Notes on Green's Functions Theory for Quantum Many-Body Systems

Carlo Barbieri

Department of Physics, University of Surrey,
Guildford GU2 7XH, UK

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Literature

A modern and compresensive monography is

- W. H. Dickhoff and D. Van Neck, *Many-Body Theory Exposed!*, 2nd ed. (World Scientific, Singapore, 2007).

This book covers several applications of Green's functions done in recent years, including nuclear and electroncic systems. Most the material of these lectures can be found here.

Two popular textbooks, that cover the almost complete formalism, are

- A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Physics* (McGraw-Hill, New York, 1971),

- A. A. Abrikosov, L. P. Gorkov and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).

Other useful books on many-body Green's functions theory, include

- R. D. Mattuck, *A Guide to Feynmnan Diagrams in the Many-Body Problem*, (McGraw-Hill, 1976) [reprinted by Dover, 1992],

- J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge MA, 1986),

- J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Benjamin, Redwood City CA, 1988).

Chapter 1

Preliminaries: Basic Formulae of Second Quantization and Pictures

Many-body Green's functions (MBGF) are a set of techniques that originated in quantum field theory but have also found wide applications to the many-body problem. In this case, the focus are complex systems such as crystals, molecules, or atomic nuclei. However, many-body Green's functions still share the same language with elementary particles theory, and have several concepts in common. To apply this formalism, one needs to use of the creation/destruction operators of second quantization and the Heisenberg and interaction pictures of quantum mechanics.

The purpose of this chapter is to gather the basic results of second quantization and pictures, so that they can be used for reference later on. One the way, we will introduce some of the notation to be used in our discussions.

1.1 A Note on Single-Particle Indices

The following conventions will be used in most of these notes.

When needed, the boldface $\mathbf{r}$ will be used to refer to the position of particles in coordinate space and $\mathbf{k}$ for momentum space. When internal degrees of freedom are present, $\mathbf{x}\equiv(\mathbf{r},\ \sigma,\ \tau,\ ...)$ will be used. However, most of the results to be discussed are valid for any general single particle basis. Thus, we will use greek indices, α,β,γ,..., to refer to *all* the states in the baisis. In general, $\{\alpha_i\}$ is a complete set of orthonormalized one-body wave functions and will be assumed to be discrete, unless it implies a loss of

generality.[1]

In many-body theory one often starts from a product wave function decribing a set of non interacting particles that occupy given orbits (called the *reference* state). This could be a Slater determinant for fermions or a macroscopic condensate orbit for bosons. It is customary to reserve the latin letters h,i,j,k,l for the levels occupied in the reference state (which are called *hole* orbits) and m,n,p,q,... for the unoccupied orbits of the basis (the *particle* orbits).

Since removing a hole orbit from the reference state leads to a systems with fewer particles, we extend the use latin hole indices to indicate states of $N-1$,$N-2$,... particles. Here, N is the number of particles in the referecnce state. Analogously, particle indices will be used to distinguish states of N,$N+1$,$N+2$,... particles. This notation will include labelling exact many-body eigenstates of the Hamiltoninan. It should not be felt as unnatural: the eigenstates of $N-1$ and $N+1$ bodies can be seen as excitations of the systems and directly are related to *quasiholes* and *suasiparticle* in the Landau sense.

1.2 Second Quantization

Most of the processes described by many-body Green's functions involve the transfer of particles to/from the intital sysytem. Thus it is useful to extend the Hilbert space to allow for states with different particle numbers. In fact we will use the Fock space which includes a complete basis set for each possible number of particles, from zero (the vacuum) to infinity. The basis states of the Fock space can be taken to be product of one-body wave functions and must be automatically symmetrized or antisymmetrized (for bosons and fermions, respectively). Using Dirac's bra and ket notation one can specify the basis states just by saying how many particles n_α are contained in each single particle orbit α. For example, the state[2]

$$|n_{\alpha_1}=3,\ n_{\alpha_2}=0,\ n_{\alpha_3}=2, n_{\alpha_4}=2,\ n_{\alpha_5}=0,\ \ldots\ \rangle\,, \tag{1.1}$$

contains a total of $N=\sum_i n_{\alpha_i}=7$ particles, distributed over the orbits α_1, α_3 and α_4. Obviously this must be a bosons state, or it would violate the Pauli exclusion principle with disastrous consequences. Note that, also due to

[1] What the $\{\alpha_i\}$ represent depends on the systems one wants to study (e.g., harmonic oscillator wave functions for nucleons in a nucleus or atoms in a trap, orthogonalized gaussian orbits in a molecule, Bloch vectors in a crystal, and so on...).

[2] In this case the corresponding product wave function would be the symmetrized $\mathcal{S}[\phi_{\alpha_1}(\mathbf{r}_1)\phi_{\alpha_1}(\mathbf{r}_2)\phi_{\alpha_1}(\mathbf{r}_3)\phi_{\alpha_3}(\mathbf{r}_4)\phi_{\alpha_3}(\mathbf{r}_5)\phi_{\alpha_4}(\mathbf{r}_6)\phi_{\alpha_4}(\mathbf{r}_7)]$.

Pauli, we can only say how many particles are in each orbit but not "which" particles.

The completeness relation in Fock space is

$$\mathbf{I} = \sum_{n_1=0}^{n_{max}} \sum_{n_2=0}^{n_{max}} \sum_{n_3=0}^{n_{max}} \cdots \sum_{n_\alpha=0}^{n_{max}} \cdots \\ |n_1,\ n_2,\ n_3,\ \ldots\ n_\alpha,\ \ldots\rangle\langle n_1,\ n_2,\ n_3,\ \ldots\ n_\alpha,\ \ldots\ | \tag{1.2}$$

and includes the vacuum state $|0\rangle \equiv |n_\alpha = 0, \forall\alpha\rangle$. n_{max} is 1 for fermions and ∞ for bososns. States with different number of particles are orthogonal by definition.

The second quantization formalism introduces the *creation* operator $c_\alpha^\dagger$ which adds a particle in state α to a vector of the Fock space. Its self-adjoint c_α removes a particle from the same state and is called *destruction* or *annihilation* operator. Their effect on Fock states is the same as that for the cration and annihilation of harmonic oscillator quanta in the linear oscillator problem

$$c_\alpha^\dagger |n_1,\ n_2,\ldots\ n_\alpha,\ldots\rangle = \sqrt{n_\alpha + 1}\ |n_1,\ n_2,\ldots\ n_\alpha + 1,\ldots\rangle\ , \tag{1.3}$$

$$c_\alpha |n_1,\ n_2,\ldots\ n_\alpha,\ldots\rangle = \sqrt{n_\alpha}\ |n_1,\ n_2,\ldots\ n_\alpha - 1,\ldots\rangle\ , \tag{1.4}$$

where we momentarily neglect a conventional signs that appears for fermions [see Eqs. (1.11) and (1.12) below]. Note that destroying and empty states ($c_\alpha|n_\alpha = 0\rangle = 0$) gives the c-numer zero, and not the vacuum state $|0\rangle$. From these relations it follows that $c_\alpha^\dagger c_\alpha |n_\alpha\rangle = n_\alpha |n_\alpha\rangle$ yields the number of particles the state α. The operator for the total number of particles is then,

$$N = \sum_\alpha c_\alpha^\dagger c_\alpha\ . \tag{1.5}$$

The eigenvalues of N are non negative integers and its eigenstates are wave functions with a definite number of particle. By applying Eqs. (1.3) and (1.4) to these states, one can see that the following commutation relations must apply,

$$[N, c_\alpha] = -c_\alpha\ , \quad \left[N, c_\alpha^\dagger\right] = c_\alpha^\dagger\ . \tag{1.6}$$

Equations from (1.2) to (1.6) are valid for both boson and fermions. Eq. (1.4) makes it impossible to create Fock states by removing a particle from an alredy empty orbit. However, there is still no restriction on the nuber of particles that can be added in the case of Fermions. The correct Pauli statistics is imposed by choosing different commutation and anticom-

mutation relations[3],

$$\left[c_\alpha, c_\beta^\dagger\right] = \delta_{\alpha,\beta} \ , \qquad [c_\alpha, c_\beta] = \left[c_\alpha^\dagger, c_\beta^\dagger\right] = 0 \ , \qquad \text{for bososns} \tag{1.7}$$

$$\left\{c_\alpha, c_\beta^\dagger\right\} = \delta_{\alpha,\beta} \ , \qquad \{c_\alpha, c_\beta\} = \left\{c_\alpha^\dagger, c_\beta^\dagger\right\} = 0 \ , \qquad \text{for fermions} \tag{1.8}$$

With both these relations, Eq. (1.6) is still valid. At the same time the anticommutator $c_\alpha^\dagger c_\beta^\dagger = -c_\beta^\dagger c_\alpha^\dagger$ ($\Rightarrow c_\alpha^\dagger c_\alpha^\dagger$=0) imposes the antisymmetrization of fermionic wave functions and restrict the occupation of each orbit to n_α=0,1 only.

To create the basis (1.2), one simply acts several times on $|0\rangle$ with creation operators. The normalized many-body states are given by

$$|n_1,\ n_2, \cdots,\ n_\alpha, \cdots\rangle = \frac{1}{\sqrt{n_1!\ n_2! \ldots n_\alpha! \ldots}} (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \cdots (c_\alpha^\dagger)^{n_\alpha} \cdots |0\rangle \ , \tag{1.9}$$

which simplifies in the fermion case because it can only be n_α!=1,

$$|n_1,\ n_2, \cdots,\ n_\alpha, \cdots\rangle = (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \cdots (c_\alpha^\dagger)^{n_\alpha} \cdots |0\rangle \ . \tag{1.10}$$

Note that only for the case of bosons Eq. (1.9) is independent on the order in which the creations operators are applied. For Fermoins a phase sign is introduced by changing the order and one must put extra care to avoid confusions. Ususally one chooses a specific order in the $\{\alpha\}$ and then stick to it. Once this is done the correct fermionic version of Eqs. (1.3) and (1.4)

$$c_\alpha^\dagger |n_1, n_2, \ldots n_\alpha, \ldots\rangle = \delta_{0,n_\alpha} (-)^{s_\alpha} \sqrt{n_\alpha + 1} |n_1, n_2, \ldots n_\alpha + 1, \ldots\rangle \ , \tag{1.11}$$

$$c_\alpha |n_1, n_2, \ldots n_\alpha, \ldots\rangle = \delta_{1,n_\alpha} (-)^{s_\alpha} \quad \sqrt{n_\alpha} \quad |n_1, n_2, \ldots n_\alpha - 1, \ldots\rangle \ , \tag{1.12}$$

with

$$s_\alpha = n_1 + n_2 + n_3 + \cdots + n_{\alpha-1} \ . \tag{1.13}$$

The creation operator for a particle in position $\mathbf{r}$ of coordinate space is indicated by $\psi(\mathbf{r})$. If $\{u_\alpha(\mathbf{r})\}$ are the single particle wave functions of a general orthonormal basis, the creation (and annihilation) operators in the two representation are related via a unitary transormation,

$$\psi^\dagger(\mathbf{r}) = \sum_\alpha c_\alpha^\dagger u_\alpha^*(\mathbf{r}) \ , \tag{1.14}$$

$$c_\alpha^\dagger = \int d\mathbf{r}\ \psi^\dagger(\mathbf{r}) u_\alpha(\mathbf{r}) \ . \tag{1.15}$$

[3]Here, $[A, B] \equiv AB - BA$ and $\{A, B\} \equiv AB - BA$ are the commutator and anticommutors, respectively. Later on we will also use the more compact notation $[A, B]_\mp \equiv AB \mp BA$ to indicate both at the same time. Otherwise, [,] without sign will always be a commutator.

It follows that to create a particle in a state α one simply superimposes eigenstates of position with weights given by the corresponding wave function,

$$|\alpha\rangle = c_\alpha^\dagger|0\rangle = \int d\mathbf{r}\; u_\alpha(\mathbf{r})|\mathbf{r}\rangle \; . \tag{1.16}$$

where

$$|\mathbf{r}\rangle = \psi^\dagger(\mathbf{r})|0\rangle \; . \tag{1.17}$$

is a particle localized in $\mathbf{r}$. Analogously, one can extract the wave funcion corresponding to a one-body Fock state by

$$u_\alpha(\mathbf{r}) = \langle\mathbf{r}|\alpha\rangle \; . \tag{1.18}$$

These relations are extentded to states of any particle number, where

$$|\mathbf{r}_1, \mathbf{r}_2, \ldots\; \mathbf{r}_N\rangle = \frac{1}{\sqrt{N!}}\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\cdots\psi^\dagger(\mathbf{r}_N)|0\rangle \; . \tag{1.19}$$

and the first quantization wave function of an N-body Fock state is

$$\langle\mathbf{r_1}, \mathbf{r}_2, \ldots\; \mathbf{r}_N|n_1, n_2, \ldots\rangle = \Phi(\mathbf{r_1}, \mathbf{r}_2, \ldots\; \mathbf{r}_N; \{n\}) \; . \tag{1.20}$$

1.2.1 Examples

- If $|\mathbf{r}'\rangle$ and $|\mathbf{p}\rangle$ are eigenstates of position and momentum one has

$$\langle\mathbf{r}'|\mathbf{r}\rangle = \delta(\mathbf{r}-\mathbf{r}') \; , \tag{1.21}$$

$$\langle\mathbf{r}|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{r}\mathbf{p}/\hbar} \; . \tag{1.22}$$

- Given the Fock state $|\alpha\beta\rangle = c_\alpha^\dagger c_\beta^\dagger|0\rangle$, the corresponding antisymmetrized wave function in first quantization is

$$\Phi_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) = \langle\mathbf{r}_1\mathbf{r}_2|\alpha\beta\rangle \tag{1.23}$$

$$= \frac{1}{\sqrt{2}}\langle 0|\psi(\mathbf{r}_2)\psi(\mathbf{r}_1)c_\alpha^\dagger c_\beta^\dagger|0\rangle \tag{1.24}$$

$$= \frac{1}{\sqrt{2}}\sum_{\gamma\delta} u_\gamma(\mathbf{r}_1)u_\delta(\mathbf{r}_2)\langle 0|c_\delta c_\gamma c_\alpha^\dagger c_\beta^\dagger|0\rangle \; . \tag{1.25}$$

  Using the (anti)commutator relations (1.7) and (1.8) one finds that $c_\delta c_\gamma c_\alpha^\dagger c_\beta^\dagger|0\rangle = (\delta_{\alpha,\gamma}\delta_{\beta,\delta} \pm \delta_{\alpha,\gamma}\delta_{\beta,\delta})\,|0\rangle$, with the upper (lower) sign referring to bosons (fermions). This leads to the usual symmetrized and antisymmetrized product wave functions of Slater type,

$$\Phi_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\{u_\alpha(\mathbf{r}_1)u_\beta(\mathbf{r}_2) \pm u_\beta(\mathbf{r}_1)u_\alpha(\mathbf{r}_2)\} \; . \tag{1.26}$$

1.3 Operators in Fock Space

1.3.1 Operators

Let $O = O(\mathbf{r})$ be a one-body operator that acts independently on each particle of the systems. The expression for its matrix elements in coordinate systems depends on the number of particles N and is

$$\langle \mathbf{r}'_1, \mathbf{r}'_2, \dots \ \mathbf{r}'_N | O | \mathbf{r}_1, \mathbf{r}_2, \dots \ \mathbf{r}_N \rangle = \left(\prod_{j=1}^{N} \delta(\mathbf{r}_i - \mathbf{r}'_i) \right) \sum_{i=1}^{N} O(\mathbf{r}_i) \ . \tag{1.27}$$

The corresponding results for a generic Fock states can be related to the latter by inserting a completeness relation based on the position states (1.19),

$$\begin{aligned}
&\langle n'_1, n'_2, \dots | O | n_1, n_2, \dots \rangle \\
&= \sum_{i=1}^{N} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \cdots \int d\mathbf{r}_N \langle n'_1, n'_2, \dots | \mathbf{r}_1, \mathbf{r}_2, \dots \ \mathbf{r}_N \rangle \\
&\qquad \times O(\mathbf{r}_i) \langle \mathbf{r}_1, \mathbf{r}_2, \dots \ \mathbf{r}_N | n_1, n_2, \dots \rangle \qquad (1.28) \\
&= \frac{1}{N!} \sum_{i=1}^{N} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \cdots \int d\mathbf{r}_N \langle n'_1, n'_2, \dots | \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2) \cdots \ \psi^\dagger(\mathbf{r}_N) | 0 \rangle \\
&\qquad \times O(\mathbf{r}_i) \langle 0 | \psi(\mathbf{r})_N \cdots \psi(\mathbf{r})_2 \psi(\mathbf{r})_1 | n_1, n_2, \dots \rangle \\
&= \frac{1}{(N-1)!} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \cdots \int d\mathbf{r}_N \langle n'_1, n'_2, \dots | \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2) \cdots \ \psi^\dagger(\mathbf{r}_N) \\
&\qquad \times O(\mathbf{r}_1) \psi(\mathbf{r})_N \cdots \psi(\mathbf{r})_2 \psi(\mathbf{r})_1 | n_1, n_2, \dots \rangle
\end{aligned}$$

In the last line we have removed the sum over the interacting particle since it gives N times the same contribution. The projection on the vacuum state $|0\rangle\langle 0|$ can be subsituted with the identity becose the operators $\psi(\mathbf{r})$ $(\psi(\mathbf{r})^\dagger)$ have already annihilated all the particle contained in the ket (bra) vectors.

We still need to perform the integration on the coordinates $\mathbf{r}_2$ to $\mathbf{r}_N$. This is easlily done remembering that $\int d\mathbf{r} \psi(\mathbf{r})^\dagger \psi(\mathbf{r})$ is the particle number operator in coordinate space (1.5). One starts integrating over $\mathbf{r}_N$ to get a factor of 1, then the integral over $\mathbf{r}_{N-1}$ gives 2, and so on up to cancelling the factor $(N-1)!$ at the denomonator. Finally,

$$\langle n'_1, n'_2, \dots | O | n_1, n_2, \dots \rangle = \int d\mathbf{r} \ \langle n'_1, n'_2, \dots | \psi(\mathbf{r})^\dagger O(\mathbf{r}) \psi(\mathbf{r}) | n_1, n_2, \dots \rangle \ . \tag{1.29}$$

The one-body operator in second quantization representation is therefore

$$\begin{aligned}
O &= \int d\mathbf{r} \ \psi(\mathbf{r})^\dagger O(\mathbf{r}) \psi(\mathbf{r}) \\
&= \sum_{\alpha\beta} o_{\alpha\beta} \ c^\dagger_\alpha c_\beta \ , \qquad (1.30)
\end{aligned}$$

where $o_{\beta\alpha}$ are the metrix elements in the generic basis $\{\alpha\}$, as can be verified inseting Eq. (1.14) in the latter equation

$$o_{\alpha\beta} = \int d\mathbf{r}\; u^*_\alpha(\mathbf{r}) O(\mathbf{r}) u_\beta(\mathbf{r}) \; . \tag{1.31}$$

For a two body operator (symmetric in the exchange of $\mathbf{r}_i$ and $\mathbf{r}_j$),

$$V = \sum_{i<j}^{N} V(\mathbf{r}_i, \mathbf{r}_j) \; , \tag{1.32}$$

one obtains

$$\begin{aligned} V &= \int d\mathbf{r}_1 \int d\mathbf{r}_2 \psi(\mathbf{r}_1)^\dagger \psi(\mathbf{r}_2)^\dagger V(\mathbf{r}_i, \mathbf{r}_2) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1) \\ &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \tilde{v}_{\alpha\beta,\gamma\delta}\; c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \\ &= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta}\; c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \; , \end{aligned} \tag{1.33}$$

with the matrix elements

$$\tilde{v}_{\alpha\beta,\gamma\delta} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 u^*_\alpha(\mathbf{r}_1) u^*_\beta(\mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2) u_\gamma(\mathbf{r}_1) u_\delta(\mathbf{r}_2) \; , \tag{1.34}$$

Note the particular order of the destruction operators in Eq. (1.33), which is inverted with respect to the creation ones. Attention must be paied to this in case of fermionic systems since this introduces an extra phase (for bososn the ordering is irrelevant). In many case is turns out to be more convenient including the $\frac{1}{4}$ factor and employing the (anti)symmetrized form to the matrix elements

$$v_{\alpha\beta,\gamma\delta} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 u^*_\alpha(\mathbf{r}_1) u^*_\beta(\mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2) \left[u_\gamma(\mathbf{r}_1) u_\delta(\mathbf{r}_2) \pm u_\delta(\mathbf{r}_1) u_\gamma(\mathbf{r}_2) \right] \; , \tag{1.35}$$

where + (-) refer to bosons (fermions).

When also a three-body interaction (symmetric in the particle indeces) is necessary,

$$W = \sum_{i<j<k}^{N} W(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) \; , \tag{1.36}$$

the corresponding operator in second quantization is

$$W = \frac{1}{3!} \sum_{\alpha\beta\gamma\mu\nu\lambda} \tilde{w}_{\alpha\beta\gamma,\mu\nu\lambda}\; c^\dagger_\alpha c^\dagger_\beta c^\dagger_\gamma c_\lambda c_\nu c_\mu \; , \tag{1.37}$$

with

$$\tilde{w}_{\alpha\beta\gamma,\mu\nu\lambda} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \int d\mathbf{r}_3 \times u^*_\alpha(\mathbf{r}_1) u^*_\beta(\mathbf{r}_2) u^*_\gamma(\mathbf{r}_3) W(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) u_\mu(\mathbf{r}_1) u_\nu(\mathbf{r}_2) u_\lambda(\mathbf{r}_3) \ . \tag{1.38}$$

$$\tag{1.39}$$

1.3.2 Expectation values

Let's asume that that we have a state $|\Psi^N\rangle$ of a system of N particles. This does not need to be a basis vector and can be any Fock state, for example, an exact solution of the Scrödinger equation. The expectation value of a one-body operator O can be calculated with a simple sum involving the one-body *reduced density matrix*, which is defined as

$$\rho_{\alpha\beta} = \langle \Psi^N | c^\dagger_\beta c_\alpha | \Psi^N \rangle \ . \tag{1.40}$$

By comparing to Eq. (1.30), it is easily seen that

$$\langle \Psi^N | O | \Psi^N \rangle = \sum_{\alpha\beta} \rho_{\beta\alpha} o_{\alpha\beta} = Tr\left(\rho O\right) \ . \tag{1.41}$$

The diagonal matrix elements of the density matrix $\rho_{\alpha\alpha}$ give the expecteation value of the operator $c^\dagger_\alpha c_\alpha$, which is interpreted as quantifying of the occupation of the single particle orbit α in the state $|\Psi^N\rangle$. From Eq. (1.5) one finds the obvious results that summing over all occupations must give the total number of particles,

$$Tr\left(\rho\right) = \sum_\alpha \rho_{\alpha\alpha} = N \ . \tag{1.42}$$

These results are particularly interesting since the theory of many-body Green's functions does not attempt any calculation of the full many-body wave function. Rather the focus is on determining directly quantities ralted to the density matrices, which are calculated in terms of basic excitation modes of the system. Thus, even if one does not compute the complete ground state wave function, Eqs. (1.41) and (1.42) tell us that it is still possible to extract the expectation values of interesting observables.

It is also useful to insert the complete set of eigenstates $\{|\Psi^{N-1}_k\rangle\}$ of the (N-1)-particle system into (1.40)

$$\rho_{\alpha\alpha} = \langle c^\dagger_\alpha c_\alpha \rangle = \sum_k \left| \langle \Psi^{N-1}_k | c_\alpha | \Psi^N \rangle \right|^2 \ . \tag{1.43}$$

This result is interesting because the *overlap function* $\langle \Psi_k^{N-1}|c_\alpha|\Psi^N\rangle$ gives the probablility amplitude that the system collapses into a state $|\Psi_k^{N-1}\rangle$ after a particle has been removed from the state α. This quantity can be probed in a measurment that involves the suddend ejection of a particle.[4] One also sees that what is observed in particle emission experiments to one final state should not be directly interpreted as occupation numbers, since Eq. (1.43) requires a sum over all possible final states.

In an analogous way, we introduce the two-body reduced density matrix

$$\Gamma_{\gamma\delta,\alpha\beta} = \langle \Psi^N|c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma|\Psi^N\rangle \ . \tag{1.44}$$

With this definition the expectation value of a two-body Hamiltonian becomes[5]

$$\begin{aligned} \langle \Psi^N|H|\Psi^N\rangle &= \sum_{\alpha\beta} \rho_{\beta\alpha} t_{\alpha\beta} + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} \Gamma_{\gamma\delta,\alpha\beta} v_{\alpha\beta,\gamma\delta} \\ &= Tr\left(\rho T\right) + \frac{1}{4} Tr\left(\Gamma V\right) \ . \end{aligned} \tag{1.45}$$

1.4 Pictures in Quantum Mechanics

The time evolution of a quantum mechanical system is determined by the Scrödinger equation. There exist different approaches to keep track of time dependence, which are commonly referred to as *pictures*. The three most relevant are the *Schrödinger*, the *Heisenberg* and the *interaction* (also called *Dirac*) pictures. The last two are important for our discussions because they are used in the definition of Green's functions and to develop their expansion in Feynman diagrams.

In the Scrödinger picture the wave function carries all the time dependence, as described by the corresponding equation,

$$i\hbar \frac{d}{dt}|\Psi^S(t)\rangle = H\ |\Psi^S(t)\rangle \ . \tag{1.46}$$

If one knows the state of the system $|\Psi_{t_0}\rangle = |\Psi^S(t=t_0)\rangle$ at time t_0 the evolution at later times is fixed by Eq. (1.46). This can be formally solved to give the result

$$|\Psi^S(t)\rangle = U|\Psi_{t_0}\rangle \ , \tag{1.47}$$

[4] This is only a first order approximation to the measured cross section and care must be taken to undertsand additional effects, such as final state interactions. Nevertheless, knock out experiments are one of the best tools available to understand the many-body dynamics of a system.

[5] Note that the factor $\frac{1}{4}$ appears since we are using fully symmetrized (or antisymmetrized) matrix elements of V, Eq. (1.35).

where U is the time evolution operator

$$U \equiv U(t, t_0) = e^{-iH(t-t_0)/\hbar} \ . \tag{1.48}$$

The idea of the Heisenberg picture is simply the opposite: keeping the wave function constant at the time t_0 while the operators evolve. Since U is a unitary operator, one simply inverts the time propagation of the Schrödinger state and instead applies it to the operator,

$$\begin{aligned} |\Psi^H\rangle &= U^\dagger \, |\Psi^S(t)\rangle = |\Psi_{t_0}\rangle \ , & (1.49) \\ O^H(t) &= U^\dagger \, O^S \, U \ . & (1.50) \end{aligned}$$

With these definitions the expectation values of Heisenberg operators remain unchanged and commutation rules evolve according to Eq. (1.50), as long as they are evaluated *at equal times* $[A^H(t), B^H(t)]_\mp = U^\dagger \, [A^S, B^S]_\mp \, U$. The evolution of Heisenberg operators is given by

$$i\hbar \frac{d}{dt} O^H(t) = \left[O^H(t), H \right] \ . \tag{1.51}$$

which is valid only for time-independent Schrödinger operators ($O^S \neq O^S(t)$). Note that the Heisenberg Hamiltonian does not depend of the time since it commutes with itself.

In the interaction picture is a hybrid between the former two. In this case one splits the hamiltonian in two parts, $H = H_0 + H_1$. One drives the evolution of the operators and the other the evolution of wave functions. Let H_0 be the part that applies to the operators. Thus one defines the corresponding time evolution operator

$$U_0 \equiv U_0(t, t_0) = e^{-iH_0(t-t_0)/\hbar} \ , \tag{1.52}$$

which is applied to the operators and used to partially invert the evolution of the Schrödinger state (the correct expression for $\tilde{U}$ is given further below),

$$\begin{aligned} |\Psi^I(t)\rangle &= U_0^\dagger \, |\Psi^S(t)\rangle = \tilde{U} |\Psi_{t_0}\rangle \ , & (1.53) \\ O^I(t) &= U_0^\dagger \, O^S \, U_0 \ . & (1.54) \end{aligned}$$

The corresponding equations for time evolution are

$$\begin{aligned} i\hbar \frac{d}{dt} |\Psi^I(t)\rangle &= H_1^I(t) \, |\Psi^I(t)\rangle \ , & (1.55) \\ i\hbar \frac{d}{dt} O^I(t) &= \left[O^I(t), H_0 \right] \ , & (1.56) \end{aligned}$$

where H_0 reamins time independent but $H_1^I(t)$ evolves according to

$$H_1^I(t) = U_0^\dagger \; H_1 \; U_0 \; . \tag{1.57}$$

Normally is it assumed that H_0 is simple enough to allow for an exact solution of the many-body problem. The remaining part $H_1^I(t)$ (possibly a small perturbation) may then be used to evolve $|\Psi^I(t)\rangle$. This last correction leads to the exact solution of the problem. However, $H_1^I(t)$ is now dependent of time and Eq. (1.55) one cannot be solved for $\tilde{U}$ by simply exponentiating as done for U and U_0. The formal solution for the time evolution operator of a state in interaction pictue can be found in standard textboooks. Here, we just show the result,

$$\begin{aligned} &\tilde{U}(t-t_0) \\ &= \; 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n T\left[H_1^I(t_1) H_1^I(t_2) \cdots H_1^I(t_n)\right] \\ &= \; exp\left\{\frac{-i}{\hbar} \int_{t_0}^{t} dt' T\left[H_1^I(t')\right]\right\} \; , \end{aligned} \tag{1.58}$$

where the last line is used as a symbolic notation for the one above and $T[\cdots]$ is the time ordering operator, defined in such a way that the latest time apperas at the far left.

The expansion (1.58) is of particular importance since it is central in applying perturbation theory to Green's functions and to derive the corresponding rules for Feynman diagrams. The interaction picture has also another powerful application in quantum field theory: by applying a small fictitious external perturbation to the system, it is possible to derive useful relations among Green's functions. This apporach leads to self-consistent equations for the propagators and shows how to construct approximations of propagators that satisfy conservation laws. We will discuss these points in better details later on.

1.5 Exercises

- Derive equations (1.33) for the two-body operator in second quantization.
- Derive the Hartee-Fock equations in second quantization
- Derive the matrix elements of the Hamiltonian H between the 1p and 2p1h configurations.
- Derive the matrix elements of H between the 1h and 2h1p states.

Chapter 2

Basic Properties and Definitions in Many-Body Green's Function Theory

2.1 Propagation of One Particle

Let us consider a particle in free space described by a single particle Hamiltonian h_1. Its eigenstates and eigenenergies are

$$h_1|\phi_n\rangle = \varepsilon_n|\phi_n\rangle \ . \tag{2.1}$$

In general, if we put the particle in one of its $|\phi_n\rangle$ orbits, it will remain in the same state forever. Instead, we immagine to prepare the system in a generic state $|\psi_{tr}\rangle$ (tr stands for 'trial') and then follow its time evolution. If the trial state is created at time t=0, the wavefunction at a later time t is given by [see Eq. (1.47)]

$$\begin{aligned} |\psi(t)\rangle &= e^{-ih_1 t/\hbar}|\psi_{tr}\rangle \\ &= \sum_n |\phi_n\rangle e^{-i\varepsilon_n t/\hbar}\langle\phi_n|\psi_{tr}\rangle \ . \end{aligned} \tag{2.2}$$

The second line shows that if one knows the eigentstates $|\phi_n\rangle$, it is relatively simple to compute the time evution: one expands $|\psi_{tr}\rangle$ in this basis and let every component propagate independently. Eventually, at time t, we want to know the probability amplitude that a measurement would find the particle at position $\mathbf{r}$,

$$\begin{aligned} \langle\mathbf{r}|\psi(t)\rangle &= \langle\mathbf{r}|e^{-ih_1 t/\hbar}|\psi_{tr}\rangle \\ &= \int d\mathbf{r}'\langle\mathbf{r}|e^{-ih_1 t/\hbar}|\mathbf{r}'\rangle\langle\mathbf{r}'|\psi_{tr}\rangle \end{aligned}$$

$$
\begin{aligned}
&= \int d\mathbf{r}' \sum_n \langle \mathbf{r}|\phi_n\rangle e^{-i\varepsilon_n t/\hbar} \langle \phi_n|\mathbf{r}'\rangle \langle \mathbf{r}'|\psi_{tr}\rangle \qquad (2.3)\\
&\equiv \int d\mathbf{r}' G(\mathbf{r},\mathbf{r}';t)\psi_{tr}(\mathbf{r}') \ ,
\end{aligned}
$$

which defines the propagator G. Obviously, once $G(\mathbf{r},\mathbf{r}';t)$ is known it can be used to calculate the evolution of any initial state. However,there is more information included in the propagator. This is apparent from the expansion in the third line of Eq (2.3): first, the braket $\langle\phi_n|\mathbf{r}\rangle = \langle\phi_n|\psi^\dagger(\mathbf{r})|0\rangle$ gives us the probability that putting a particle at position $\mathbf{r}$ and mesuring its energy rgiht away, would make the system to collapse into the eigenstate $|\phi_n\rangle$. Second, the time evolution is a superposition of waves propagating with different energies and could be inverted to find the eigenspectrum. Immagine an experiment in which the particle is put at position $\mathbf{r}$ and picked up at $\mathbf{r}'$ after some time t. If one can do this for different positions and elapsed times– and with good resolution–then a Fourier transform would simply give back the full eigenvalue spectrum. Such an experiment is a lot of work to carry out! But would give us complete information on our particle.

We now want to apply the above ideas to see what we can learn by adding and removing a particle in an environment when many others are present. This can cause the particle to behave in an unxepected way, induce collective excitations of the full systems, and so on. Moreover, the role played by the physical vacuum in the above example, is now taken by an many-body state (usually its ground state). Thus, it is also possible to probe the system by removing particles.

2.2 One-Body Green's Function

In the following we consider the Heisenberg description of the field operators,

$$\psi_s^\dagger(\mathbf{r},t) = e^{iHt/\hbar}\ \psi_s^\dagger(\mathbf{r})\ e^{-iHt/\hbar} \ , \qquad (2.4)$$

where the subscript s serves to indicate possible internal degrees of freedom (spin, isospin, etc...). We omit the superscrips H (Hiesenberg) and S (Scrödinger) from the operators since the two pictures can be distinguished from the presence of the time variable, which appears only in the first case. Similarly,

$$\psi_s(\mathbf{r},t) = e^{iHt/\hbar}\ \psi_s(\mathbf{r})\ e^{-iHt/\hbar} \ , \qquad (2.5)$$

For the case of a general single-particle basis $\{u_\alpha(\mathbf{r})\}$ one uses the following creation and annihilation operators

$$
\begin{aligned}
c_\alpha^\dagger(t) &= e^{iHt/\hbar}\ c_\alpha^\dagger\ e^{-iHt/\hbar} \ , \qquad (2.6)\\
c_\alpha(t) &= e^{iHt/\hbar}\ c_\alpha\ e^{-iHt/\hbar} \ , \qquad (2.7)
\end{aligned}
$$

which are related to $\psi_s^\dagger(\mathbf{r},t)$ and $\psi_s(\mathbf{r},t)$ through Eqs. (1.14) and (1.15).

In most applications the Hamiltonian is split in a unperturbed part H_0 and a residual interaction

$$H = H_0 + V \ . \tag{2.8}$$

The N-body eigenstates of the full Hamiltonian are indicated with $|\Psi_n^N\rangle$, while $|\Phi_n^N\rangle$ are the unperturbed ones

$$\begin{aligned} H\ |\Psi_n^N\rangle &= E_n^N\ |\Psi_n^N\rangle \ , & (2.9)\\ H_0\ |\Phi_n^N\rangle &= E_n^{(0),N}\ |\Phi_n^N\rangle \ , & (2.10) \end{aligned}$$

The definitions given in the following are general and do not depend on the type of interaction being used. Thus, most properties of Green's functions result from genaral principles of quantum mechanics and are valid for any system.

2.2.1 Definitions

The two-points Green's function describies the propagation of one particle or one hole on top of the ground state $|\Psi_0^N\rangle$. This is defined by

$$g_{ss'}(\mathbf{r},t;\mathbf{r}',t') = -\frac{i}{\hbar}\langle\Psi_0^N|T[\psi_s(\mathbf{r},t)\psi_{s'}^\dagger(\mathbf{r}',t')]|\Psi_0^N\rangle \ , \tag{2.11}$$

where $T[\cdots]$ is the time ordering operator that imposes a change of sing for each exchange of two fermion operators

$$T[\psi_s(\mathbf{r},t)\psi_{s'}^\dagger(\mathbf{r}',t')] = \begin{cases} \psi_s(\mathbf{r},t)\psi_{s'}^\dagger(\mathbf{r}',t') \ , & t>t' \ , \\ \pm\psi_{s'}^\dagger(\mathbf{r}',t')\psi_s(\mathbf{r},t) \ , & t'>t \ , \end{cases} \tag{2.12}$$

where the upper (lower) sign is for bosons (fermions). A similar definition can be given for the non interacting state $|\Phi_0^N\rangle$, in this case the Heisenberg operators (2.4) to (2.7) must evolve only according to H_0 and the notation $g^{(0)}$ is used.

If the Hamiltonian does not depend on time, the propagator (2.11) depends only on the difference $t-t'$

$$\begin{aligned} g_{ss'}(\mathbf{r},\mathbf{r}';t-t') &= -\frac{i}{\hbar}\theta(t-t')\langle\Psi_0^N|\psi_s(\mathbf{r})e^{-i(H-E_0^N)(t-t')/\hbar}\psi_{s'}^\dagger(\mathbf{r}')|\Psi_0^N\rangle \\ &\quad \mp\frac{i}{\hbar}\theta(t'-t)\langle\Psi_0^N|\psi_{s'}^\dagger(\mathbf{r}')e^{i(H-E_0^N)(t-t')/\hbar}\psi_s(\mathbf{r})|\Psi_0^N\rangle \ . \end{aligned} \tag{2.13}$$

In this case it is useful to Froutier transform with respect to time and define

$$g_{ss'}(\mathbf{r},\mathbf{r}';\omega) = \int d\tau e^{i\omega\tau} g_{ss'}(\mathbf{r},\mathbf{r}';\tau) \ . \tag{2.14}$$

By using the relation

$$\theta(\pm\tau) = \mp \lim_{\eta\to 0^+} \frac{1}{2\pi i}\int_{-\infty}^{+\infty} d\omega \frac{e^{-i\omega\tau}}{\omega \pm i\eta} \,, \tag{2.15}$$

one obtains

$$\begin{aligned} g_{ss'}(\mathbf{r},\mathbf{r}';\omega) &= g^p_{ss'}(\mathbf{r},\mathbf{r}';\omega) + g^h_{ss'}(\mathbf{r},\mathbf{r}';\omega) \\ &= \langle\Psi_0^N|\psi_s(\mathbf{r})\frac{1}{\hbar\omega - (H-E_0^N) + i\eta}\psi^\dagger_{s'}(\mathbf{r}')|\Psi_0^N\rangle \\ &\quad \mp\langle\Psi_0^N|\psi^\dagger_{s'}(\mathbf{r}')\frac{1}{\hbar\omega + (H-E_0^N) - i\eta}\psi_s(\mathbf{r})|\Psi_0^N\rangle \,, \end{aligned} \tag{2.16}$$

In Eq. (2.16), g^p propagates a particle from $\mathbf{r}'$ to $\mathbf{r}$, while g^h propagates a hole from $\mathbf{r}$ to $\mathbf{r}'$. Note that the interpretation is that a particle is added at $\mathbf{r}'$, and later on some (indistiguishable) particle is removed from $\mathbf{r}'$ (and similarly for holes). In the mean time, it is the fully correlated $(N \pm 1)$-body system that propagates. We will discuss in the next chapter that in many cases–and especially in the vicinity of the Fermi surface–this motion mantains many characteristics that are typical of a particle moving in free space, even if the motion itself could actually be a collective excitation of many constituents. But since it looks like a single particle state we may still refer to it as *quasiparticle*.

The same definitions can be made for *any* orthonormal basis $\{\alpha\}$, leading to the realtions

$$g_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\alpha(t)c^\dagger_\beta(t')]|\Psi_0^N\rangle \,, \tag{2.17}$$

where

$$g_{ss'}(\mathbf{r},t;\mathbf{r}',t') = \sum_{\alpha\beta} u_\alpha(\mathbf{r},s) g_{\alpha\beta}(t,t') u^*_\beta(\mathbf{r}',s') \,, \tag{2.18}$$

and

$$\begin{aligned} g_{\alpha\beta}(\omega) &= \langle\Psi_0^N|c_\alpha\frac{1}{\hbar\omega - (H-E_0^N) + i\eta}c^\dagger_\beta|\Psi_0^N\rangle \\ &\quad \mp\langle\Psi_0^N|c^\dagger_\beta\frac{1}{\hbar\omega + (H-E_0^N) - i\eta}c_\alpha|\Psi_0^N\rangle \,. \end{aligned} \tag{2.19}$$

Equations (2.17) and (2.19) are completely equivalent to the previous ones. These may look a bit more abstract than the corresponding Eqs. (2.11) and (2.16) but are more *general* since they show that the formalism can be developed and applied in any orthonormal basis, without restricting oneself to coordindate space.

2.2.2 Lehmann Representation

As discussed in Sec. 2.1 for the one particle case, the information contained in the propagators becomes more clear if one Fourier transforms the time variable and inserts a completness for the intermediate states. This is so because it makes the spectrum and the transition amplitudes to apper explicitely. Using the completeness relations for the $(N \pm 1)$-body systems in Eq. (2.19), one has

$$\begin{aligned} g_{\alpha\beta}(\omega) &= \sum_n \frac{\langle \Psi_0^N | c_\alpha | \Psi_n^{N+1} \rangle \langle \Psi_n^{N+1} | c_\beta^\dagger | \Psi_0^N \rangle}{\hbar\omega - (E_n^{N+1} - E_0^N) + i\eta} \\ &\mp \sum_k \frac{\langle \Psi_0^N | c_\beta^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | c_\alpha | \Psi_0^N \rangle}{\hbar\omega - (E_0^N - E_k^{N-1}) - i\eta} \ . \end{aligned} \tag{2.20}$$

which is known as the *Lehmann* repressentation of a many-body Green's function[1]. Here, the first and second terms on the left hand side describe the propagation of a (quasi)particle and a (quasi)hole excitations.

The poles in Eq. (2.20) are the energies relatives to the $|\Psi_0^N\rangle$ ground state. Hence they give the energies actually relased in a capture reaction experiment to a bound state of $|\Psi_n^{N+1}\rangle$. The residues are transition amplitudes for the addition of a particle and take the name of *spectroscopic amplitudes*. They play the same role of the $\langle \phi_n | \mathbf{r} \rangle$ wave function in Eq. (2.3). In fact these energies and amplitudes are solutions of a Schrödinger-like equation: the Dyson equation. The hole part of the propagator gives instead information on the process of particle emission, the poles being the exact energy absorbed in the process. For example, in the single particle Green's function of a molecule, the quasiparticle and quasihole poles are respectively the electron affinities an ionization energies.

We will look at the physical significance of spectroscopic amplitudes in the next Chapter and derive the Dyson equation (which is the fundamental equation in many-body Green's function theory) only later on, when developin the formalism.

2.2.3 Spectral function and dispersive relation

As a last definition, we rewrite the contents of Eq. (2.20) in a form that can compared more easily to experiments. By using the relation

$$\frac{1}{x \pm i\eta} = \mathcal{P}\frac{1}{x} \ \mp \ i\pi\delta(x) \ , \tag{2.21}$$

[1] H. Lehmann, *Nuovo Cimento* **11**, 324 (1954).

it is immediate to extract the one-body spectral function

$$S_{\alpha\beta}(\omega) = S^p_{\alpha\beta}(\omega) + S^h_{\alpha\beta}(\omega) \ , \tag{2.22}$$

where the partcle and hole components are

$$\begin{aligned} S^p_{\alpha\beta}(\omega) &= -\frac{1}{\pi}\ \mathrm{Im}\ g^p_{\alpha\beta}(\omega) \\ &= \sum_n \langle \Psi^N_0 | c_\alpha | \Psi^{N+1}_n \rangle \langle \Psi^{N+1}_n | c^\dagger_\beta | \Psi^N_0 \rangle\ \delta\left(\hbar\omega - (E^{N+1}_n - E^N_0)\right) \ , \qquad (2.23) \\ S^h_{\alpha\beta}(\omega) &= \frac{1}{\pi}\ \mathrm{Im}\ g^h_{\alpha\beta}(\omega) \\ &= \mp \sum_k \langle \Psi^N_0 | c^\dagger_\beta | \Psi^{N-1}_k \rangle \langle \Psi^{N-1}_k | c_\alpha | \Psi^N_0 \rangle\ \delta\left(\hbar\omega - (E^N_0 - E^{N-1}_k)\right) \ . \qquad (2.24) \end{aligned}$$

The diagonal part of the spectral function is interpreted as the probability of adding $[S^p_{\alpha\alpha}(\omega)]$ or removing $[S^h_{\alpha\alpha}(\omega)]$ one particle in the state α leaving the residual system in a state of energy ω.

By comparing Eqs. (2.23) and (2.24) to the Lehmann representation (2.20), it is seen that the propagator is completely constrained by its imaginary part. Indeed,

$$g_{\alpha\beta}(\omega) = \int d\omega' \frac{S^p_{\alpha\beta}(\omega')}{\omega - \omega' + i\eta} \ + \ \int d\omega' \frac{S^h_{\alpha\beta}(\omega')}{\omega - \omega' - i\eta} \ . \tag{2.25}$$

In general the single particle propagator of a finite system has isolated poles in correspondence to the bound eigenstates of the $(N+1)$-body system. For larger enegies, where $|\Psi^{N+1}_n\rangle$ are states in the continuum, it develops a branch cut. The particle propagator $g^p(\omega)$ is analytic in the upper half of the complex plane, and so is the full propagator (2.16) for $\omega \geq E^{N+1}_0 - E^N_0$. Analogously, the hole propagator has poles for $\omega \leq E^N_0 - E^{N-1}_0$ and is analytic in the lower complex plane. Note that high excitation energies in the (N-1)-body system correspond to negative values of the poles $E^N_0 - E^{N-1}_k$, so $g^h(\omega)$ develops a branch cut for large negative energies.

2.3 Observables from $g_{\alpha\beta}$

2.3.1 Calculation of Expectation Values

The one-body density matrix (1.40) can be obtained from the one-body propagator. One simply chooses the appropriate time ordering in Eq. (2.17)

$$\rho_{\alpha\beta} = \langle \Psi_0^N | c_\beta^\dagger c_\alpha | \Psi_0^N \rangle = \pm i\hbar \, \lim_{t' \to t^+} \, g_{\alpha\beta}(t,t') \tag{2.26}$$

(where the upper sign is for bosons and the lower one is for fermions). Alternatively, the hole spectral function can be used

$$\rho_{\alpha\beta} = \mp \int d\omega \; S^h_{\alpha\beta}(\omega) \; . \tag{2.27}$$

Thus, the expectation value of a one-body operator, Eq. (1.41), on the ground states $|\Psi_0^N\rangle$ is usually written in one the following ways

$$\begin{aligned} \langle \Psi_0^N | O | \Psi_0^N \rangle &= \mp \sum_{\alpha\beta} \int d\omega \; o_{\alpha\beta} \; S^h_{\beta\alpha}(\omega) \\ &= \pm i\hbar \, \lim_{t' \to t^+} \sum_{\alpha\beta} \; o_{\alpha\beta} \; g_{\beta\alpha}(t,t') \end{aligned} \tag{2.28}$$

which are equivalent.

From the particle spectral function, one can extract the quantity

$$d_{\alpha\beta} = \langle \Psi_0^N | c_\alpha c_\beta^\dagger | \Psi_0^N \rangle = \int d\omega \; S^p_{\beta\alpha}(\omega) \tag{2.29}$$

which leads to the following sum rule

$$\int d\omega S_{\alpha\beta}(\omega) = d_{\alpha\beta} \mp \rho_{\alpha\beta} = \langle \Psi_0^N | [c_\alpha, c_\beta^\dagger]_\mp | \Psi_0^N \rangle = \delta_{\alpha\beta} \; . \tag{2.30}$$

2.3.2 Sum Rule for the Energy

For the case of an Hamiltonian containing only two-body interactions,

$$\begin{aligned} H &= U \; + \; V \\ &= \sum_{\alpha\beta} t_{\alpha\beta} \; c_\alpha^\dagger c_\beta \; + \; \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta} \; c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \; , \end{aligned} \tag{2.31}$$

there exist an important sum rule that relates the total energy of the state $|\Psi_0^N\rangle$ to its one-body Green's function. To derive this, one makes use of the equation of motion for Heisenberg operators (1.51), which gives

$$i\hbar \frac{d}{dt} c_\alpha(t) = e^{iHt/\hbar} \; [c_\alpha, H] \; e^{-iHt/\hbar} \; , \tag{2.32}$$

with[2]

$$[c_\alpha, H] = \sum_\beta t_{\alpha\beta}\ c_\beta\ +\ \frac{1}{2}\sum_{\beta\gamma\delta} v_{\alpha\beta\gamma\delta} c^\dagger_\beta c_\delta c_\gamma\ , \tag{2.33}$$

which is valid for both fermions and bosons.

If one uses Eq. (2.33) and derives the propagator (2.17) with respect to time,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t} g_{\alpha\beta}(t-t') &= \delta(t-t')\delta_{\alpha\beta}\ +\ \sum_\gamma t_{\alpha\gamma} g_{\gamma\beta}(t-t') \\ &\quad -\frac{i}{\hbar}\ \sum_{\eta\gamma\zeta}\frac{1}{2} v_{\alpha\eta,\gamma\zeta}\ \langle\Psi_0^N|\ T[c^\dagger_\eta(t) c_\zeta(t) c_\gamma(t) c^\dagger_\beta(t')]|\Psi_0^N\rangle\ . \end{aligned} \tag{2.34}$$

The braket in the last line contains the four points Green's function [see Eq. (2.38)], which can describe the simultaneous propagation of two particles. Thus, one sees that applying the equation of motion to a propagator leads to relations which contain Green's functions of higher order. This result is particularly important because it shows there exist a hierarchy between propagators, so that the exact equations that determine the one-body function will depend on the two-body one, the two-body function will contain contributions from three-body propagators, and so on.

For the moment we just want to select a particular order of the operators in Eq. (2.34) in order to extract the one- and two-body density matrices. To do this, we chose t' to be a later time than t and take its limit to the latter from above. This yields

$$\pm i\hbar\ \lim_{t'\to t^+}\sum_\alpha \frac{\partial}{\partial t} g_{\alpha\alpha}(t-t') = \langle T\rangle + 2\langle V\rangle \tag{2.35}$$

(note that for $t \neq t'$, the term $\delta(t-t')$=0 and it does not contribute to the limit). This result can also be expressed in energy representation by inverting the Fourier transformation (2.14), which gives

$$lim_{\tau\to 0^-}\ \frac{\partial}{\partial\tau}\ g_{\alpha\beta}(\tau) = -\int d\omega\ \omega\ S^h_{\alpha\beta}(\omega) \tag{2.36}$$

By combining (2.35) with Eq. (2.28) one finally obtains

$$\begin{aligned} \langle H\rangle = \langle U\rangle + \langle V\rangle &= \pm i\hbar\ \frac{1}{2}\lim_{t'\to t^+}\sum_{\alpha\beta}\left\{\delta_{\alpha\beta}\frac{\partial}{\partial t} + t_{\alpha\beta}\right\} g_{\beta\alpha}(t-t') \\ &= \mp\frac{1}{2}\sum_{\alpha\beta}\int d\omega\ \left\{\delta_{\alpha\beta}\omega + t_{\alpha\beta}\right\} S^h_{\beta\alpha}(\omega)\ . \end{aligned} \tag{2.37}$$

[2]We use the relation $[A, BC]_- = [A,B]C - B[C,A] = \{A,B\}C - B\{C,A\}$ which is valid for both commutators and anticommutators

Surprisingly, for an Hamiltonian containing only two-body forces it is possible to extract the ground state energy by knowing only the one-body propagator. This result was derived independently by Galitski and Migdal[3] and by Kolutn[4]. When interactions among three or more particles are present, this relation has to be augmented to include additional terms. In these cases higher order Green's functions will appear explicitly.

2.4 Higher Order Green's Functions

The definition (2.17) can be extended to Green's functions for the propagation of more than one particle. In general, for each additional particle it will be necessary to introduce one additional creation and one annihilation operator. Thus a $2n$-points Green's function will propagate a maximum of n quasiparticles. The explicit definition of the 4-points propagator is

$$g^{4-pt}_{\alpha\beta,\gamma\delta}(t_1,t_2;t'_1,t'_2) = -\frac{i}{\hbar}\langle\Psi^N_0|T[c_\beta(t_2)c_\alpha(t_1)c^\dagger_\gamma(t'_1)c^\dagger_\delta(t'_2)]|\Psi^N_0\rangle\ , \tag{2.38}$$

while the 6-point case is

$$\begin{aligned} &g^{6-pt}_{\alpha\beta\gamma,\mu\nu\lambda}(t_1,t_2,t_3;t'_1,t'_2,t'_3) = \\ &\quad -\frac{i}{\hbar}\langle\Psi^N_0|T[c_\gamma(t_3)c_\beta(t_2)c_\alpha(t_1)c^\dagger_\mu(t'_1)c^\dagger_\nu(t'_2)c^\dagger_\lambda(t'_3)]|\Psi^N_0\rangle\ , \end{aligned} \tag{2.39}$$

It should be noted that the actual number of particles that are propagated by these objects depends on the ordering of the time variables. Therefore the information on transitions between eigenstates of the systems with N, $N\pm1$ and $N\pm2$ bodies are all encoded in Eq. (2.38), while additional states of $N\pm3$-body states are included in Eq. (2.38). Obviously, the presence of so many time variables makes the use of these functions extremely difficult (and even impossible, in many cases). However, it is still useful to consider only certain time orderings which allow to extract the information not included in the 2-point propagator.

2.4.1 Two-particles–two-holes Propagator

The Two-particle–two-hole propagator is a two-times Green's function defined as

$$g^{II}_{\alpha\beta,\gamma\delta}(t,t') = -\frac{i}{\hbar}\langle\Psi^N_0|T[c_\beta(t)c_\alpha(t)c^\dagger_\gamma(t')c^\dagger_\delta(t')]|\Psi^N_0\rangle\ , \tag{2.40}$$

[3] V. M. Galitski and A. B. Migdal, Sov. Phys.-JEPT **7**, 96 (1958).
[4] D. S. Koltun, Phys. Rev. Lett. **28**, 182 (1972); Phys. Rev. C **9**, 484 (1974)

which corresponds to the limit $t_1' = t_2'^+$ and $t_2 = t_1^+$ of g^{4-pt}.

As for the case of $g_{\alpha\beta}(t,t')$, if the Hamiltonian is time-independent, Eq. (2.40) is a function of the time difference only. Therefore it has a Lehmann representation containing the exact spectrum of the $(N \pm 2)$-body systems

$$\begin{aligned} g^{II}_{\alpha\beta,\gamma\delta}(\omega) &= \sum_n \frac{\langle \Psi_0^N | c_\beta c_\alpha | \Psi_n^{N+2} \rangle \, \langle \Psi^{N+2_n} | c_\gamma^\dagger c_\delta^\dagger | \Psi_0^N \rangle}{\omega - (E_n^{N+2} - E_0^N) + i\eta} \\ &- \sum_k \frac{\langle \Psi_0^N | c_\gamma^\dagger c_\delta^\dagger | \Psi_k^{N-2} \rangle \, \langle \Psi_k^{N-2} | c_\beta c_\alpha | \Psi_0^N \rangle}{\omega - \left(E_0^N - E_k^{N-2} \right) - i\eta} \, . \end{aligned} \tag{2.41}$$

Similarly one defines the two-particle and two-hole spectral functions

$$S^{II}_{\alpha\beta}, \gamma\delta(\omega) = S^{pp}_{\alpha\beta,\gamma\delta}(\omega) + S^{hh}_{\alpha\beta,\gamma\delta}(\omega) \, , \tag{2.42}$$

and

$$\begin{aligned} S^{pp}_{\alpha\beta,\gamma\delta}(\omega) &= -\frac{1}{\pi} \, \mathrm{Im} \, g^{pp}_{\alpha\beta,\gamma\delta}(\omega) \\ &= \sum_n \langle \Psi_0^N | c_\beta c_\alpha | \Psi_n^{N+2} \rangle \langle \Psi_n^{N+2} | c_\gamma^\dagger c_\delta^\dagger | \Psi_0^N \rangle \, \delta \left(\hbar\omega - (E_n^{N+2} - E_0^N) \right) \, , \end{aligned} \tag{2.43}$$

$$\begin{aligned} S^{hh}_{\alpha\beta,\gamma\delta}(\omega) &= \frac{1}{\pi} \, \mathrm{Im} \, g^{hh}_{\alpha\beta,\gamma\delta}(\omega) \\ &= -\sum_k \langle \Psi_0^N | c_\gamma^\dagger c_\delta^\dagger | \Psi_k^{N-2} \rangle \langle \Psi_k^{N-2} | c_\beta c_\alpha | \Psi_0^N \rangle \, \delta \left(\hbar\omega - (E_0^N - E_k^{N-2}) \right) \, . \end{aligned} \tag{2.44}$$

Following the demonstration of Sec. 2.3.1, it is immediate to obtain relations for the two-body density matrix (1.44)

$$\Gamma_{\alpha\beta,\gamma\delta} = \langle \Psi^N | c_\gamma^\dagger c_\delta^\dagger c_\beta c_\alpha | \Psi^N \rangle = -\int d\omega S^{hh}_{\alpha\beta,\gamma\delta}(\omega) \tag{2.45}$$

and, hence, for the expectation value of any two-body operator

$$\begin{aligned} \langle \Psi_0^N | V | \Psi_0^N \rangle &= -\sum_{\alpha\beta\gamma\delta} \int d\omega v_{\alpha\beta,\gamma\delta} S^h_{\gamma\delta,\alpha\beta}(\omega) \\ &= +i\hbar \, \lim_{t' \to t^+} \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta} g^{II}_{\gamma\delta,\alpha\beta}(t,t') \, . \end{aligned} \tag{2.46}$$

2.4.2 Polarization Propagator

The polarization propagator $\Pi_{\alpha\beta,\gamma\delta}$ corresponds to the time ordering of g^{4-pt} in which a particle-hole excitation is created at one single time. Therefore,

no process involving particle transfer in included. However it describes transition to the excitations of the system, as long as they can be reached with a one-body operator. For example, this includes collective modes of a nucleus. This is defined as

$$\begin{aligned}\Pi_{\alpha\beta,\gamma\delta}(t,t') &= -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\beta^\dagger(t)c_\alpha(t)c_\gamma^\dagger(t')c_\delta(t')]|\Psi_0^N\rangle \\ &\quad + \frac{i}{\hbar}\langle\Psi_0^N|c_\beta^\dagger c_\alpha|\Psi_0^N\rangle\langle\Psi_0^N|c_\gamma^\dagger c_\delta|\Psi_0^N\rangle \ . \end{aligned} \tag{2.47}$$

After including a completeness of $|\Psi_n^N\rangle$ states in (2.47), the contribution of to the ground states (at zero energy) is cancelled by the last term in the equation. Thus one can Fourier transform to the Lehmann representation

$$\begin{aligned}\Pi_{\alpha\beta,\gamma\delta}(\omega) &= \sum_{n\neq 0}\frac{\langle\Psi_0^N|c_\beta^\dagger c_\alpha|\Psi_n^N\rangle\ \langle\Psi_n^N|c_\gamma^\dagger c_\delta|\Psi_0^N\rangle}{\omega-(E_n^N-E_0^N)+i\eta} \\ &\quad - \sum_{n\neq 0}\frac{\langle\Psi_0^N|c_\gamma^\dagger c_\delta|\Psi_n^N\rangle\ \langle\Psi_n^N|c_\beta^\dagger c_\alpha|\Psi_0^N\rangle}{\omega+(E_n^N-E_0^N)-i\eta} \ , \end{aligned} \tag{2.48}$$

Note that $\Pi_{\alpha\beta,\gamma\delta}(\omega)=\Pi_{\delta\gamma,\beta\alpha}(-\omega)$ due to time reversal symmetry. Also the forward and backward parts carry the same information.

Once again, the residues of the propagator (2.48) can be used to calculate expectation values. In this case, given a one-body operator (1.30) on obtains the transition matrix elements to any excited state

$$\langle\Psi_n^N|O|\Psi_0^N\rangle = \sum_{\alpha\beta} o_{\beta\alpha}\langle\Psi_n^N|c_\beta^\dagger c_\alpha|\Psi_0^N\rangle \ . \tag{2.49}$$

Chapter 3

Relation to Experimental Data

In this chapter we will partially explore the connection between the information contained in various propagators and experimental data. The focus is on the experimental properties that are probed by the removal of particles. Also, from now on, we will only consider fermionic systems.

An important case is when the spectrum for the $N \pm 1$-particle system near the Fermi energy involves discrete bound states. This happens in finite system like nuclei or molecules. In these cases the main quantity of interest is the overlap wave function, which appears in the residues of Eq. (2.20) and in Eq. (2.24). This is

$$\begin{aligned} \psi_k^{overlap}(\mathbf{r}) &= \langle \Psi_k^{N-1} | \psi_s(\mathbf{r}) | \Psi_0^N \rangle \\ &= \sqrt{N} \int d\mathbf{r}_2 \int d\mathbf{r}_3 \cdots \int d\mathbf{r}_N \\ &\quad \times [\Psi_k^{N-1}(\mathbf{r}_2, \mathbf{r}_3, \ldots \mathbf{r}_N)]^* \Psi_0^N(\mathbf{r}, \mathbf{r}_2, \mathbf{r}_3, \ldots \mathbf{r}_N) \ . \end{aligned} \tag{3.1}$$

The second line in Eq. (3.1) can be proved by using relations (1.19) and (1.20). This integral comes out in the description of most particle knock out processes because it represents the matrix element between the initial and final states, in the case when the emitted particle is ejected with energy large enough the it interacts only weakly with the residual system. The quantity of interest here is the so called spectroscopic factor to the final state k,

$$S_k = \int d\mathbf{r} |\psi_k^{overlap}(\mathbf{r})|^2 \ . \tag{3.2}$$

When the system is made of completely non interacting particles, S_k is unity. In real cases however, correlations among the constituents reduce this value. The possibility of extracting this quantity from experimental data gives us information on the spectral function and therefore on the structure of the correlated system.

3.0.3 Spectroscopic strength from particle emission

In order to make the connection with experimental data obtained from knock-out reactions, it is useful to consider the response of a system to a weak probe. The hole spectral function introduced in Eq. (2.24) can be substantially "observed" these reactions. The general idea is to transfer a large amount of momentum and energy to a particle of a bound system in the ground state. This is then ejected from the system, and one ends up with a fast-moving particle and a bound $(N-1)$-particle system. By observing the momentum of the ejected particle it is then possible the reconstruct the spectral function of the system, provided that the interaction between the ejected particle and the remainder is sufficiently weak or treated in a controlled fashion, *e. g.* by constraining this treatment with information from other experimental data.

We assume that the N-particle system is initially in its ground state,

$$|\Psi_i\rangle = |\Psi_0^N\rangle, \tag{3.3}$$

and makes a transition to a final N-particle eigenstate

$$|\Psi_f\rangle = a_{\boldsymbol{p}}^\dagger |\Psi_n^{N-1}\rangle, \tag{3.4}$$

composed of a bound $(N-1)$-particle eigenstate, $|\Psi_n^{N-1}\rangle$, and a particle with momentum $\boldsymbol{p}$.

For simplicity we consider the transition matrix elements for a scalar external probe

$$\rho(\boldsymbol{q}) = \sum_{j=1}^{N} \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}_j\right), \tag{3.5}$$

which transfers momentum $\boldsymbol{q}$ to a particle. Suppressing other possible sp quantum numbers, like *e.g.* spin, the second-quantized form of this operator is given by

$$\hat{\rho}(\boldsymbol{q}) = \sum_{\boldsymbol{p},\boldsymbol{p}'} \langle \boldsymbol{p}| \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}\right)|\boldsymbol{p}'\rangle a_{\boldsymbol{p}}^\dagger a_{\boldsymbol{p}'} = \sum_{\boldsymbol{p}} a_{\boldsymbol{p}}^\dagger a_{\boldsymbol{p}-\boldsymbol{q}}. \tag{3.6}$$

The transition matrix element now becomes

$$\begin{aligned}
\langle \Psi_f|\hat{\rho}(\boldsymbol{q})|\Psi_i\rangle &= \sum_{\boldsymbol{p}'} \langle \Psi_n^{N-1}| a_{\boldsymbol{p}} a_{\boldsymbol{p}'}^\dagger a_{\boldsymbol{p}'-\boldsymbol{q}} |\Psi_0^N\rangle \\
&= \sum_{\boldsymbol{p}'} \langle \Psi_n^{N-1}| \delta_{\boldsymbol{p}',\boldsymbol{p}} a_{\boldsymbol{p}'-\boldsymbol{q}} + a_{\boldsymbol{p}'}^\dagger a_{\boldsymbol{p}'-\boldsymbol{q}} a_{\boldsymbol{p}} |\Psi_0^N\rangle \\
&\approx \langle \Psi_n^{N-1}| a_{\boldsymbol{p}-\boldsymbol{q}} |\Psi_0^N\rangle.
\end{aligned} \tag{3.7}$$

The last line is obtained in the so-called *Impulse Approximation* (or *Sudden Approximation*), where it is assumed that the ejected particle is the one that

has absorbed the momentum from the external field. This is a very good approximation whenever the momentum $\boldsymbol{p}$ of the ejectile is much larger than typical momenta for the particles in the bound states; the neglected term in Eq. (3.7) is then very small, as it involves the removal of a particle with momentum $\boldsymbol{p}$ from $|\Psi_0^N\rangle$.

There is one other assumption in the derivation: the fact that the final eigenstate of the N-particle system was written in the form of Eq. (3.4), i.e. a plane-wave state for the ejectile on top of an $(N-1)$-particle eigenstate. This is again a good approximation if the ejectile momentum is large enough, as can be understood by rewriting the Hamiltonian in the N-particle system as

$$H_N = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i<j=1}^{N} V(i,j) = H_{N-1} + \frac{\boldsymbol{p}_N^2}{2m} + \sum_{i=1}^{N-1} V(i,N). \tag{3.8}$$

The last term in Eq. (3.8) represents the *Final State Interaction*, or the interaction between the ejected particle N and the other particles $1 \ldots N-1$. If the relative momentum between particle N and the others is large enough their mutual interaction can be neglected, and $H_N \approx H_{N-1} + \boldsymbol{p}_N^2/2m$. The result given by Eq. (3.7) is called the *Plane Wave Impulse Approximation* or PWIA knock-out amplitude, for obvious reasons, and is precisely a removal amplitude (in the momentum representation) appearing in the Lehmann representation of the sp propagator [Eq. (3.1) and (2.24)].

The cross section of the knock-out reaction, where the momentum and energy of the ejected particle and the probe are either measured or known, is according to Fermi's golden rule proportional to

$$d\sigma \sim \sum_n \delta(\omega + E_i - E_f) |\langle \Psi_f | \hat{\rho}(\boldsymbol{q}) | \Psi_i \rangle|^2, \tag{3.9}$$

where the energy-conserving δ-function contains the energy transfer ω of the probe, and the initial and final energies of the system are $E_i = E_0^N$ and $E_f = E_n^{N-1} + \boldsymbol{p}^2/2m$, respectively. Note that the internal state of the residual $N-1$ system is not measured, hence the summation over n in Eq. (3.9). Defining the missing momentum $\boldsymbol{p}_{miss}$ and missing energy E_{miss} of the knock-out reaction as[1]

$$\boldsymbol{p}_{miss} = \boldsymbol{p} - \boldsymbol{q} \tag{3.10}$$

and

$$E_{miss} = \boldsymbol{p}^2/2m - \omega = E_0^N - E_n^{N-1}, \tag{3.11}$$

[1]We will neglect here the recoil of the residual $N-1$ system, i.e. we assume the mass of the N and $N-1$ system to be much heavier than the mass m of the ejected particle.

respectively, the PWIA knock-out cross section can be rewritten as

$$\begin{aligned} d\sigma &\sim \sum_n \delta(E_{miss} - E_0^N + E_n^{N-1}) |\langle \Psi_n^{N-1} | a_{\boldsymbol{p}_{miss}} | \Psi_0^N \rangle|^2 \\ &= S^h(\boldsymbol{p}_{miss}, E_{miss}). \end{aligned} \tag{3.12}$$

The PWIA cross section is therefore exactly proportional to the diagonal part of the hole spectral function defined in Eq. (2.24). This is of course only true in the PWIA, but when the deviations of the impulse approximation and the effects of the final state interaction are under control, it is possible to obtain precise experimental information on the hole spectral function of the system under study.

3.0.4 An example: the $(e, e'p)$ reaction

Several studies of reacton theory have been done in past years constrain and improve the analysis of electron scattering reactions[2]. Although the actual (e,e′p) experiments involve more complicated one-body excitation operators than the one considered in the simple simple example above, the basic conclusions are not altered[3].

In the practical analysis of an (e,e′p) experiment it is conventional to find a local potential well (mostly of Woods-Saxon type) which will generate a sp state at the removal energy for the transition that is studied. This state is further required to provide the best possible fit to the experimental momentum dependence of the cross section (with proper inclusion of complications due to electron and proton distortion). The overall factor necessary to bring the resulting calculated cross section into agreement with the experimental data, can then be interpreted as the spectroscopic factor corresponding to the "experimental" quasihole wave function according to Eq.(3.2).

The resulting cross sections obtained at the NIKHEF facility are shown for four different nuclei in Fig. 3.1[4] It is important to realize that the shapes of the wave functions in momentum space correspond closely to the ones expected on the basis of a standard Woods-Saxon potential well (or more involved mf wave functions). This is itself an important observation since the (e,e′p) reaction probes the interior of the nucleus, a feat not available with hadronically induced reactions.

While the shapes of the valence nucleon wave functions correspond to the basic ingredients expected on the basis of years of nuclear structure physics

[2]See for example, S. Boffi, C. Giusti, F. D. Pacati, and M. Radici, *Electromagnetic Response of Atomic nuclei*, Oxford Studies in Nuclear Physics (Clarendon, Oxford, 1996).

[3]S. Frullani and J. Mougey, Adv. Nucl. Phys. **14**, 1 (1984).

[4]L. Lapikás, Nucl. Phys. **A553**, 297c (1993).

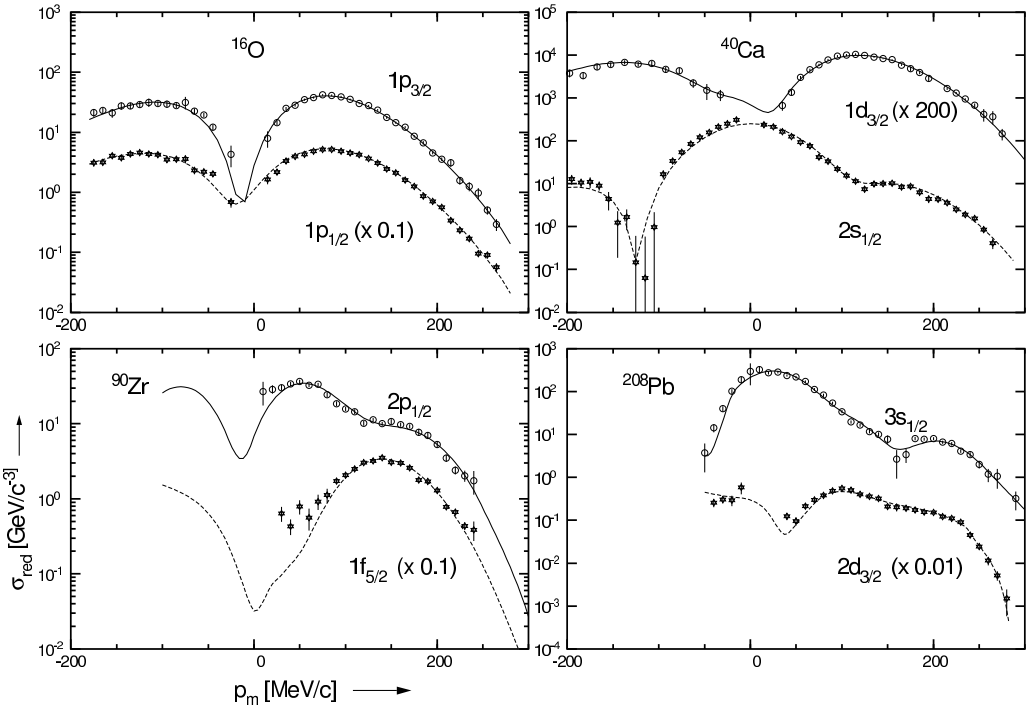

Figure 3.1: Momentum distributions for various nuclei obtained from the (e,e′p) reaction performed at NIKHEF (Note n. 4, p. 28).

experience, there is a significant departure with regard to the integral of the square of these wave functions. This quantity is of course the spectroscopic factor and is shown in Fig. 3.2 for the data obtained at NIKHEF. The results shown in Fig. 3.2 indicate that there is an essentially global reduction of the sp strength of about 35 % which needs to be explained by the theoretical calculations. This depletion is somewhat less for the strength associated with slightly more bound levels. An additional feature obtained in the (e,e′p) reaction is the fragmentation pattern of these more deeply bound orbitals in nuclei. This pattern is such that single isolated peaks are obtained only in the immediate vicinity of the Fermi energy whereas for more deeply bound states a stronger fragmentation of the strength is obtained with larger distance from ε_F. This is beautifully illustrated by the (e,e′p) data from Quint[5]. Whereas the $3s_{1/2}$ orbit exhibits a single peak, there is a substantial fragmentation of the $1f$ strength as indicated in this figure. Additional information about the occupation number of the former orbit is also available and can be obtained by analyzing elastic electron scattering cross sections of neighboring nuclei.

[5]E. N. M. Quint, Ph.D. thesis, University of Amsterdam (1988).

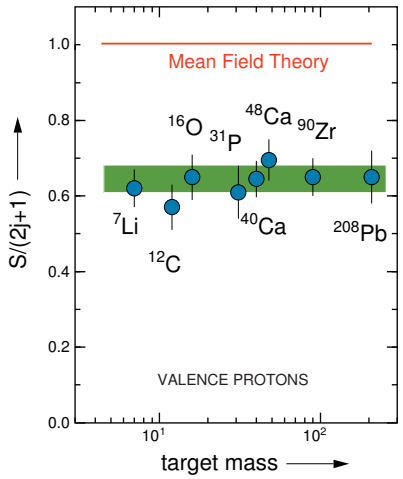

Figure 3.2: Spectroscopic factors from the (e,e′p) reaction as a function of target mass. Data have been obtained at the NIKHEF facility (Note n. 4, p. 28).

The actual occupation number for the $3s_{1/2}$ proton orbit obtained from this analysis is about 10% larger than the quasihole spectroscopic factor [6] and therefore corresponds to 0.75. All these features of the strength need to be explained theoretically. This will be attempted in the material covered in later sections.

[6] P. Grabmayr *et al.*, Phys. Lett. **B164**, 15 (1985). P. Grabmayr, Prog. Part. Nucl. Phys. **29**, 251 (1992).