $|\Psi^{(A-1)}_\lambda\rangle$ of the $(A-1)$-system. Here, the symbol $(|\,\rangle$ means that the integration runs over the coordinates of $(A-1)$-nucleons contained in $|\Psi^{(A-1)}_\lambda\rangle$. One of these operators is the hole Hamiltonian proper, $h^{(h)}(E)$, of which the hole Green's function $G^{(h)}(E)$ is the resolvent:

$$[E - h^{(h)}(E)]\,G^{(h)}(E) = 1, \qquad h^{(h)}(E^{(-)}_\lambda\,|\chi^{(-)}_\lambda\rangle = E^{(-)}_\lambda\,|\chi^{(-)}_\lambda\rangle. \tag{7.9}$$

The discrete eigenvalues $E^{(-)}_\lambda$ are equal to the difference $E^{(-)}_\lambda = \mathscr{E}^{(A)}_0 - \mathscr{E}^{(A-1)}_\lambda$ between the energies of $|\Psi^{(A)}_0\rangle$ and $|\Psi^{(A-1)}_\lambda\rangle$. The square of the norm of $|\chi^{(-)}_\lambda\rangle$ is the spectroscopic factor of the level $|\Psi^{(A-1)}_\lambda\rangle$. Equations (3.55b) and (3.60d) show that it can be calculated from the energy derivative of $h^{(h)}(E)$ or $h^{(h)}_{\mathscr{F}}(E)$ at $E = E^{(-)}_\lambda$.

In Section 3.4, we expressed the hole Hamiltonian in terms of projection operators $P^{(h)}$ and $Q^{(h)}$. These play a role analogous to that of Feshbach's operators $P^{(p)}$ and $Q^{(p)}$ in the $(A+1)$-system [25]. The result reads

$$h^{(h)}(E) = E\frac{K-1}{K} + K^{-1}R^{(h)}K^{-1} + K^{-1}D^{(h)}(E - i\eta)\,K^{-1}. \tag{7.10}$$

The operators $P^{(h)}$ and $Q^{(h)}$ are contained only in the quantity $D^{(h)}(E - i\eta)$. The energy-independent contribution $R^{(h)}$ is closely related to the so-called mean removal energy (Section 3.5). By transferring the contribution of the first term of (7.10) to the

right-hand side of $h^{(h)}(E_\lambda^{(-)}\,|\chi_\lambda^{(-)}\rangle = E_\lambda^{(-)}\,|\chi_\lambda^{(-)}\rangle$, the latter yields $h_{\mathscr{F}}^{(h)}(E_\lambda^{(-)})\,|\chi_\lambda^{(-)}\rangle = E_\lambda^{(-)}\,|\chi_\lambda^{(-)}\rangle$, where

$$h_{\mathscr{F}}^{(h)}(E) = Kh^{(h)}(E) + E(1-K). \tag{7.11}$$

In the coordinate space representation, the real and imaginary parts of $h^{(h)}(\mathbf{r}, \mathbf{r}'; E)$ are symmetric functions of $\mathbf{r}$ and $\mathbf{r}'$. In contrast, $h_{\mathscr{F}}^{(h)}(\mathbf{r}, \mathbf{r}'; E)$ is not symmetric.

One might be tempted to associate the potential-type operator $M^{(h)}(E) = h^{(h)}(E) - T$ with the shell-model potential. This would be misleading. Indeed, the largest eigenvalue of the Hamiltonian $h^{(h)}(E)$ is negative. Except for a sign, this largest eigenvalue $E_0^{(-)}$ is the separation energy of one nucleon from the ground state of the A-nucleon system. For instance, $E_0^{(-)} = -7.37$ MeV for a neutron hole in the ^{208}Pb core. *This has the important physical consequence that, at low energy, the real part $M^{(h)}(E)$ has only little resemblance, if any, with the real part of empirical shell-model potentials.* Indeed, the latter always have discrete or continuous eigenvalues larger than $E_0^{(-)}$.

We also considered the overlap functions $\chi_E^{t(-)}(\mathbf{r}) = \langle \Psi_E^{t(A-1)}|\, a(\mathbf{r})\, |\Psi_0^{(A)}\rangle$, where $|\Psi_E^{t(A-1)}\rangle$ is a scattering eigenstate of the $(A-1)$-nucleon Hamiltonian. These continuum overlaps appear in the interpretation of knockout reactions which feed highly excited states of the $(A-1)$-system. In Appendix C, it is shown that $\chi_E^{t(-)}$ is the solution of an inhomogeneous equation.

The hole spectral function $S^{(h)}(E)$ describes the energy distribution of the single-particle strength contained in the $(A-1)$-system. It can readily be calculated from $h^{(h)}(E)$. The integral of $S^{(h)}(E)$ over all energies is equal to K. In Section 3.6, we exhibited that this sum rule is responsible for the existence of the first term on the right-hand side of the expression (7.10) of $h^{(h)}(E)$. Equivalently, it implies that, at high energy, $G^{(h)}(E) \sim K/E$. This is quite different from the asymptotic behaviour $\sim E^{-1}$ of the standard potential scattering Green's function. The resolvent $G_{\mathscr{F}}^{(h)}(E)$ of the Feshbach-type Hamiltonian $h_{\mathscr{F}}^{(h)}(E)$ approaches E^{-1} at large E, but $h_{\mathscr{F}}^{(h)}(\mathbf{r}, \mathbf{r}'; E)$ is not symmetric in $\mathbf{r}$ and $\mathbf{r}'$.

One may thus wonder whether it is possible to construct a Hamiltonian $\tilde{h}^{(h)}(\mathbf{r}, \mathbf{r}', E)$ which would be self-transposed, remain finite at large energy, have the overlaps $|\chi_\lambda^{(-)}\rangle$ as eigenstates, and enable one to calculate the hole spectral function. In Section 3.13, we showed that this question can be answered in the affirmative. For this purpose, we used an extension of Feshbach's method. Namely, we wrote $|\Psi^{(A-1)}\rangle$ as the sum of two components which are not orthogonal to each other. We constructed a hole-type Hamiltonian $\tilde{h}^{(h)}(E)$ which fulfills the required properties. The resolvent $\tilde{G}^{(h)}(z)$ of $\tilde{h}^{(h)}(z)$ contains a pole which is located at $z = \mathscr{E}_0^{(A)} + i\eta$; it is spurious in the sense that it does not correspond to a bound state of $h(E)$ or $h^{(h)}(E)$.

In Sections 3 and 4, we tried to achieve mathematical rigor. A priori, rigorous proofs are expected to be less difficult to find in the hole case since the overlaps $|\chi_\lambda^{(-)}\rangle$ and $|\chi_E^{t(-)}\rangle$ are normalizable, in contrast to $|\chi_E^{0(+)}\rangle$ and $|\chi_E^{t(+)}\rangle$. Even in the hole case, mathematical difficulties are encountered mainly because the operators $h^{(h)}(E)$ and $h_{\mathscr{F}}^{(h)}(E)$ involve the inverse K^{-1}. This operator is unbounded, since the

eigenvalues of K have an accumulation point at zero. The expression of $\tilde{h}^{(h)}(E)$ does not involve K^{-1}. Therefore, the study of $\tilde{h}^{(h)}$ and of related quantities could be performed in a rigorous mathematical framework. This was one of our main motivations for investigating $\tilde{h}^{(h)}(E)$ in detail.

In particular, in Appendix B we give rigorous proofs of the following two properties: (a) The operator $\tilde{Q}^{(h)}H\tilde{Q}^{(h)}$ is self-adjoint (which is a stronger property than hermiticity). (b) Generalized Møller operators do exist. These properties enabled us to provide, in Appendix C, a rigorous mathematical support to the usual assumption that the time evolution of a scattering state is asymptotically free of any hole component.

Section 5 is devoted to the time-ordered Green's function $G(E)$ and related operators. Let $h(E)$ be the one-body Hamiltonian whose resolvent is $G(E)$; thus, $[E-h(E)]\,G(E)=1$. We show in Section 5.2 that all the eigenvectors of $h^{(p)}(E)$ and of $h^{(h)}(E)$ are also eigenvectors of $h(E)$. In particular, $h(E)\,|\chi_E^{0(+)}\rangle = E\,|\chi_E^{0(+)}\rangle$: this is the result that Bell and Squires [4] had first proved. We exhibit in Section 5.5 that $h(E)$ furthermore enables one to calculate the spectral function $S(E)=S^{(p)}(E)+S^{(h)}(E)$, as well as $S^{(p)}(E)$ and $S^{(h)}(E)$ separately. In particular, the spectroscopic factors can be evaluated from the derivative of $h(E)$ at $E=E_\lambda^{(\pm)}$.

The one-body Hamiltonian $h(E)$ can be written as $h(E)=R^{(p)}+R^{(h)}+D(E)$. The nonherinitian energy-dependent contribution $D(E)$ tends to zero at large E, while $R^{(p)}$ and $R^{(h)}$ are the real hermitian operators which appear in (7.4) and (7.10). Since $R^{(p)}+R^{(h)}$ is the sum of the kinetic energy operator T and of a static operator $V^{(S)}$, it is natural to write $h(E)=T+M(E)$. The quantity $M(E)$ is called the mass operator. It is symmetric in the coordinate space representation.

The mass operator is a good candidate for being identified with the microscopic shell-model potential when $E<0$ and with the microscopic optical-model potential when $E>0$. It thus provides a unified microscopic approach to the shell- and optical-model potentials. At large energy, it approaches the static operator $V^{(S)}$. When only two-body interactions exist, $V^{(S)}$ can be written in the closed form (5.38). In atomic physics, $V^{(S)}$ can be viewed as an extension of the Hartree–Fock approximation. In contrast, it does not have much physical meaning in the nuclear case, because in that case $V^{(S)}$ is extremely large and repulsive.

In Section 6, we illustrate the difference between $h^{(p)}(E)$, $h^{(h)}(E)$, and $h(E)$ by deriving their expressions in nuclear matter, within the framework of second-order perturbation theory. Nuclear matter is much simpler than a finite system because the relevant quantities only depend upon two variables, the momentum k and the energy E. Their dependence upon k corresponds to their spatial nonlocality. In second order and for k larger than the Fermi momentum k_F, the particle Hamiltonian $h^{(p)}(k;E)$ is essentially obtained from $h(k;E)$ by replacing in some contributions the energy variable E by the quasiparticle energy $E_{qp}(k)$ defined by (6.11). Moreover, $h^{(p)}(E)$ contains a term linear in E, in contrast to $h(E)$. This suggests that, in a finite system, the difference between $h(E)$ and $h^{(p)}(E)$ mainly derives from the fact that part of the energy dependence of $h(E)$ is replaced by a spatial nonlocality in $h^{(p)}(E)$. It appears that the spatial nonlocality of $h^{(p)}(E)$ is quite complicated. This

is suggested by the fact that, in nuclear matter, the particle Hamiltonian $h^{(p)}(k; E)$ has a discontinuity at $k = k_F$. In a finite system, it is most probably the spatial nonlocality of $h^{(p)}(E)$ which is responsible for the fact that it has no eigenvalue smaller than the Fermi energy.

In Section 4.17, we show that, besides $h^{(p)}(E)$, $h^{(p)}_{\mathscr{F}}(E)$, and $\tilde{h}^{(p)}(E)$, there exist many optical-model Hamiltonians $\hat{h}^{(p)}(E)$ which all have the overlaps $|\chi^{(+)}_\lambda\rangle$ and $|\chi^{0(+)}_E\rangle$ as eigenstates and, furthermore, which enable one to calculate the particle spectral function. In Section 5.7, we exhibit that, besides $h(E)$, there exist many Hamiltonians $\hat{h}(E)$ which all have the overlaps $|\chi^{(-)}_\lambda\rangle$, $|\chi^{(+)}_\lambda\rangle$, and $|\chi^{0(+)}_E\rangle$ as eigenstates and, furthermore, which enable one to calculate the spectral function. Since many Hamiltonians exist which all admit the elastic overlap $|\chi^{0(+)}_E\rangle$ as the eigenstate, one should discuss which one is privileged from a physical point of view. The following two main criteria could be adopted:

(a) *Some microscopic expressions may be more "useful" than others.* We restricted our attention to the microscopic nucleon–nucleus mean field, to the exclusion of any other aspect of nuclear reaction theory. It is thus appropriate to stress that Feshbach's projection operator techniques have proved extremely useful for describing many different types of nuclear reaction phenomena, besides having provided the first theoretical derivation of a microscopic optical-model potential. In the present specific context, we adopt the point of view of Gottfried [47], according to whom "useful" means that the expression of the optical-model potential "should lead to sensible approximate methods of calculation." In that respect, the mass operator presents the advantage that one knows its linked-cluster perturbation expansion in powers of the strength of the nucleon–nucleon interaction. In contrast, it does not appear possible to derive a linked-cluster expansion for $h^{(p)}(E)$ or $h^{(p)}_{\mathscr{F}}(E)$, for instance. The expansion of $M(E)$ has a simple structure. It can be rearranged, for instance by summing subseries in closed form with the help of Brueckner's reaction matrix [73] or of similar methods [78]. When one uses "effective" interactions as input, one could use straightforward perturbation theory, but an *RPA*-type approximation is probably more appropriate, at least in a finite system, in order to take collectivity effects into account [69–71]. This *RPA*-type approximation is derived by truncating the set of equations which relate the one-, two-, many-body Green's functions.

(b) One should be able to establish a correspondence between the microscopic and phenomenological optical-model potentials. In particular, the spatial nonlocality of the microscopic potential should be sufficiently simple to enable one to construct its local equivalent, at least in principle. This condition seems to rule out operators which are not symmetric in the space coordinate representation. Moreover, we showed that the particle Hamiltonians $h^{(p)}(E)$, $h^{(p)}_{\mathscr{F}}(E)$, $h^{(p)}_{\mathscr{K}}(E)$, and $\tilde{h}^{(p)}(E)$ studied in Section 4 have no eigenvalue smaller than the Fermi energy. In contrast, phenomenological optical-model Hamiltonians have deeply bound eigenstates. Correspondingly, the microscopic operators of Sections 3 and 4 do not provide a unified description of the shell- and optical-model potentials. In contrast, the mass operator treats negative and positive energies on the same footing.

APPENDIX

A. *Extension of the Hellmann–Feynman Theorem*

Let $h(E)$ be some energy-dependent one-body Hamiltonian. In the present appendix, we extend the Hellmann–Feynman theorem [79–81] to the case when $h(E)$ is not hermitian. For fixed E, the eigenstates of $h(E)$ and of $h^\dagger(E)$ in general form a complete biorthogonal set of bound and scattering states [36–38]:

$$h(E)\,|\varphi_\mu(E)\rangle = e_\mu(E)\,|\varphi_\mu(E)\rangle, \qquad h(E)\,|\varphi_e(E)\rangle = e(E)\,|\varphi_e(E)\rangle, \tag{A.1a}$$

$$h^\dagger(E)\,|\tilde{\varphi}_\mu(E)\rangle = e_\mu^*(E)\,|\tilde{\varphi}_\mu(E)\rangle, \qquad h^\dagger(E)\,|\tilde{\varphi}_e(E)\rangle = e(E)\,|\tilde{\varphi}_e(E)\rangle, \tag{A.1b}$$

$$\langle \tilde{\varphi}_\mu(E)\,|\,\varphi_{\mu'}(E)\rangle = \delta_{\mu\mu'}, \tag{A.1c}$$

$$\langle \tilde{\varphi}_{e'}(E)\,|\,\varphi_{e''}(E)\rangle = \delta(e'-e''). \tag{A.1d}$$

The continuous eigenvalues $e(E)$ are real [82]. We choose the normalization

$$\langle \varphi_\mu(E)\,|\,\varphi_\mu(E)\rangle = 1. \tag{A.1e}$$

Then, the norm of $|\tilde{\varphi}_\mu\rangle$ is determined by (A.1c). One has successively

$$\begin{aligned}
&\frac{d}{dE}\langle \tilde{\varphi}_\mu(E)|\, h(E)\,|\varphi_\mu(E)\rangle \\
&\quad = \langle \tilde{\varphi}_\mu(E)|\,\frac{d}{dE}h(E)\,|\varphi_\mu(E)\rangle \\
&\qquad + \left\langle \frac{d}{dE}\tilde{\varphi}_\mu(E)\right| h(E)\,|\varphi_\mu(E)\rangle + \langle \tilde{\varphi}_\mu(E)|\, h(E)\left|\frac{d}{dE}\varphi_\mu(E)\right\rangle \qquad \text{(A.2a)} \\
&\quad = \langle \tilde{\varphi}_\mu(E)|\,\frac{d}{dE}h(E)\,|\varphi_\mu(E)\rangle \\
&\qquad + e_\mu(E)\left[\left\langle \frac{d}{dE}\,\widetilde{\varphi}_\mu(E)\right|\varphi_\mu(E)\right\rangle + \left\langle \tilde{\varphi}_\mu(E)\left|\frac{d}{dE}\varphi_\mu(E)\right\rangle\right]. \qquad \text{(A.2b)}
\end{aligned}$$

The contents of the square brackets are the derivative of the left-hand side of (A.1c). It thus vanishes. This yields

$$\frac{d}{dE}\langle \tilde{\varphi}_\mu(E)|\, h(E)\,|\varphi_\mu(E)\rangle = \langle \tilde{\varphi}_\mu(E)|\,\frac{d}{dE}h(E)\,|\varphi_\mu(E)\rangle. \tag{A.3a}$$

This is the extension of the Hellmann–Feynman theorem to nonhermitian operators. It can also be written in the form

$$\frac{d}{dE} e_\mu(E) = \langle \tilde{\varphi}_\mu(E) | \frac{d}{dE} h(E) \, | \varphi_\mu(E) \rangle. \tag{A.3b}$$

B. *Mathematical Properties of* $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$

We establish some mathematical properties of $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$ which will be needed in the next appendix.

B.1. *Classes of Linear Operators*

All the operators that we consider below are defined on the whole Hilbert space $\mathscr{H}$.

(a) "Trace class" (or "nuclear") operators fulfill

$$\text{trace}(O^\dagger O)^{1/2} = \sum_n \langle \alpha_n | \, (O^\dagger O)^{1/2} \, | \alpha_n \rangle < \infty, \tag{B.1}$$

where $\{\alpha_n\}$ is an arbitrary basis in the Hilbert space $\mathscr{H}$.

(b) "Hilbert–Schmidt" operators satisfy

$$\text{trace } O^\dagger O < \infty. \tag{B.2}$$

(c) "Compact" or "completely continuous" operators have the property that

$$O\alpha_n \Rightarrow O\alpha \qquad \text{if} \quad \alpha_n \to \alpha, \tag{B.3}$$

where $\Rightarrow$ and $\to$ denote strong and weak convergence, respectively.

(d) "Bounded" operators have a finite norm:

$$\operatorname*{Sup}_{\Psi \neq 0} \frac{\|O\Psi\|}{\|\Psi\|} \equiv \|O\| < \infty. \tag{B.4a}$$

They have the property that

$$O\alpha_n \Rightarrow O\alpha \qquad \text{if} \quad \alpha_n \Rightarrow \alpha. \tag{B.4b}$$

The following inclusions hold:

$$\text{trace class} \subset \text{Hilbert–Schmidt} \subset \text{compact} \subset \text{bounded}. \tag{B.5}$$

B.2. *Applications*

Because $a_{\mathbf{r}} \, | \Psi_0^{(A)} \rangle$ is normalizable, the quantity

$$\mathscr{O}(\mathbf{r}, \mathbf{r}') = \langle \Psi_0^{(A)} | \, a_{\mathbf{r}'}^\dagger O a_{\mathbf{r}} \, | \Psi_0^{(A)} \rangle \tag{B.6}$$

is a square summable function of $\mathbf{r}$ and $\mathbf{r}'$. The operator $\mathcal{O}$ thus belongs to the Hilbert–Schmidt class. Therefore, the density matrix K (Eq. (2.8a)) and the hole Green's function $G^{(h)}(E-i\eta)$ (Eq. (3.2)) are Hilbert–Schmidt operators. Apart from the constant term $\mathscr{E}_0^{(A)}$, the hole-type Hamiltonian $\tilde{h}^{(h)}(E-i\eta)$ (Eq. (3.72)) is also a Hilbert–Schmidt operator. In contrast, the hole Hamiltonian $h^{(h)}(E-i\eta)$ is unbounded because its resolvent $G^{(h)}(E-i\eta)$ is compact; see Section 12.5 of [35].

According to Theorem VI.15 of [45], the spectrum of a compact operator is a discrete set having no limit point, except perhaps the point zero. This point is not necessarily a discrete eigenvalue. Since compact operators are bounded, their spectrum is a bounded set. Therefore, the spectrum of $\tilde{h}^{(h)}(E-i\eta)$ has that structure, except for a translation due to the constant term $\mathscr{E}_0^{(A)}$. Although $h^{(h)}(E-i\eta)$ is not compact, it also has a discrete (but unbounded) spectrum; this is a consequence of the fact that $G^{(h)}(E-i\eta)$ is compact; see Theorem 1 in Section 12.5 of [35].

B.3. *Hilbert–Schmidt Nature of* $[\tilde{Q}^{(h)}H\tilde{Q}^{(h)}-H]$

We now show that

$$J^{(h)}=\tilde{Q}^{(h)}H\tilde{Q}^{(h)}-H \tag{B.7a}$$

is a Hilbert–Schmidt operator. The interest of this property will become apparent below. According to (3.67a),

$$J^{(h)}=L^{(h)}HL^{(h)}-HL^{(h)}-L^{(h)}H. \tag{B.7b}$$

It can be checked that each term on the right-hand side of (B.7b) is a Hilbert–Schmidt operator. For instance, let us consider the second term $HL^{(h)}$. One has

$$\text{trace}[(L^{(h)})^{\dagger}HHL]=\int d\mathbf{r}\,d\mathbf{s}\,\gamma(\mathbf{r},\mathbf{s})\langle\Psi_0^{(A)}|\,a_{\mathbf{s}}^{\dagger}H^2a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle, \tag{B.8a}$$

where

$$\gamma(\mathbf{r},\mathbf{s})=\int d\mathbf{r}'\,d\mathbf{s}'\,\beta^{(h)}(\mathbf{r},\mathbf{r}')\,K_{\mathbf{s}'\mathbf{r}'}[\beta^{(h)}(\mathbf{s}',\mathbf{s}]^*. \tag{B.8b}$$

The operator $\beta^{(h)}$ is given by (3.67c). Since $a_{\mathbf{r}}\,|\Psi_0^{(A)}\rangle$ is normalizable, the matrix element which appears on the right-hand side of (B.8a) is a square summable function of $\mathbf{s}$ and $\mathbf{r}$. Moreover, $\gamma(\mathbf{r},\mathbf{s})$ is also square summable because the eigenvalues of $\beta^{(h)}$ are a bounded set. We conclude that

$$\text{trace}[(L^{(h)})^{\dagger}HHL^{(h)}]<\infty. \tag{B.8c}$$

This establishes that $HL^{(h)}$ is a Hilbert–Schmidt operator. A similar proof holds for the two other terms on the right-hand side of (B.7b).

B.4. *Self-adjoint Nature of* $\tilde{Q}^{(h)}H\tilde{Q}^{(h)}$

An operator O_h is "hermitian" if

$$\langle \alpha |\, O_h \,| \beta \rangle = \langle O_h \alpha \,|\, \beta \rangle \tag{B.9}$$

for all the vectors α and β contained in the domain of definition of O_h. An hermitian operator O_s, is "self-adjoint" if

$$O_s = O_s^\dagger , \tag{B.10}$$

i.e., if the domains of definition of O_h and $O_h^\dagger$ are identical. One has

$$\text{self-adjoint} \subset \text{hermitian}. \tag{B.11}$$

In the present context, the basic interest of distinguishing the self-adjoint from the hermitian properties is that the spectral properties of self-adjoint operators are more restricted than those of hermitian operators.

According to (B.7a), the operator $J^{(h)}$ is hermitian. Moreover, we showed above that $J^{(h)}$ is a Hilbert–Schmidt operator. Since, by definition, a Hilbert–Schmidt operator may be defined in the whole Hilbert space, we conclude that $J^{(h)}$ is self-adjoint. It results that $\tilde{Q}^{(h)}H\tilde{Q}^{(h)}$ is self-adjoint, because it is the sum of the self-adjoint operator H and of the self-adjoint operator $J^{(h)}$, which is defined in the whole Hilbert space.

This proof does not apply to $Q^{(h)}HQ^{(h)}$, $Q^{(p)}HQ^{(p)}$, and $\tilde{Q}^{(p)}H\tilde{Q}^{(p)}$. Following all previous authors, we shall nevertheless assume that these operators are also self-adjoint.

B.5. *Generalized Møller Operators*

One can show that $J^{(h)}$ actually belongs to the trace class. We skip the proof, but hint that it uses the basis provided by the complete set of eigenvectors of $L^{(h)}$. This trace class property is relevant because the Kato–Rosenblum theorem (Section XI.3 of [45]) then implies that the following strong limit exists,

$$\underset{\tau \to +\infty}{\text{st.lim}}\, e^{-i\tilde{Q}^{(h)}H\tilde{Q}^{(h)}\tau} e^{iH\tau} \,|\Lambda^{(-)}\rangle = \Omega_{\tilde{Q}}^{(h)} \,|\Lambda^{(-)}\rangle, \tag{B.12a}$$

for every normalizable $|\Lambda^{(-)}\rangle$ spanned by the continuous eigenvectors of H. This theorem also implies that

$$\underset{\tau \to +\infty}{\text{st.lim}}\, e^{iH\tau} e^{-i\tilde{Q}^{(h)}H\tilde{Q}^{(h)}\tau} \,|\tilde{\Lambda}^{(-)}\rangle = \hat{\Omega}_{\tilde{Q}}^{(h)} \,|\tilde{\Lambda}^{(-)}\rangle, \tag{B.12b}$$

exists for every normalizable $|\tilde{\Lambda}^{(-)}\rangle$ spanned by the continuous eigenvectors of $\tilde{Q}^{(h)}H\tilde{Q}^{(h)}$. The existence of these strong limits will be used in Appendix C.

C. *One-Body Wave Equation for the Continuum Overlaps* $|\chi_E^{c(-)}\rangle$

In the present appendix, we derive a relation between $|\chi_E^{c(-)}\rangle$ and the resolvent $\tilde{G}^{(h)}(E)$ of the hole-type Hamiltonian. For that purpose, we shall extend a method which had been introduced in [25]. Let us apply (3.68b) and (3.68c) to a scattering eigenstate $|\Psi_{\mathscr{E}}^{(-)}\rangle = |\Psi_{\mathscr{E}}^{c(-)}\rangle$ of the $(A-1)$-nucleon Hamiltonian. The general solution of (3.68c) is

$$\tilde{Q}^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle = b_{\mathscr{E}}^{c(-)} |\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle + (\mathscr{E} - \tilde{Q}^{(h)} H \tilde{Q}^{(h)} - i\eta)^{-1} \tilde{Q}^{(h)} H \tilde{P}^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle. \quad \text{(C.1)}$$

As in (3.100b) $|\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle$ denotes an eigenstate of $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$ with eigenvalue $\mathscr{E}$. Its precise definition will be derived below. It is only for $\mathscr{E}$ larger than the threshold energy $\mathscr{T}_c^{(-)}$ that (C.1) is meaningful. In order to handle boundary conditions, it is safer to use a time-dependent description.

Let B and C be two positive operators. We shall write

$$B \leqslant C \quad \text{(C.2a)}$$

as an abbreviated way of stating that

$$\langle \Psi | B | \Psi \rangle \leqslant \langle \Psi | C | \Psi \rangle \quad \text{(C.2b)}$$

for any normalizable $|\Psi\rangle$. Since it follows from (3.67a)–(3.67c) that $0 \leqslant \tilde{Q}^{(h)} \leqslant 1$,

$$(1 - \tilde{Q}^{(h)})^2 \leqslant 1 - \tilde{Q}^{(h)} \leqslant [1 - (\tilde{Q}^{(h)})^2] = \tilde{P}^{(h)}. \quad \text{(C.2c)}$$

The normalizable packet of scattering eigenfunctions of H

$$|\Psi^{(-)}(\tau)\rangle = e^{-iH\tau} |\Lambda^{(-)}\rangle \quad \text{(C.3)}$$

is a solution of the time-dependent Schrödinger equation for the $(A-1)$-system. The inequalities (C.2c) imply that

$$\begin{aligned} \| e^{i\tilde{Q}^{(h)} H \tilde{Q}^{(h)} \tau} (1 - \tilde{Q}^{(h)}) e^{-iH\tau} |\Lambda^{(-)}\rangle \| &= \| (1 - \tilde{Q}^{(h)}) e^{-iH\tau} |\Lambda^{(-)}\rangle \| \\ &\leqslant \| \sqrt{\tilde{P}^{(h)}}\, e^{-iH\tau} |\Lambda^{(-)}\rangle \|. \end{aligned} \quad \text{(C.4a)}$$

Since $\tilde{P}^{(h)}$ is a trace class (and thus a compact) operator, the Riemann–Lebesgue lemma (see Theorem IX.7, on page 10 of [45]) yields

$$\lim_{\tau \to +\infty} \| \sqrt{\tilde{P}^{(h)}}\, e^{-iH\tau} |\Lambda^{(-)}\rangle \| = 0; \quad \text{(C.4b)}$$

see Problem 18, page 386 of [45] (Vol. III). Equations (C.4a) and (C.4b) give

$$\text{st.lim}_{\tau \to +\infty} e^{i\tilde{Q}^{(h)} H \tilde{Q}^{(h)} \tau} (1 - \tilde{Q}^{(h)}) e^{-iH\tau} |\Lambda^{(-)}\rangle = 0. \quad \text{(C.5)}$$

We recall that st.lim denotes a strong limit.

We define a generalized Møller operator $\Omega_{\tilde{Q}}^{(h)}$ by means of

$$\Omega_{\tilde{Q}}^{(h)} |\Lambda^{(-)}\rangle = \underset{\tau \to +\infty}{\text{st.lim}}\, e^{i\tilde{Q}^{(h)} H \tilde{Q}^{(h)} \tau} \tilde{Q}^{(h)} e^{-iH\tau} |\Lambda^{(-)}\rangle. \tag{C.6}$$

According to (C.4a) and (C.4b), Eq. (C.6) amounts to

$$\Omega_{\tilde{Q}}^{(h)} |\Lambda^{(-)}\rangle = \underset{\tau \to +\infty}{\text{st.lim}}\, e^{i\tilde{Q}^{(h)} H \tilde{Q}^{(h)} \tau} e^{-iH\tau} |\Lambda^{(-)}\rangle. \tag{C.7}$$

The existence of the strong limit in (C.7), as well as of the strong limit in (B.12b) has been proved in Section B.5. Dealing with the continuous spectrum of $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$, we have no indication of pathologies as singular continuous spectrum and/or discrete eigenvalues of $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$ with infinite degeneracy embedded in the continnuum. So, in practice, the existence of the strong limits in (C.7) and (B.9b) implies that the continuous spectra of H and $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$ are equal. Equation (3.73) shows that, as a consequence, the branch cut of the hole-type Hamiltonian $\tilde{h}^{(h)}(E)$ extends from $-\infty$ up to $T_0^{(-)}$. In any case, a more rigorous proof relies on the compactness of $J^{(h)}$. Indeed, the "classical Weyl theorem" then implies that the continuous spectra of H and $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$ coincide, even in the presence of mathematically possible pathologies such as those quoted above (see, e.g., Section XIII.4 of [45]).

Equation (C.7) shows that the operator $\Omega_{\tilde{Q}}^{(h)}$ is "isometric" since it is the limit of unitary operators. We recall that, by definition, an isometric operator fulfills

$$(\Omega_{\tilde{Q}}^{(h)})^{\dagger}\, \Omega_{\tilde{Q}}^{(h)} = 1. \tag{C.8}$$

As a consequence, it preserves the orthonormalization properties of the state vectors on which it is applied [83, 84]. Equation (C.6) implies the existence of the integral

$$\int_0^{+\infty} d\tau \frac{d}{d\tau} (e^{i\tilde{Q}^{(h)} H \tilde{Q}^{(h)} \tau} \tilde{Q}^{(h)} e^{-iH\tau}) |\Lambda^{(-)}\rangle = \Omega_{\tilde{Q}}^{(h)} |\Lambda^{(-)}\rangle - \tilde{Q}^{(h)} |\Lambda^{(-)}\rangle. \tag{C.9a}$$

By performing the time derivative, one finds

$$-i \int_0^{+\infty} d\tau\, e^{i\tilde{Q}^{(h)} H \tilde{Q}^{(h)} \tau} \tilde{Q}^{(h)} H \tilde{P}^{(h)} e^{-iH\tau} |\Lambda^{(-)}\rangle = \Omega_{\tilde{Q}}^{(h)} |\Lambda^{(-)}\rangle - \tilde{Q}^{(h)} |\Lambda^{(-)}\rangle. \tag{C.9b}$$

A time-independent wave equation is obtained from (C.9b) by introducing Fourier transforms, after having introduced a convergence factor $\exp(-\eta\tau)$ [83, 84]. This yields

$$\tilde{Q}^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle = \Omega_{\tilde{Q}}^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle + (\mathscr{E} - \tilde{Q}^{(h)} H \tilde{Q}^{(h)} - i\eta)^{-1}\, \tilde{Q}^{(h)} H \tilde{P}^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle. \tag{C.10}$$

Equations (C.1) and (C.10) show that $b_{\mathscr{E}}^{c(-)} = 1$ and that

$$|\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle = \Omega_{\tilde{Q}}^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle. \tag{C.11a}$$

Since $\Omega_Q^{(h)}$ is isometric, these quantities $|\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle$ given by (C.11a) satisfy the same orthonormalization properties as the scattering states $|\Psi_{\mathscr{E}}^{c(-)}\rangle$. Therefore, they belong to the eigenstates that we had introduced in (3.100b), with $\mathscr{E} - \mathscr{E}_0^{(A)} - \tilde{\varepsilon}^{(h)}$. A similar reasoning based on (B.12b) shows that

$$|\Psi_{\mathscr{E}}^{c(-)}\rangle = \hat{\Omega}_Q^{(h)} |\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle. \tag{C.11b}$$

Therefore, a one-to-one correspondence relates the continuum eigenstates of H to those of $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$. It follows that (C.11a) yields all the continuum eigenstates of $\tilde{Q}^{(h)} H \tilde{Q}^{(h)}$. By introducing (C.10)–(C.11a) in (3.68b), we obtain

$$\begin{aligned}[\mathscr{E} - \tilde{P}^{(h)} H \tilde{P}^{(h)} - \tilde{P}^{(h)} H \tilde{Q}^{(h)} (\mathscr{E} - \tilde{Q}^{(h)} H \tilde{Q}^{(h)} - i\eta)^{-1} \tilde{Q}^{(h)} H \tilde{P}^{(h)}] \tilde{P}^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle \\ = \tilde{P}^{(h)} H \tilde{Q}^{(h)} |\tilde{\Phi}_{\mathscr{E}}^{c(-)}\rangle.\end{aligned} \tag{C.12}$$

This equation is similar to (3.68e), except for the appearance of an inhomogeneous term on the right-hand side. By following the same procedure as the one which led from (3.68e) to (3.71), one derives the following inhomogeneous wave equation for the continuum overlap $|\chi_E^{c(-)}\rangle$:

$$[E - \tilde{h}^{(h)}(E)] |\chi_E^{c(-)}\rangle = -|\tilde{\mathscr{J}}^{c(-)}(E)\rangle. \tag{C.13}$$

The quantity $|\tilde{\mathscr{J}}^{c(-)}(E)\rangle$ is defined as

$$\langle \mathbf{r} | \tilde{\mathscr{J}}^{c(-)}(E)\rangle = \langle \tilde{\Phi}_{\mathscr{E}}^{c(-)} | \tilde{Q}^{(h)} H a_{\mathbf{r}} |\Psi_0^{(A)}\rangle \tag{C.14}$$

with $E = E_0^{(A)} - \mathscr{E}$. The solution of (C.13) reads

$$|\chi_E^{c(-)}\rangle = -\tilde{G}^{(h)}(E) |\tilde{\mathscr{J}}^{c(-)}(E)\rangle, \tag{C.15}$$

where $\tilde{G}^{(h)}(E)$ is the resolvent of $\tilde{h}^{(h)}(E)$.

For completeness, we briefly outline the derivation [25] of an analogous relationship between the overlap wave functions $|\chi_{/E}^{c(-)}\rangle$ and the hole Green's function proper, $G^{(h)}(E)$. Note that, in contrast $\tilde{P}^{(h)}$, in general $P^{(h)}$ is not a compact operator. Therefore, the proof of a relation analogous to (C.4b) but involving $P^{(h)}$ requires restrictive hypotheses on the eigenvalues of the density matrix K; see [25]. One defines an isometric generalized Møller operator $\Omega_Q^{(h)}$ by

$$\Omega_Q^{(h)} |A^{(-)}\rangle = \underset{\tau \to +\infty}{\text{st.lim}} e^{iQ^{(h)} H Q^{(h)} \tau} Q^{(h)} e^{-iH\tau} |A^{(-)}\rangle, \tag{C.16}$$

where $Q^{(h)}$ is the projection operator given by (3.11) and (3.17). The analog of (C.11a) is

$$|\Phi_{\mathscr{E}}^{c(-)}\rangle = \Omega_Q^{(h)} |\Psi_{\mathscr{E}}^{c(-)}\rangle. \tag{C.17}$$

Equations (C.13) and (C.14) are replaced by

$$[E - h^{(h)}(E)] |\chi_E^{c(-)}\rangle = -K^{-1} |\mathscr{J}^{c(-)}(E)\rangle, \tag{C.18a}$$

where $\mathscr{J}^{c(-)}(E)$ is defined by (3.38):

$$\langle \mathbf{r} | \mathscr{J}^{c(-)}(E) \rangle = \langle \Phi_{\mathscr{E}}^{c(-)} | \, Q^{(h)} H a_{\mathbf{r}} \, | \Psi_0^{(A)} \rangle. \tag{C.18b}$$

From (C.18a), one gets

$$|\chi_E^{c(-)}\rangle = -G^{(h)}(E)\, K^{-1} \, |\mathscr{J}^{c(-)}(E)\rangle. \tag{C.19}$$

Equations (C.15) and (C.19) show that the continuum overlaps $|\chi_E^{c(-)}\rangle$ are solutions of inhomogeneous equations, in contrast to the discrete overlaps $|\chi_\lambda^{(-)}\rangle$. This is in keeping with the fact that the energy index of $|\chi_E^{c(-)}\rangle$ takes continuous values, while the energies $E_\lambda^{(-)}$ associated with $|\chi_\lambda^{(-)}\rangle$ are determined by an eigenvalue problem.

D. *Scattering States of the* $(A+1)$*-Nucleon System*

In the present appendix, we clarify the detailed nature of the scattering states $|\Psi_{\mathscr{E}}^{c(A\pm1)}\rangle$ that we introduced in (2.2a) and (2.2c). For definiteness, we consider the $(A+1)$-system and drop the upper index $(A+1)$. In the main text, we pay particular attention to the scattering by the target ground state $|\Psi_0^{(A)}\rangle$, but excited target states also have to be included, for instance when one uses the completeness relation (2.3a). We denote the energies of these excited states by $\mathscr{E}_t^{(A)}$,

$$H \, |\Psi_t^{(A)}\rangle = \mathscr{E}_t^{(A)} \, |\Psi_t^{(A)}\rangle. \tag{D.1}$$

In order to fully define the scattering eigenstate $|\Psi_{\mathscr{E}}^{c}\rangle$, one has to specify the nature of the boundary condition that it fulfills. Two types of boundary condition are convenient. The first one corresponds to an incident plane wave; it is discussed in Appendix D.1. The second one corresponds to an incoming spherical wave with well-defined angular momentum; it is discussed in Appendix D.2. The corresponding "plane" and "spherical" overlaps functions are introduced in Appendix D.3. We omit the spin degree of freedom; it could be included without difficulty.

D.1. *Incident Plane Wave*

Equations (3.40a) and (3.41) of [55] show that

$$|\Psi_{\mathbf{k}_t}^{t}\rangle = \frac{i\eta}{\mathscr{E}_k^t - H + i\eta} \, a_{\mathbf{k}_t}^{\dagger} \, |\Psi_t^{(A)}\rangle \tag{D.2a}$$

is a scattering eigenstate of the Hamiltonian of the $(A+1)$-system:

$$H \, |\Psi_{\mathbf{k}_t}^{t}\rangle = \mathscr{E}_k^t \, |\Psi_{\mathbf{k}_t}^{t}\rangle. \tag{D.2b}$$

The energy $\mathscr{E}_k^t$ and the momentum k_t are related by

$$\mathscr{E}_k^t = \mathscr{E}_t^{(A)} + k_t^2/2m. \tag{D.3}$$

Whenever $\mathbf{k}_t$ and t appear together as lower and upper indices of a quantity, the index t of $\mathbf{k}_t$ is not necessary. We shall thus often write

$$|\Psi^t_{\mathbf{k}_t}\rangle = |\Psi^t_{\mathbf{k}}\rangle, \tag{D.4}$$

in keeping with our notation for $\mathscr{E}^t_k$. The solutions of (D.2a) are orthonormal:

$$\langle \Psi^t_{\mathbf{k}} | \Psi^{t'}_{\mathbf{k}'}\rangle = \delta(\mathbf{k}_t - \mathbf{k}'_{t'})\, \delta_{tt'}\,. \tag{D.5a}$$

Together with the bound states $|\Psi_\lambda\rangle$ they form a complete basis:

$$\sum_\lambda |\Psi_\lambda\rangle\langle\Psi_\lambda| + \sum_t \int d\mathbf{k}\, |\Psi^t_{\mathbf{k}}\rangle\langle\Psi^t_{\mathbf{k}}| = \mathscr{I}^{(A+1)}. \tag{D.5b}$$

We now discuss some properties of $|\Psi^t_{\mathbf{k}}\rangle$ in the coordinate space representation. With the same notation as in (4.18b), one has

$$\langle \mathbf{r}, \xi |\, a^\dagger_{\mathbf{k}_t} |\Psi^{(A)}_t\rangle = (A+1)^{-1/2}\, \mathscr{A}\{\langle r | \mathbf{k}_t\rangle\, \Psi^{(A)}_t(\xi)\}. \tag{D.6}$$

By introducing this expression in (D.2a) and using the invariance of H under permutation of coordinates, one finds

$$\Psi^t_{\mathbf{k}}(\mathbf{r}, \xi) = (A+1)^{-1/2}\, \mathscr{A}\hat{\Psi}^t_{\mathbf{k}}(\mathbf{r}, \xi), \tag{D.7}$$

where the non-antisymmetrized wave function

$$\hat{\Psi}^t_{\mathbf{k}}(\mathbf{r}, \xi) = \frac{i\eta}{\mathscr{E}^t_k - H + i\eta}\, \langle \mathbf{r} | \mathbf{k}_t\rangle\, \Psi^{(A)}_t(\xi) \tag{D.8a}$$

is the solution of the Lippmann–Schwinger equation

$$\hat{\Psi}^t_{\mathbf{k}}(\mathbf{r}, \xi) = \langle \mathbf{r} | \mathbf{k}_t\rangle\, \Psi^{(A)}_t(\xi) + (\mathscr{E}^t_k - H + i\eta)^{-1}\, V \langle \mathbf{r} | \mathbf{k}_t\rangle\, \Psi^{(A)}_t(\xi). \tag{D.8b}$$

Here $\langle \mathbf{r} | \mathbf{k}_t\rangle$ is defined by (4.15c), and the symbol V denotes the interaction of the nucleon with coordinate $\mathbf{r}$ with the target nucleons whose coordinates have been generically denoted by ξ. By introducing (D.8b) in (D.7) and then expanding $|\Psi^t_{\mathbf{k}}\rangle$ onto the complete set of target states, one obtains the "fractional parentage expansion,"

$$\Psi^t_{\mathbf{k}}(\mathbf{r}; \xi) = \sum_t w^t_{\mathbf{k}}(\mathbf{r})\, \Psi^{(A)}_t(\xi), \tag{D.8c}$$

and the asymptotic behaviour at large r,

$$\Psi^t_{\mathbf{k}}(\mathbf{r}, \xi) \sim (A+1)^{-1/2} \langle \mathbf{r} | \mathbf{k}_t\rangle\, \Psi^{(A)}_t(\xi) + \sum_{t'} f_{tt'}\, \frac{e^{ik_{t'} r}}{r}\, \Psi^{(A)}_{t'}(\xi). \tag{D.9a}$$

Here $f_{tt'}$ denotes the scattering amplitude. The momenta of the incident and outgoing nucleons are related by

$$\mathscr{E}_k^t = \mathscr{E}_t^{(A)} + k_t^2/2m = \mathscr{E}_{t'}^{(A)} + k_{t'}^2/2m = \mathscr{E}_k^{t'}. \tag{D.9b}$$

In the case of the target ground state, namely for $t=0$, Eq. (D.9a) is the explicit form of (4.18b).

D.2. *Incoming Spherical Waves*

We perform the partial wave expansion

$$\Psi_{\mathbf{k}}^t(\mathbf{r}, \xi) = (mk_t)^{-1/2} \sum_{L,\mu} i^L \Psi_{\mathscr{E}}^c(\mathbf{r}, \xi)\ Y_L^\mu(\hat{\mathbf{k}}_t)^*, \tag{D.10a}$$

where $\mathscr{E} = \mathscr{E}_k^t$ is defined by (D.9b), and

$$\Psi_{\mathscr{E}}^c(\mathbf{r}, \xi) = \varphi_{\mathscr{E}}^c(r, \xi)\ Y_L^\mu(\hat{\mathbf{r}}). \tag{D.10b}$$

The factor $(mk_t)^{-1/2}$ has been introduced in such a way that

$$\langle \Psi_{\mathscr{E}}^c \mid \Psi_{\mathscr{E}'}^{c'} \rangle = \delta(\mathscr{E} - \mathscr{E}')\, \delta_{cc'}. \tag{D.11a}$$

This relation can readily be derived from (D.5a). When spin is included, the quantum numbers generically denoted by c are specified in Section III.1 of [85]. In the present simplified case c stands for the nature of the target (t), the orbital angular momentum (L) and its projection (μ). Thus: $c = \{t, L, \mu\}$. The completeness relation (D.5b) yields

$$\sum_\lambda |\Psi_\lambda\rangle\langle\Psi_\lambda| + \sum_c \int_{\mathscr{T}_c}^\infty d\mathscr{E}\ |\Psi_{\mathscr{E}}^c\rangle\langle\Psi_{\mathscr{E}}^c| = \mathscr{I}^{(A+1)}. \tag{D.11b}$$

Equations (D.11a) and (D.11b) amount to (2.2c) and (2.3a). The asymptotic behaviour of $\Psi_{\mathscr{E}}^c(\mathbf{r}; \mathscr{E})$ at large distance is given by Eq. (3.10.5) of [7],

$$\Psi_{\mathscr{E}}^c(\mathbf{r}; \mathscr{E}) \sim \frac{i}{\sqrt{A+1}} \sum_{c'} \left(\frac{m}{2\pi k_{t'}}\right)^{1/2} \frac{1}{r} \times [e^{-i(k_{t'}r - L'\pi/2)}\delta_{cc'} - S_{cc'} e^{i(k_{t'}r - L'\pi/2)}]\ \Psi_{t'}^{(A)}(\xi)\ Y_{L'}^\mu(\hat{\mathbf{r}}), \tag{D.12}$$

where $S_{cc'}$ is the collision matrix.

D.3. *Overlaps*

We extend (4.20) to excited target states by introducing the overlaps

$$\chi_{\mathbf{k}}^t(\mathbf{r}) = \langle \Psi_0^{(A)} |\ a_{\mathbf{r}}\ | \Psi_{\mathbf{k}}^t \rangle. \tag{D.13}$$

These quantities are related to the spherical overlaps $\chi^c_{\mathscr{E}}(\mathbf{r})$ of (2.5b) by the partial wave expansion

$$\chi^t_{\mathbf{k}}(\mathbf{r}) = (mk_t)^{-1/2} \sum_{L,\mu} i^L \chi^c_{\mathscr{E}}(\mathbf{r})\ Y^{\mu}_{L}(\hat{\mathbf{k}}_t)^*. \tag{D.14}$$

At large distance, one has

$$\chi^t_{\mathbf{k}}(\mathbf{r}) \sim \langle \mathbf{r} \,|\, \mathbf{k}_t \rangle\, \delta_{t0} + f_{t0} e^{ik_0 r}/r. \tag{D.15}$$

We recall that $t=0$ corresponds to the target ground state. In this elastic channel, the asymptotic behaviour of $\chi^0_{\mathbf{k}}(\mathbf{r})$ is

$$\langle \mathbf{r} \,|\, \chi^0_{\mathbf{k}} \rangle \sim \langle \mathbf{r} \,|\, \mathbf{k} \rangle + f(\mathbf{k}, \mathbf{k}')\, e^{ikr}/r, \tag{D.16a}$$

where $f(\mathbf{k}, \mathbf{k}')$ is the elastic scattering amplitude, with

$$\mathbf{k} = \mathbf{k}_0, \qquad \mathbf{k}' = k\frac{\mathbf{r}}{r}. \tag{D.16b}$$

The relationship between $f(\mathbf{k}, \mathbf{k}')$ and the transition matrix is

$$f(\mathbf{k}, \mathbf{k}') = -4\pi^2 m \,\langle \mathbf{k}' |\, \boldsymbol{t}(E_k) \,| \mathbf{k} \rangle, \tag{D.17}$$

with $E_k = k^2/2m$. The asymptotic behaviour of the spherical overlap reads

$$\chi^c_{\mathscr{E}}(\mathbf{r}) \sim i \sum_{c'} \left(\frac{m}{2\pi k_{t'}}\right)^{1/2} \frac{1}{r} \left[e^{-i(kr - L\pi/2)} \delta_{cc'} \delta_{t0} - S_{cc'} \delta_{t'0} e^{i(kr - L'\pi/2)} \right] Y^{\mu}_{L'}(\hat{\mathbf{r}}). \tag{D.18}$$

From (D.14) one can show that

$$\int d\mathbf{k}\, \delta(\mathscr{E} - \mathscr{E}^t_k)\, |\chi^t_{\mathbf{k}}\rangle\langle\chi^t_{\mathbf{k}}| = \sum_{c(t)} |\chi^c_{\mathscr{E}}\rangle\langle\chi^c_{\mathscr{E}}|, \tag{D.19}$$

where $c(t)$ means that the sum runs over all the channels associated with the target state $|\Psi^{(A)}_t\rangle$. Since we omit spin, here this sum only runs over L and μ. Henceforth, we usually do not refer to these quantum numbers and write (D.19) in the simplified form

$$\int d\mathbf{k}\, \delta(\mathscr{E} - \mathscr{E}^t_k)\, |\chi^t_{\mathbf{k}}\rangle\langle\chi^t_{\mathbf{k}}| = |\chi^{c(t)}_{\mathscr{E}}\rangle\langle\chi^{c(t)}_{\mathscr{E}}|. \tag{D.20}$$

E. *One-Body Wave Equation for the Continuum Overlaps* $|\chi^{c(+)}_E\rangle$

As in Appendix D, we attach a "target index" t to quantities associated with the level $|\Psi^{(A)}_t\rangle$ of the A-nucleon system. We recall that $t=0$ corresponds to the target ground state. One of the most important properties of the particle Hamiltonian

$h^{(p)}(E)$ is that it has as eigenstate the elastic scattering overlap $|\chi_{\mathbf{k}}^{0(+)}\rangle$. In the present Appendix E, we show that this property also holds for the particle-type Hamiltonian $\tilde{h}^{(p)}(E)$ defined by (4.80). Besides, we relate the resolvents $\tilde{G}^{(p)}(E)$ and $G^{(p)}(E)$ of $\tilde{h}^{(p)}(E)$ and $h^{(p)}(E)$ to the inelastic overlaps $|\chi_{\mathbf{k}}^{t(+)}\rangle$ with $t \neq 0$.

E.1. *Asymptotic Behaviour of Wave Packets*

The wave packet

$$|\Lambda^{(+)}(\tau)\rangle = e^{-iH\tau}\,|\Lambda^{(+)}\rangle \tag{E.1}$$

is a solution of the time-dependent Schrödinger equation. Initial conditions have to be specified. In keeping with our previous notation, $|\Lambda^{t(+)}\rangle$ corresponds to

$$\underset{\tau \to -\infty}{\text{st.lim}}\,[\,e^{-iH\tau}\,|\Lambda^{t(+)}\rangle - a_{F_t}^{\dagger}\,|\Psi_t^{(A)}\rangle\,] = 0, \tag{E.2a}$$

where $F_t(\mathbf{r}, \tau)$ is a normalizable wave packet localized at large distance of the target. Since antisymmetrization effects vanish when $\tau \to -\infty$, one has moreover

$$\lim_{\tau \to -\infty}\,[\,\langle \Psi_0^{(A)}|\, a_{\mathbf{r}} a_{F_t}^{\dagger}\,|\Psi_t^{(A)}\rangle - F_t(\mathbf{r}, \tau)\,\delta_{t0}\,] = 0. \tag{E.2b}$$

Equations (E.2a) and (E.2b) give

$$\lim_{\tau \to -\infty}\,[\,\langle \Psi_0^{(A)}|\, a_{\mathbf{r}} e^{-iH\tau}\,|\Lambda^{t(+)}\rangle - F_t(\mathbf{r}, \tau)\,\delta_{t0}\,] = 0. \tag{E.2c}$$

By multiplying (E.2c) by $a_{\mathbf{r}}^{\dagger}\,|\Psi_0^{(A)}\rangle$ and then integrating over $\mathbf{r}$ one finds that

$$\underset{\tau \to -\infty}{\text{st.lim}}\,[\,\tilde{P}^{(p)} e^{-iH\tau}\,|\Lambda^{t(+)}\rangle - a_{F_t}^{\dagger}\,|\Psi_0^{(A)}\rangle\,\delta_{t0}\,] = 0, \tag{E.2d}$$

where $\tilde{P}^{(p)}$ is defined by (4.75a). We now derive useful limits in the case of the scattering from the ground state ($t = 0$) and from an excited state ($t \neq 0$), respectively. For simplicity, in the following we omit the upper index $(+)$ which recalled that we deal with the $(A+1)$-system.

(a) *From scattering from the target ground state*, Eqs. (4.75c), (E.2a), and (E.2d) give

$$\underset{\tau \to -\infty}{\text{st.lim}}\,(1 - \tilde{P}^{(p)})\,e^{-iH\tau}\,|\Lambda^0\rangle = \underset{\tau \to -\infty}{\text{st.lim}}\,\tilde{Q}^{(p)}\tilde{Q}^{(p)} e^{-iH\tau}\,|\Lambda^0\rangle = 0, \tag{E.3a}$$

which implies that

$$\lim_{\tau \to -\infty}\,\|\,\{\tilde{Q}^{(p)}\}^2\,e^{-iH\tau}\,|\Lambda^0\rangle\,\| = 0. \tag{E.3b}$$

By definition, one has

$$\|\tilde{Q}^{(p)} e^{-iH\tau}\,|\Lambda^0\rangle\|^2 = \langle \Lambda^0|\, e^{iH\tau}\tilde{Q}^{(p)}\tilde{Q}^{(p)} e^{-iH\tau}\,|\Lambda^0\rangle. \tag{E.3c}$$

Schwartz' inequality then yields

$$\|\tilde{Q}^{(p)}e^{-iH\tau}\,|\Lambda^0\rangle\|^2 \leqslant \|\Lambda^0\| \cdot \|\tilde{Q}^{(p)}\tilde{Q}^{(p)}e^{-iH\tau}\,|\Lambda^0\rangle\|. \tag{E.3d}$$

Therefore, (E.3b) and (E.3d) give

$$\lim_{\tau \to -\infty} \|\tilde{Q}^{(p)}e^{-iH\tau}\,|\Lambda^0\rangle\| = 0, \tag{E.3e}$$

which can also be written as

$$\lim_{\tau \to -\infty} \|e^{i\tilde{Q}^{(p)}H\tilde{Q}^{(p)}t}\tilde{Q}^{(p)}e^{-iH\tau}\,|\Lambda^0\rangle\| = 0. \tag{E.3f}$$

(b) *For scattering from an excited state of the target*, Eq. (E.2d) yields

$$\text{st.}\lim_{\tau \to -\infty} \tilde{P}^{(p)}e^{-iH\tau}\,|\Lambda^t\rangle = 0 \qquad \text{for} \quad t \neq 0. \tag{E.4}$$

By using Schwartz' inequality as in case (a), Eq. (E.4) leads to

$$\lim_{\tau \to -\infty} \|(\tilde{P}^{(p)})^{1/2}\,e^{-iH\tau}\,|\Lambda^t\rangle\| = 0 \qquad \text{for} \quad t \neq 0. \tag{E.5}$$

E.2. *Generalized Møller Operator Associated with* $\tilde{h}^{(p)}(E)$

We now use the relations (E.3f) and (E.5) to derive equations fulfilled by the overlaps $|\chi^t_{\mathbf{k}}\rangle$. Like in (C.6) we define a generalized Møller operator $\Omega^{(p)}_{\tilde{Q}}$ by

$$\Omega^{(p)}_{\tilde{Q}}\,|\Lambda^t\rangle = \text{st.}\lim_{\tau \to -\infty} e^{i\tilde{Q}^{(p)}H\tilde{Q}^{(p)}\tau}\tilde{Q}^{(p)}e^{-iH\tau}\,|\Lambda^t\rangle. \tag{E.6a}$$

We assume that this strong limit exists. This implies the existence of the integral

$$\int_{-\infty}^{0} d\tau \frac{d}{d\tau}\,(e^{i\tilde{Q}^{(p)}H\tilde{Q}^{(p)}\tau}\tilde{Q}^{(p)}e^{-iH\tau})\,|\Lambda^t\rangle = \tilde{Q}^{(p)}\,|\Lambda^t\rangle - \Omega^{(p)}_{\tilde{Q}}\,|\Lambda^t\rangle. \tag{E.6b}$$

A time-independent wave equation is obtained from (E.6b) by means of Fourier transforms. An adiabatic convergence factor $e^{\eta\tau}$ must be introduced [83, 84]. This yields

$$\tilde{Q}^{(p)}\,|\Psi^t_{\mathbf{k}}\rangle = \Omega^{(p)}_{\tilde{Q}}\,|\Psi^t_{\mathbf{k}}\rangle + (\mathscr{E}^t_k - \tilde{Q}^{(p)}H\tilde{Q}^{(p)} + i\eta)^{-1}\,\tilde{Q}^{(p)}H\tilde{P}^{(p)}\,|\Psi^t_{\mathbf{k}}\rangle, \tag{E.7}$$

where we used the simplified notation (D.4) and where $\mathscr{E}^t_k$ is defined by (D.3).

(a) *In the case of scattering from the target ground state*, (E.3f) implies that

$$\Omega^{(p)}_{\tilde{Q}}\,|\Psi^0_{\mathbf{k}}\rangle = 0. \tag{E.8a}$$

Therefore,

$$\tilde{Q}^{(p)} \,|\Psi^0_{\mathbf{k}}\rangle = (\mathscr{E}_k - \tilde{Q}^{(p)} H \tilde{Q}^{(p)} + i\eta)^{-1}\, \tilde{Q}^{(p)} H \tilde{P}^{(p)} \,|\Psi^0_{\mathbf{k}}\rangle, \tag{E.8b}$$

where

$$\mathscr{E}_k = \mathscr{E}^0_k = \mathscr{E}^{(A)}_0 + k^2/2m = \mathscr{E}^{(A)}_0 + E_k. \tag{E.8c}$$

Note the analogy between (E.8b) and (4.77d). By following the same procedure as that which led from (4.77e) to (4.80), we find

$$\tilde{h}^{(p)}(E) \,|\chi^0_{\mathbf{k}}\rangle = E_k \,|\chi^0_{\mathbf{k}}\rangle. \tag{E.9a}$$

We can also write (E.9a) in terms of the spherical elastic overlap; see (4.24c):

$$\tilde{h}^{(p)}(E) \,|\chi^0_E\rangle = E \,|\chi^0_E\rangle. \tag{E.9b}$$

We have thus proved that the elastic overlaps are eigenstates of the particle-type Hamiltonian $\tilde{h}^{(p)}(E)$. The latter thus fulfills the requirement (4.3b).

(b) *In the case of scattering from an excited target state*, the first term of the right-hand side of (E.7) does not vanish. From (E.6a), one gets, using (C.4a) and (E.5):

$$\Omega^{(p)}_{\tilde{Q}} \,|\Lambda^t\rangle = \underset{\tau \to -\infty}{\text{st.lim}}\, e^{i\tilde{Q}^{(p)} H \tilde{Q}^{(p)} \tau} e^{-iH\tau} \,|\Lambda^t\rangle \qquad \text{for} \quad t \neq 0. \tag{E.10a}$$

Hence, $\Omega^{(p)}_{\tilde{Q}}$ is an isometric operator when it acts on vector states associated with inelastic boundary conditions, since it is then the limit of isometric operators. Equations (4.77c) and (E.7) show that, for $t \neq 0$, the quantity

$$|\tilde{\Phi}^t_{\mathbf{k}}\rangle = \Omega^{(p)}_{\tilde{Q}} \,|\Psi^t_{\mathbf{k}}\rangle \qquad \text{with} \quad t \neq 0 \tag{E.10b}$$

is an eigenstate of $\tilde{Q}^{(p)} H \tilde{Q}^{(p)}$ with eigenvalue $\mathscr{E}^t_k$. We emphasize that this is true only for $t \neq 0$. Indeed, (E.8a) shows that the right-hand side of (E.10b) would vanish in the case $t = 0$. By introducing (E.7) and (E.10b) in (4.77a), we find

$$\begin{aligned}[\mathscr{E}^t_k - \tilde{P}^{(p)} H - \tilde{P}^{(p)} H \tilde{Q}^{(p)} (\mathscr{E}^t_k - \tilde{Q}^{(p)} H \tilde{Q}^{(p)} + i\eta)^{-1}\, \tilde{Q}^{(p)} H]\, \tilde{P}^{(p)} \,|\Psi^{t\neq 0}_{\mathbf{k}}\rangle \\ = \tilde{P}^{(p)} H \tilde{Q}^{(p)} \,|\tilde{\Phi}^{t\neq 0}_{\mathbf{k}}\rangle.\end{aligned} \tag{E.11}$$

By following a procedure similar to the one which led from (4.77e) to (4.80), we obtain the inhomogeneous equation

$$\{E^t_k - \tilde{h}^{(p)}(E^t_k)\} \,|\chi^t_{E_k}\rangle = |\tilde{\mathscr{J}}^t(E^t_k)\rangle \qquad \text{for} \quad t \neq 0, \tag{E.12a}$$

where E^t_k is defined by (4.53b). Equation (E.12a) yields

$$|\chi^t_{\mathbf{k}}\rangle = \tilde{G}^{(p)}(E^t_k + i\eta) \,|\tilde{\mathscr{J}}^t(E^t_k)\rangle \qquad (\text{for } t \neq 0). \tag{E.12b}$$

In summary, the isometric operator

$$\Omega_{\tilde{Q}}^{(p)} = \underset{\tau \to -\infty}{\text{st.lim}}\, e^{i\tilde{Q}^{(p)} H \tilde{Q}^{(p)} \tau} e^{-iH\tau} \tag{E.13a}$$

generates the continuous eigenvectors of $\tilde{Q}^{(p)} H \tilde{Q}^{(p)}$ from those of H. The operator

$$\underset{\tau \to -\infty}{\text{st.lim}}\, e^{i\tilde{Q}^{(p)} H \tilde{Q}^{(p)} \tau} \tilde{Q}^{(p)} e^{-iH\tau} \tag{E.13b}$$

has the same property when it coincides with $\tilde{\Omega}_{\tilde{Q}}^{(p)}$. This only holds in the inelastic subspace spanned by $\{\Psi_{\mathbf{k}}^{t \neq 0}\}$. In contrast, these two operators differ when they act on wave packets $|\Lambda^0\rangle$. Indeed,

$$\underset{\tau \to -\infty}{\text{st.lim}}\, e^{i\tilde{Q}^{(p)} H \tilde{Q}^{(p)} \tau} \tilde{Q}^{(p)} e^{-iH\tau} |\Lambda^0\rangle = 0, \tag{E.13c}$$

while

$$\underset{\tau \to -\infty}{\text{st.lim}}\, e^{i\tilde{Q}^{(p)} H \tilde{Q}^{(p)} \tau} e^{-iH\tau} |\Lambda^0\rangle \tag{E.13d}$$

has an oscillating behaviour. The proper interpretation of these features is that $\tilde{Q}^{(p)} H \tilde{Q}^{(p)}$ does not have eigenstates which correspond to elastic scattering boundary conditions.

E.3. *Generalized Møller Operator Associated with* $h^{(p)}(E)$

The relations derived in Section E.2 can readily be adapted to Feshbach's projection operator $P^{(p)}$. The corresponding Møller operator is

$$\Omega_{Q}^{(p)} = \underset{\tau \to +\infty}{\text{st.lim}}\, e^{iQ^{(p)} H Q^{(p)} \tau} Q^{(p)} e^{-iH\tau}. \tag{E.14a}$$

Equations (E.8a) and (E.10b) become

$$\Omega_{Q}^{(p)} |\Psi_k^0\rangle = 0, \tag{E.14b}$$

$$|\Phi_{\mathbf{k}}^t\rangle = \Omega_{Q}^{(p)} |\Psi_{\mathbf{k}}^t\rangle \qquad \text{with} \quad t \neq 0. \tag{E.14c}$$

Equation (E.9a) now reads

$$h^{(p)}(E) |\chi_{\mathbf{k}}^0\rangle = E_k |\chi_{\mathbf{k}}^0\rangle. \tag{E.15}$$

The latter equation is equivalent to (4.24b), of which we thus provided another derivation in the framework of time-dependent scattering theory. Equation (E.12a) becomes

$$\{E_k^t - h^{(p)}(E_k^t)\} |\chi_{\mathbf{k}}^t\rangle = (1-K)^{-1} |\mathscr{J}^t(E_k^t)\rangle \qquad \text{for} \quad t \neq 0, \tag{E.16a}$$

where $\mathscr{J}^t(E_k^t)$ is defined by (4.62b). Equations (4.10c) and (E.16a) give

$$|\chi_{\mathbf{k}}^t\rangle = G^{(p)}(E_k^t + i\eta)(1-K)^{-1}\,|\mathscr{J}^t(E_k^t)\rangle \qquad \text{for} \quad t \neq 0. \tag{E.16b}$$

E.4. *Incoming Wave Boundary Condition*

Let us write the Lippmann–Schwinger equation (4.19) in the schematic form

$$|\Psi_{\mathscr{E}}^0\rangle = \frac{i\eta}{\mathscr{E} - H + i\eta}\, a_{\mathbf{k}}^\dagger\, |\Psi_0^{(A)}\rangle. \tag{E.17}$$

At large distance, it has the "outgoing" behaviour given by (D.12). The corresponding overlap is $|\chi_E^0\rangle$. In scattering theory, it is also useful to introduce the solution of

$$|\bar{\Psi}_{\mathscr{E}}^0\rangle = \frac{-i\eta}{\mathscr{E} - H - i\eta}\, a_{\mathbf{k}}^\dagger\, |\Psi_0^{(A)}\rangle, \tag{E.18}$$

which is associated with an "incoming" wave boundary condition. By definition, the corresponding overlap is

$$|\bar{\chi}_E^0\rangle = \langle \Psi_0^{(A)}|\, a_{\mathbf{r}}\, |\bar{\Psi}_{\mathscr{E}}^0\rangle. \tag{E.19}$$

By taking the limit $\tau \to -\infty$ instead of $\tau \to +\infty$ in the preceding subsections, one finds that $|\bar{\chi}_E^0\rangle$ is an eigenstate of $[h^{(p)}(E)]^\dagger$ as well as of $[\tilde{h}^{(p)}(E)]^\dagger$:

$$[h^{(p)}(E)]^\dagger\, |\bar{\chi}_E^0\rangle = E\, |\bar{\chi}_E^0\rangle, \qquad [\tilde{h}^{(p)}(E)]^\dagger\, |\bar{\chi}_E^0\rangle = E\, |\bar{\chi}_E^0\rangle. \tag{E.20}$$

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