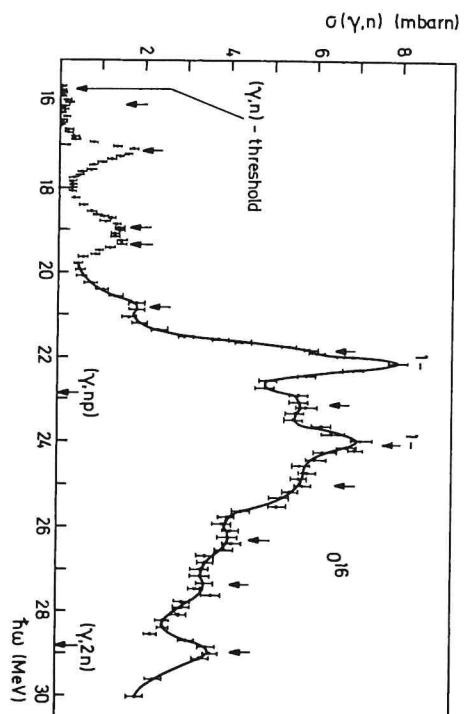


## CHAPTER 8

# Harmonic Vibrations



**Figure 8.1.** The cross section for  $(\gamma, n)$  processes as a function of the  $\gamma$ -energy (from [BCH 64]).

### 8.1 Introduction

In giving a microscopic description of the nuclear properties, until now we have used only static independent particle models. We have seen that by a proper definition of the particles or quasi-particles and by using an effective interaction, we are able within such a picture to explain the basic properties of the groundstates of many nuclei. Spectra of nuclear excitations are also very important for an understanding of the nuclear structure. If we perform an analysis of such spectra within the nuclear shell model or within the more elaborated independent particle models such as Hartree-Fock or Hartree-Fock-Bogoliubov, we find that a series of excited states can be very adequately explained by such models as *ph-* or two-quasi-particle excitations. But there are also many excited states with features that cannot be reproduced within the framework of shell model excitations, in spite of the fact that by introducing sophisticated methods involving the breaking of symmetries we are able to take into account important correlations among the nucleons.

If, for example, we restrict ourselves to spherically symmetric doubly magic nuclei like  $^{16}\text{O}$ ,  $^{40}\text{Ca}$ , or  $^{208}\text{Pb}$ , then the lowest excitations according to the harmonic oscillator approximation of the nuclear shell model should lie at about  $\hbar\omega_0$ . For  $^{16}\text{O}$  the experimental shell difference between  $1p$  and  $2s-1d$  shells is roughly 11.5 MeV. In the spectrum of  $^{16}\text{O}$ , however, we see amongst other states a ( $J^\pi = 3^-$ ,  $T=0$ )-state at 6.14 MeV, and around 22

MeV a 5 MeV broad resonance which is usually called the giant dipole resonance (see Fig. 8.1) having the quantum numbers  $J^\pi = 1^-$ ,  $T=1$ . It can be shown (see Sec. 8.3.3) that mainly  $1\hbar\omega$  excitations are involved in this resonance. Therefore, the pure shell model also fails to explain the high energy of the giant dipole resonance.

It will turn out that these excitations can only be explained if we suppose that coherent participation by many nucleons takes place in the nucleus. What we understand by “coherent” can at the moment only be expressed in terms of the classical liquid drop approach to the nucleus (Chap. 1): Many nucleons are believed to take part in similar fashion to the shape vibrations of the nuclear drop. We will learn below what coherent means in the quantum mechanical sense. Such collective excitations furthermore generally fulfill the following criteria.

- (i) Their electromagnetic transition probabilities have a collective strength such that they are one to two orders of magnitude larger than the single-particle transitions (see Sec. 2.7.2).
- (ii) They show up in the spectra of different nuclei over entire regions of the periodic table with great regularity. The giant dipole resonance, for instance, has been observed throughout the periodic table and its excitation energy varies slowly with mass number [ $\propto 80A^{-1/3} + -1/6$ , see Eq. (1.44)].

The spectra of spherical as well as deformed nuclei contain a variety of states that fulfill these criteria. We will restrict ourselves to the general methods which, within the context of the *residual interaction* Eq. (2.35)

$$V_R = \frac{1}{4} \sum_{kk',ll'} \bar{v}_{kk'l'l'} a_k^+ a_{k'}^+ a_l a_{l'} - V_{HF}, \quad (8.1)$$

allow an explanation of the high-lying (which are usually resonances) as well as low-lying (usually bound states) collective vibrations. As indicated by Eq. (8.1), we will in the following mostly use the Hartree–Fock single-particle picture because it makes things somewhat less complicated. It should be emphasized, however, that all methods which we will present in the following sections generalize straightforwardly when using HFB quasi-particles (see Chap. 7) instead of particles. In certain cases we will also show this explicitly.

In Section 8.2, we study the interaction between  $ph$ -pairs based on an uncorrelated HF ground state (Tamm–Dancoff approximation TDA). In Section 8.3, different types of collective excitations are presented. Ground state correlations are taken into account in Section 8.4 within the random phase approximation (RPA) and it is shown that some problems inherent to the TDA method can be solved in this way. In Section 8.5, we show how the same equations can be derived with the formalism of linear response theory and what kind of features come into play when treating density dependent interactions. In Section 8.6 we present some numerical applications of the theory. Sum rules are an interesting means of extracting general properties of such resonances and of clarifying the relations between the quantum mechanical eigenstates of the RPA-Hamiltonian and the classical picture of surface vibrations. They are discussed in Section 8.7. Finally, Sections 8.8 and 8.9 are devoted to special extensions of the RPA, such as particle–particle RPA and quasi-particle RPA.

## 8.2 Tamm–Dancoff Method

### 8.2.1 Tamm–Dancoff Secular Equation

If we fill up the shell model potential with  $A$  nucleons up to a certain Fermi level, as shown in Fig. 8.2, then all zero, single, two, three, four, ...,  $N$  particle shell model excitations form a complete orthogonal set which can be used to expand the true many-nucleon wave functions of the ground state  $|0\rangle$  or the excited states  $|\nu\rangle$ . The exact solution of the Schrödinger equation would then be obtained by a diagonalization of  $H$  in the full shell model space or, equivalently, by a variation of the following expansion coefficients. [In the following we restrict the indices  $m, n$  ( $i, j$ ) to above (below) the Fermi level.]

$$|0\rangle = C_0^0 |HF\rangle + \sum_{mi} C_m^0 a_m^+ a_i |HF\rangle + \frac{1}{4} \sum_{mnij} C_{mn,ij}^0 a_m^+ a_n^+ a_i a_j |HF\rangle + \dots \quad (8.2)$$

$$|\nu\rangle = C_0^\nu |HF\rangle + \sum_{mi} C_m^\nu a_m^+ a_i^\dagger |HF\rangle + \frac{1}{4} \sum_{mnij} C_{mn,ij}^\nu a_m^+ a_n^+ a_i a_j |HF\rangle + \dots \quad (8.3)$$

Ideally, the determinant  $|HF\rangle$  would be given by filling up the  $N$  lowest single-particle levels of the Hartree–Fock potential. However, the latter is

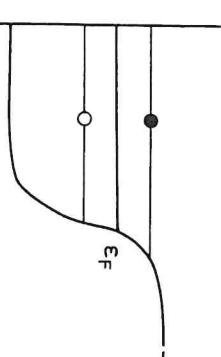


Figure 8.2. A  $ph$ -excitation in the shell model.

usually approximated by a phenomenological single-particle potential. The operator  $a_m^+ a_i$  consequently annihilates a particle below  $\epsilon_F$  (creates a hole) and creates a particle above  $\epsilon_F$ . It is therefore called a particle–hole creation operator (Fig. 8.2).

The exact diagonalization of  $H$  within the full shell model space is a task which cannot be solved. Let us, however, suppose that it is reasonable in the expansion of the excited states  $|\nu\rangle$  in Eq. (8.3) to go up to 1 particle–1 hole excitations only. We will see later that for certain kind of states this is indeed a very good approximation. A priori there are also reasons why this should be so. The subset of  $1\hbar\omega$  particle–hole excitations are the shell model configurations lowest in energy and should therefore be important for low-lying states of negative parity. Transition probabilities of states which are excited by an electromagnetic field  $F = \sum_{pp'} F_{pp'} a_p^- a_{p'}^+$  are proportional to  $|\langle 0|F|\nu\rangle|^2$  and these states are therefore believed to have dominant particle–hole contributions. We can thus hope to get a fair approximation for at least a certain class of states if we retain from the expansion (8.3) only the following terms

$$|\nu\rangle \approx C_0^\nu |HF\rangle + \sum_{mi} C_{mi}^\nu a_m^+ a_i |HF\rangle. \quad (8.4)$$

Since  $\langle HF | H a_m^+ a_i | HF \rangle = 0$  [Eq. (5.35)], we see that the ansatz (8.4) implies that the ground state remains a determinant, whereas it is sufficient for the excited state to retain only

$$|\nu\rangle = \sum_{mi} C_{mi}^\nu a_m^+ a_i |HF\rangle. \quad (8.5)$$

The main drawback of this procedure is the fact that correlations are only taken into account for the excited states, whereas the ground state will be unchanged. Later we will see how we can build correlations into the ground state also.

Since the Hamilton operator commutes with the operator of total angular momentum  $\mathbf{I}$  and in many cases also with the operator of total isospin  $\mathbf{T}$ , we should use the ansatz (8.5) in a Clebsch–Gordon coupled form [see Eq. (2.46)]. In order not to spoil the simplicity of our formulae we shall omit them in the following unless they are absolutely necessary.

Using (8.5) as a variational ansatz, we obtain with

$$|\delta\nu\rangle = \sum_{mi} a_m^+ a_i |\text{HF}\rangle C_{mi}^\nu \quad (8.6)$$

as usual a secular equation for the determination of eigenvalues and expansion coefficients:

$$\sum_{\eta j} \{ \langle \text{HF} | a_i^+ a_m a_n^+ a_j | \text{HF} \rangle - E_\nu \langle \text{HF} | a_i^+ a_m a_n^+ a_j | \text{HF} \rangle \} C_{\eta j}^\nu = 0. \quad (8.7)$$

With (8.5), we can get a more convenient form of Eq. (8.7):

$$\sum_{\eta j} \langle \text{HF} | a_i^+ a_m [H, a_n^+ a_j] | \text{HF} \rangle C_{\eta j}^\nu = (E_\nu - E_0^{\text{HF}}) C_{mi}^\nu. \quad (8.8)$$

The commutator in (8.8) can easily be calculated with the use of Eqs. (5.25)

$$[H, a_n^+ a_j] = \sum_r \{ t_{rn} a_r^+ a_j - t_{jr} a_n^+ a_r \} + \frac{1}{2} \sum_{rs} \bar{v}_{rsn} a_s^+ a_r a_j - \frac{1}{2} \sum_{sr} \bar{v}_{jrs} a_n^+ a_q a_r a_s. \quad (8.9)$$

With the definition (5.37) of the Hartree–Fock single-particle energies  $\epsilon_p$  and the rules for calculating the ground state expectation values of field operators (Appendix C) we finally obtain the so-called *Tamm–Dancoff equation*:

$$\sum_{\eta j} \{ (\epsilon_m - \epsilon_j) \delta_{mn} \delta_{ij} + \bar{v}_{mjn} \} C_{\eta j}^\nu = E^{\text{TDA}} C_{mi}^\nu. \quad (8.10)$$

$[E_0^{\text{HF}}$  has been set to zero by a suitable choice of the energy scale and  $E^{\text{TDA}}$  is the excitation energy of  $|\nu\rangle$  in Tamm–Dancoff approximation (TDA)].

For many purposes it has turned out to be useful to represent the matrix elements of the interaction  $\bar{v}$  graphically (Fig. 8.3):

$$\begin{aligned} \bar{v}_{mjn} &= \int \varphi_m^*(\xi_1) \varphi_j^*(\xi_2) v(\xi_1, \xi_2) \varphi_n(\xi_1) \varphi_j(\xi_2) d\xi_1 d\xi_2 \\ &\quad - \int \varphi_m^*(\xi_1) \varphi_j^*(\xi_2) v(\xi_1, \xi_2) \varphi_n(\xi_1) \varphi_j(\xi_2) d\xi_1 d\xi_2. \end{aligned} \quad (8.11)$$

The variable  $\xi$  stands symbolically for all coordinates and the integration shall include summation over spin and isospin. The rules for graphs are explained in many text books [AGD 63, Ma 67b] and since we do not want to present the graphical method as a tool by itself but rather as a pictorial representation of what we have derived analytically, we do not go into much detail here and simply give the prescription used to draw them. A wavy line shall stand for  $v$  and lines with arrows for the single-particle functions (arrow up-particle; arrow down-hole) which, according to their coordinates, are linked to the interaction points 1 and 2 of the wavy line. Furthermore, we usually agree that lines which are to the right of the interaction  $v$  in formula (8.11) point towards it, and that those lines to the left point away from it. With these conventions,  $\bar{v}_{mjn}$  can be displayed graphically, as shown in Fig. 8.3.

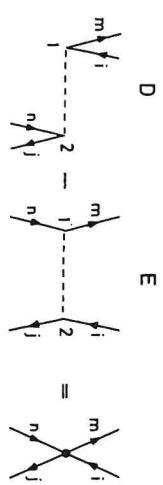


Figure 8.3. Graphical representation of the matrix elements  $v_{mjnin}$  and  $v_{mjin}$ .

If we imagine a time scale perpendicular to the wavy line, a particle–hole pair  $\eta j$  is annihilated and another one created in the direct term  $D$ , whereas in the exchange term  $E$  a pair  $\eta j$  is scattered in a new one  $m i$ . Thinking of the wavy line as a pion, the meaning of “direct” and “exchange” becomes even clearer; process  $D$  being a pair creation and annihilation process (as in electrodynamics, in which the wavy line stands for the photon, the hole for the positron, and the particle for the electron). The graph  $E$  then represents a process in which a pion is exchanged between a particle–hole pair. Very often the direct plus exchange term is combined into one graph (Feynman graph), indicated in Fig. 8.3.

## 8.2.2 The Schematic Model

The solution of the Tamm–Dancoff equation is, in general, not obtained in the full particle–hole space, since this is a very big numerical task. Therefore, in most cases, only a “model” space is retained which includes several levels above and below  $\epsilon_F$ . These calculations are also often called configuration mixing or shell model calculations. Before we go into more details, we want to study the qualitative features of the solutions of the TDA equation in a very simple model for which we can obtain the solution in an analytic form.

**8.2.2.1. Solution of the TDA Equation with a Separable Interaction.** The solution of Eq. (8.10) is greatly simplified if we assume that the matrix elements of the residual interaction are separable in the particle–hole indices (see Sec. 4.4.7 and [BB 59, BET 61])

$$\bar{v}_{mjn} = \lambda \cdot D_{mi} D_{nj}^*. \quad (8.12)$$

Further, it is assumed that the  $D_{mi}$  are matrix elements of a multipole operator as, for example, the quadrupole operator

$$D_{mi} = \langle m | r^2 Y_{2\mu}(\theta, \phi) | i \rangle. \quad (8.13)$$

The multipolarity agrees, of course, with the angular momentum to which the particle–hole pair  $(m, i)$  is coupled. The matrix element (8.12) is certainly not antisymmetric as it should be. However, it turns out that the exchange term is small and neglecting it is a good approximation [BK 68,

Ma 74]. In general, the residual interaction is attractive for  $T=0$  states (they are pushed down in energy as, for example, the  $3^- - T=0$  state in  $^{16}\text{O}$ ), and repulsive for  $T=1$  states [BB 59]. Therefore, we have to choose

$$\begin{aligned} \lambda < 0 & \quad \text{for } T=0; \\ \lambda > 0 & \quad \text{for } T=1. \end{aligned} \quad (8.14)$$

There are reasons to believe that the ansatz (8.12) for the interaction is not as bad as it might look, but here we do not want to go into the philosophy of a separable force (see Sec. 4.4.7). Rather, we wish to consider (8.12) as a convenient simplification which allows us to study the qualitative features of the TDA solution.

With the ansatz (8.12), the secular equation (8.10) has the following form.

$$(E_\nu^{\text{TDA}} - \epsilon_m + \epsilon_i) C_{mi}^\nu = \lambda D_{mi} \sum_{\eta_j} D_{\eta j}^* C_{\eta j}^\nu. \quad (8.15)$$

The states  $|\nu\rangle$  should, of course, be normalized and with Eq. (8.5) we therefore have:

$$\sum_{mi} C_{mi}^{\nu*} C_{mi}^{\nu'} = \delta_{\nu\nu'}. \quad (8.16)$$

With  $\sum_{\eta j} D_{\eta j}^* C_{\eta j}^\nu = \text{const.}$ , we can solve Eq. (8.15) for the coefficients  $C_{mi}^\nu$ :

$$\begin{aligned} C_{mi}^\nu &= N \cdot \frac{D_{mi}}{E_\nu^{\text{TDA}} - \epsilon_m + \epsilon_i}; \\ N^{-2} &= \sum_{mi} \frac{|D_{mi}|^2}{(E_\nu^{\text{TDA}} - \epsilon_m + \epsilon_i)^2} \end{aligned} \quad (8.17)$$

Multiplying Eq. (8.15) by  $D_{mi}^*(E_\nu^{\text{TDA}} - \epsilon_m + \epsilon_i)^{-1}$  and summing over  $m, i$ , we obtain an eigenvalue equation for the excitation energies  $E_\nu^{\text{TDA}}$ :

$$\frac{1}{\lambda} = \sum_{mi} \frac{|D_{mi}|^2}{E_\nu^{\text{TDA}} - \epsilon_m + \epsilon_i}. \quad (8.18)$$

We can solve Eq. (8.18) graphically by plotting the r.h.s. as a function of  $E_\nu^{\text{TDA}}$ . We thus obtain the eigenvalues from the intersection of this function with the straight line  $1/\lambda$ . All solutions are sandwiched between the original shell model excitations  $\epsilon_{mi} = \epsilon_m - \epsilon_i$ , only one solution being pushed up (if  $1/\lambda > 0$ ) or down (if  $1/\lambda < 0$ ). The assumption of a finite particle-hole space seems to enter into this argumentation, but we have to remember that *ph* shell model excitations of definite parity are grouped into bunches roughly  $2\hbar\omega_0$  apart. Figure 8.4 thus represents just one of these bunches.

The one excitation which is pushed down ( $T=0$ ) or up ( $T=1$ ) is a state formed by a *coherent* superposition of all matrix elements of the residual interaction, as can easily be shown for the degenerate case to be discussed

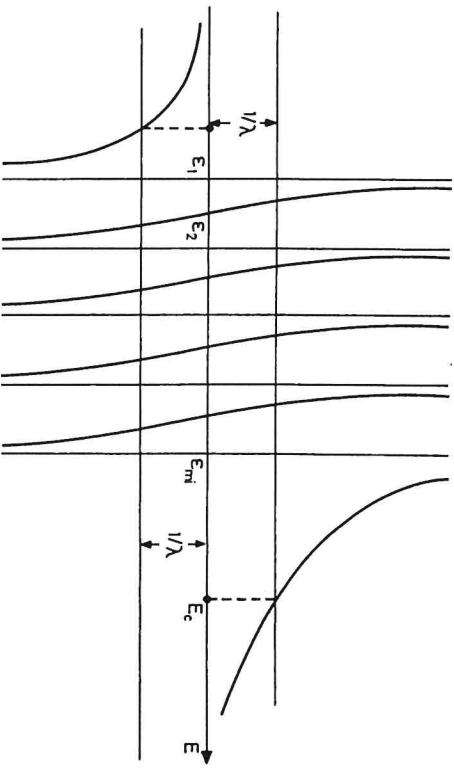


Figure 8.4. Graphical solution of Eq. (8.18).

next. By “coherent” we now mean that all matrix elements contribute with the same sign. Examples for such states are the first octupole states ( $T=0$ ) appearing in  $^{16}\text{O}$ ,  $^{40}\text{Ca}$ , and  $^{208}\text{Pb}$  at low excitation energies and the giant dipole resonance ( $T=1$ ), which we will turn to later.

**8.2.2.2. Degenerate Case.** If we set all  $\epsilon_{mi}$  equal to  $\epsilon$ , it follows from Eqs. (8.17, 8.18) that

$$C_{mi} = \left( \sum_{mi} |D_{mi}|^2 \right)^{-1/2} \cdot D_{mi}, \quad (8.19)$$

$$E_c^{\text{TDA}} = \epsilon + \lambda \sum_{mi} |D_{mi}|^2,$$

which means that collective state is being pushed up (down) by the sum of all diagonal elements of the interaction.

This degenerate case is realized, for example, if we take into account only one major shell for particles and another major shell for holes in a spherical oscillator potential without a spin orbit term. In reality things will not be so pronounced, but the essential features are likely to be preserved.

The collectivity of the shifted state can be demonstrated for the degenerate case by studying the partitioning of the total transition probability for the different excitations. For the collective state we have

$$|\nu_c\rangle = \left( \sum_{mi} |D_{mi}|^2 \right)^{-1/2} \sum_{mi} D_{mi} a_m^+ a_i |\text{HF}\rangle. \quad (8.20)$$

We therefore get, for the transition probability,

$$|\langle \nu_c | D | \text{HF} \rangle|^2 = \sum_{mi} |D_{mi}|^2, \quad (8.21)$$

a coherent superposition of the expansion coefficients (where the transition operator  $D = \sum_{kk'} D_{kk'} a_k^+ a_{k'}$  shall correspond to that for the separable interaction).

For the so-called sum rule (see Sec. 8.7), we get

$$\begin{aligned} \sum_{\nu} |\langle \nu | D | HF \rangle|^2 &= \sum_{\nu \neq \nu_c} \dots + |\langle \nu_c | D | HF \rangle|^2 \\ &= \sum_{\nu} \langle HF | D^+ | \nu \rangle \langle \nu | D | HF \rangle \\ &= \sum_{mi} \langle HF | D^+ | mi \rangle \langle mi | D | HF \rangle = \sum_{mi} |D_{mi}|^2. \end{aligned} \quad (8.22)$$

Here we replaced the complete set  $|\nu\rangle$  in the *ph* space by the complete set  $|mi\rangle$ . Because of (8.21), we see that the total sum rule is exhausted by the collective state.

This means that in the degenerate case there is no transition probability from the ground state to any non-collective state. On the other hand, the transition probability to the collective state (8.21) is drastically enhanced. We thus have a qualitative explanation for the strong  $1^-$  resonance shown in Fig. 8.1.

### 8.2.3 Particle–Particle (Hole–Hole) Tamm–Dancoff Method

As we have seen in the case of doubly magic nuclei, the simplest correlations beyond Hartree–Fock can only be taken into account by breaking the HF core and raising a nucleon from below to above the Fermi level. In moving away from doubly magic nuclei, that is, by filling nucleons into the next open shell, a quite different type of correlation may be viewed as important. Since a magic nucleus is supposed to be quite a stable entity, the correlations among the valence nucleons alone seem to be responsible for a variety of experimental facts known about these nuclei. The  $s - d$  shell nuclei ranging from  $^{16}\text{O}$  to  $^{40}\text{Ca}$  are perhaps the most studied examples of such “open shell” nuclei. A whole theory has been developed to treat such nuclei, known most widely under the heading of *shell model configuration mixing* calculations. Many ingredients of this theory can be found in the textbook of de Shalit and Talmi [ST 63], and the most advanced calculations within this theory have been performed by the Oak Ridge group [HMW 71] and by Whitehead [Wh 72]. In this section we only want to treat the simplest possible case of such nuclei, that is, we move away from the closed shell by only two particles, thus filling in two nucleons or removing two (creating two holes). In accordance with what we have said above, and by analogy to the *ph*-case, we may therefore try the following variational ansatz (*pp-TDA4 method*):

$$|\tau, A+2\rangle = \sum_{m < n} C_{mn}^r a_m^+ a_n^+ |HF\rangle. \quad (8.23)$$

The coefficients  $C_{mn}^r$  are supposed to be antisymmetric, that is,  $C_{mn}^r = -C_{nm}^r$ . In complete analogy to the *ph*-TDA case, we obtain the *pp-TDA* secular equation:

$$(E_r^{\text{TDA}} - \epsilon_m - \epsilon_n) C_{mn}^r = \sum_{m' < n'} \bar{v}_{mm'n'n} C_{mn}^r. \quad (8.24)$$

This is a linear Hermitian eigenvalue problem. The eigenvectors have to fulfill the norm and closure relations ( $n < m$ ,  $n' < m'$ )

$$\sum_{m < n} C_{mn}^r C_{m'n'}^{r*} = \delta_{nn'} \delta_{mm'}. \quad (8.25)$$

$$\sum_{m < n} C_{mn}^r C_{m'n'}^{r*} = \delta_{nn'} \delta_{mm'}. \quad (8.26)$$

As indicated, the sum in principle runs over all levels  $> \epsilon_F$  and therefore includes bound and continuum states. Since this generally gives rise to matrices too big for present day computers, we usually work in a restricted subspace, taking into account one or two major shells above the Fermi level. In order to account for the levels not included, we must take a suitably “renormalized” interaction (see Sec. 4.3.2). Equation (8.24) looks just the same for the *hh*-TDA case but the particle indices  $(m, n)$  are replaced by hole indices  $(i, j)$  and the sign of the single particle energies is reversed. The solutions of the *pp*(*hh*) equation can exhibit features similar to the *ph* case. For instance, we can also get collective low-lying states, known mostly as *pairing vibrations* (see Sec. 8.3.5). Since the qualitative discussions would be very much the same as in the *ph* case, we will not go into greater detail. (For calculations in the lead region, see, for instance, [HK 72, MT 73] and references therein.)

## 8.3 General Considerations for Collective Modes

### 8.3.1 Vibrations in Quantum Mechanics

Perhaps this is the right place to interrupt our more or less formal discussion of the TDA method for a while and consider the nature of the collective states in more detail. In Chapter 1 we described states such as vibrations of a liquid drop. The word vibration may be puzzling in the quantum mechanical context, since we are in fact only dealing with stationary states. The density  $\rho(\mathbf{r})$  of such a stationary state is time independent. The correspondence is roughly the same as talking about oscillations in the quantum mechanical harmonic oscillator problem. To get a time dependent density distribution  $\rho(\mathbf{r}, t)$  which vibrates around the ground state density  $\rho^{(0)}(\mathbf{r})$  we have to investigate a *wavepacket*

$$|\Psi(t)\rangle = |0\rangle + \sum_{\nu} c_{\nu} |\nu\rangle e^{-iE_{\nu}t/\hbar} \quad (8.27)$$

which contains the ground state  $|0\rangle$  and small admixtures of excited states  $|\nu\rangle$ . Up to first order in the coefficients  $c_{\nu}$  the corresponding density is (see Appendix D):

$$\begin{aligned} \rho(\mathbf{r}, t) &= \langle \Psi(t) | \sum_{i=1}^A \delta(\mathbf{r} - \mathbf{r}_i) | \Psi(t) \rangle \\ &= \rho^{(0)}(\mathbf{r}) + \delta\rho(\mathbf{r}, t) \end{aligned} \quad (8.28)$$

with

$$\delta\rho(\mathbf{r}, t) = \sum_{\nu} c_{\nu} \langle 0 | \sum_{i=1}^A \delta(\mathbf{r} - \mathbf{r}_i) | \nu \rangle e^{-iE_{\nu}t/\hbar} + \text{c.c.} \quad (8.29)$$

A Fourier analysis of this density gives the contributions of the different excited states

$$\rho^{(1)\nu}(\mathbf{r}) = \langle 0 | \sum_{i=1}^A \delta(\mathbf{r} - \mathbf{r}_i) | \nu \rangle. \quad (8.30)$$

These quantities are called *transition densities*.

In general, we expect oscillations not only in the local part of the density as given in Eq. (8.28), but also in the nonlocal part, that is, we are interested in the transition density matrix. As discussed in Appendix D, in a shell model basis, it has the form

$$\rho_{pq}^{(1)\nu} = \langle 0 | a_q^\dagger a_p | \nu \rangle. \quad (8.31)$$

In the TDA approach these matrix elements are given by the coefficients  $C_m^\nu$  in Eq. (8.5), that is, in TDA we have

$$\rho_{ml}^{(1)\nu} = C_{mi}^\nu, \quad \rho_{ii}^{(1)\nu} = \rho_{mm}^{(1)\nu} = \rho_{im}^{(1)\nu} = 0. \quad (8.32)$$

There are many different types of modes a nucleus can assume according to its various degrees of freedom: A nucleus can be deformed, displaced, or compressed; the densities of the protons and neutrons can vibrate *in* and *out* of phase; there can be vibrations in spin and isospin; we have pairing modes and many more things of which only a few elementary features will be discussed here (see also Chap. 13).

### 8.3.2 Classification of Collective Modes

Since we are dealing with harmonic vibrations in this chapter, in the following we want to investigate their qualitative properties in more detail. To see the basic structures we restrict our discussion to spherical closed shell nuclei. The best suited example is  $^{208}\text{Pb}$ . These considerations do, however, also apply for the other regions in the periodic table. In fact, as we saw in the introduction, many of these collective excitations show rather classical properties which depend smoothly on the mass number.

Collective *ph*-vibrations can be characterized by the properties of the corresponding pair operators [Mo 76a+b]

$$(a^\dagger a). \quad (8.33)$$

There are a number of exact symmetries of the Hamiltonian such as rotational invariance, parity conservation, and charge conservation with the corresponding quantum numbers  $I$ ,  $\pi$  and  $T$ . In addition, we have (as discussed in Sec. 2.6.3) the approximate isospin symmetry for light and heavy nuclei with the quantum number  $T$ . Since we start with a spherical closed shell nucleus in its ground state ( $I^\pi = 0^+$ ), the angular momentum and the parity of the excitation are determined by the corresponding quantum numbers of the coupled pair  $(a^\dagger a)_\nu$ . The same also holds true in light ( $N = Z$ ) nuclei (with  $T = 0$  in the ground state) for the isospin. For

heavy nuclei, the isospin of the ground state is  $T_0 = (N - Z)/2$  and it has to be coupled to the isospin of the *ph* pair to the total isospin  $T = T_0$  or  $T = T_0 + 1$ . \* We usually classify the excitation by the numbers  $\Delta T$  of the *ph* pairs  $a^\dagger a$ . Therefore, we have  $\Delta T = 0$  or  $\Delta T = 1$  excitations, and a  $\Delta T = 1$  excitation does not necessarily mean  $T = T_0 + 1$ .

In addition to these general considerations about symmetries, which give, for instance, information about the angular distributions, we want to classify the collective motion more precisely according to the different degrees of freedom in the *ph* pair

$$a^\dagger(\mathbf{r}, s, t) a(\mathbf{r}', s', t'). \quad (8.34)$$

(a) In the first place, there are vibrations of the *local* density  $\rho(\mathbf{r})$  of the nucleus in space. Since the angular dependence of such vibrations is already completely determined by the angular momentum, we only can allow for different *radial shapes*. The simplest examples in this context are the surface vibrations of a sphere with a sharp surface, which we have discussed in Section 1.4 in great detail. From Eq. (1.7) we find that the transition density (8.30) for such a surface vibration with a sharp surface is given by

$$\rho^{(1)}(r) = \begin{cases} \pm \rho_0 & \text{for } r \text{ between } R_0 \text{ and } R(\theta, \varphi), \\ 0 & \text{elsewhere,} \end{cases} \quad (8.35)$$

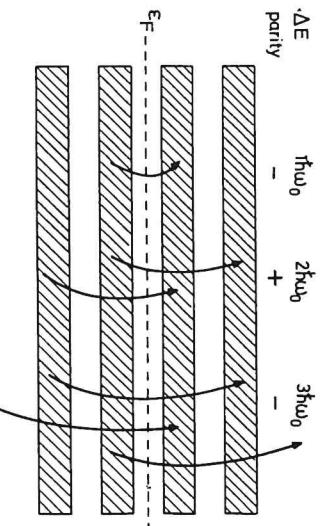
that is, the density in the nuclear interior stays constant. The entire transition is concentrated in the surface region.

We can also imagine other radial dependences of  $\rho^{(1)}$ , where the density in the interior is also changed. Such excitations are called *breathing modes*.

(b) A quite different type of motion, which also involves only the spatial degrees of freedom is given by vibrations in the nonlocal part of the transition density matrix  $\rho^{(1)}(\mathbf{r}, \mathbf{r}')$ . An example is the *nuclear twist mode*, where the local density of the nucleus stays unchanged and only the intrinsic velocity distribution oscillates (see [HE 77]).

(c) The isospin is an additional degree of freedom. There we have to distinguish between excitations in the same nucleus  $\Delta T_z = 0$  and isospin flip processes  $\Delta T_z = -1$ , which belong to the neighboring nucleus with the charge  $Z + 1$  and the neutron number  $N - 1$ . In the first case, the *ph* pair can be coupled to either  $\Delta T = 0$  or to  $\Delta T = 1$ . For all the modes discussed so far, we therefore have two options: The protons can vibrate in phase ( $\Delta T = 0$ ) or out of phase ( $\Delta T = 1$ ) with the neutrons. At a fixed point  $\mathbf{r}$  we then eventually have an oscillating charge distribution. This corresponds to *polarization waves* in the nucleus. A case of vibrations with  $\Delta T_z = -1$  is the analog resonances, which will be discussed in Section 8.3.4.

\*  $T = T_0 - 1$  is only possible in proton particle-neutron hole excitations that correspond to states in the neighboring odd-odd nucleus.



**Figure 8.5.** Schematic picture of the shell structure in a closed shell nucleus and possible  $1p - 1h$  excitations.

(d) Finally, we also have the *spin* degree of freedom. The corresponding vibrations produce spin waves.

The classification of different modes given so far was, to a large extent, based on considerations within the coordinate space and emphasized its classical aspects. In finite realistic nuclei however, these modes are not precisely realized. There are always more or less drastic admixtures of less collective states. Therefore, it is often very useful to apply quite a different classification, based on the *shell model* in its simplest version—the harmonic oscillator.

Figure 8.5 shows schematically the shell structure for a closed shell nucleus (as  $^{208}\text{Pb}$ ). We have alternating shells with positive and negative parities separated by an energy distance of roughly  $\hbar\omega_0$ . For a closed shell nucleus, the Fermi surface lies just between two shells and we therefore find  $p\hbar$ -pairs of a  $1\hbar\omega_0$  excitation with negative parity, or a  $2\hbar\omega_0$  excitation with positive parity, or a  $3\hbar\omega_0$  excitation with negative parity, and so on. For nuclei between closed shells we also have, in addition,  $0\hbar\omega_0$  excitations within the shell.

In realistic nuclei, the degenerate oscillator shells split up and a few levels with the wrong parity are shifted down into a lower shell by the  $1s$  term. This also causes  $1\hbar\omega_0$  excitations with positive parity for closed shell nuclei such as  $^{208}\text{Pb}$ . But the basic features of this pictures also hold in realistic cases.

Although we have superpositions of many  $p\hbar$  pairs in the collective excitation and drastic energy shifts due to the correlations as discussed in

Section 8.2.2.2, this gross structure is conserved to a large extent.\* For  $J^\pi = 3^-$ , for instance, we find a very collective state consisting mainly of  $1\hbar\omega_0$  excitations and a second one consisting mainly of  $3\hbar\omega_0$  excitations

It is evident that this shell structure has a great influence on the excitation energy of the low-lying collective states (shown schematically in Fig. 1.6), because they depend closely on the  $p\hbar$  energy of the lowest  $p\hbar$  pair. In fact, here we observe drastic shell effects (see Fig. 1.7). For the high-lying states, the giant resonances, this is no longer the case. The energy distance between two major shells varies only smoothly over the periodic table [ $\hbar\omega_0 \propto A^{-1/3}$ ; see Eq. (2.12)]. We therefore expect a similar smooth  $A$ -dependence of the resonance energy for giant resonances.

### 8.3.3 Discussion of Some Collective $p\hbar$ -Vibrations

In a sense the most trivial collective motion is a *translation* of the whole nucleus, generated by the linear momentum  $\mathbf{P}$ . Since it commutes with the two-body Hamiltonian  $H$ , the exact ground state  $|0\rangle$  is an eigenfunction of  $P$ . However, if we use an approximation  $|0\rangle_{\text{app}}$  for the ground state which violates this symmetry,  $\mathbf{P}|0\rangle_{\text{app}}$  are new states. They look like collective excitations. We call them *spurious*, because they do not correspond to physical excitations. Within the angular momentum coupling scheme, their quantum numbers are  $J = 1^-$ ,  $T = 0$  ( $\mathbf{P}$  is a vector operator that does not depend on the isospin). They correspond to a translation of the whole nucleus. There is no restoring force against this motion and therefore they should have zero excitation energy

$$H|0\rangle_{\text{app}} = \mathbf{P}H|0\rangle_{\text{app}} \approx E_0|\mathbf{P}|0\rangle_{\text{app}}. \quad (8.36)$$

However, this depends on the approximation. For instance, in the TDA,  $\mathbf{P}|H\rangle$  is a superposition of particle-hole states, which is generally not an eigenstate of the TDA equations (8.10). Instead, it is a mixture of all the TDA eigenstates, which form a complete set in the  $1p - 1h$  space. Since its energy is nevertheless close to  $E_0$  (Eq. 8.36), it has large components of the low-lying TDA states. This means some low-lying solutions of the TDA equation (8.10) have large spurious contributions. As long as we are working in a spherical basis with good spin and isospin, only the  $J = 1^-$ ,  $T = 0$  states are influenced. They have to be treated separately in order to extract the spurious components. For details, see Chapter 11.

The best known and the most thoroughly investigated giant resonance is the *giant dipole state* (see for instance [Sp 68]). It is a several MeV broad resonance, which has been observed over the whole periodic table at an energy of roughly

$$E_{1^-} \propto 80A^{-1/3+/-1/6} [\text{MeV}]. \quad (8.37)$$

A typical case is shown in Fig. 8.1. The experimental spectrum usually shows some fine structure. It has its origins in the specific properties of nuclei and is not constant over the periodic table. Particular  $p\hbar$ -components may show up—as in  $^{16}\text{O}$  [EF 57]—or shell effects may cause a splitting of the resonance. For instance, passing from spherical to de-

\* One can also show this analytically in a schematic model with several bunches of degenerate levels in analogy to Sec. 8.2.2.

formed nuclei, we observe two kinds of dipole vibrations, one parallel to the symmetry axis and one orthogonal to it. The splitting of the energies allows an experimental determination of the deformation parameter [Da 58, Ok 58, BBC 71].

The giant dipole resonance is excited, for instance, by photo-absorption of  $\gamma$ -radiation. In Section B.7 we derive the cross section for the excitation of a final state  $|\nu\rangle$  by a photon of energy  $E$

$$\sigma_\nu(E) = \frac{4\pi^2 e^2}{\hbar c} (E_\nu - E_0) |\langle \nu | D | 0 \rangle|^2 \delta(E - E_\nu + E_0). \quad (8.38)$$

$D$  is the dipole operator (B.88) for  $E$  1-radiation in the  $z$ -direction.

$$D = \frac{NZ}{A} \left( \frac{1}{Z} \sum_{p=1}^Z z_p - \frac{1}{N} \sum_{n=1}^N z_n \right) = - \sum_{i=1}^A i f_3^{(i)} (\mathbf{r}_i - \mathbf{R})_z. \quad (8.39)$$

It is proportional to the  $z$ -component of the distance between the two centers of gravity for protons and neutrons.

The total cross section for dipole absorption  $\sigma_{\text{total}}$  is obtained from (8.38) by summing over all final states  $|\nu\rangle$  and integrating over the energy:

$$\sigma_{\text{total}} = \sum_p \int_0^\infty \sigma_\nu(E) dE = \frac{4\pi^2 e^2}{\hbar c} \sum_p (E_\nu - E_0) |\langle \nu | D | 0 \rangle|^2. \quad (8.40)$$

It is proportional to the energy-weighted dipole sum rule (see also Sec. 8.7)

$$S_1(D) = \sum_\nu (E_\nu - E_0) |\langle \nu | D | 0 \rangle|^2 \quad (8.41)$$

and can be evaluated in closed form:

$$S_1(D) = \frac{1}{2} \langle 0 | [D, [H, D]] | 0 \rangle,$$

where  $H$  is the exact two-body Hamiltonian and  $|0\rangle$  is the exact ground state. If we assume that the two-body potential has no velocity dependence and no exchange mixtures (Wigner force), we easily calculate in analogy to (8.158):

$$\langle 0 | [D, [H, D]] | 0 \rangle = \frac{NZ}{A} \frac{\hbar^2}{m}. \quad (8.42)$$

For the dipole sum we therefore have the Thomas-Reiche-Kuhn sum rule:

$$\sigma_{\text{total}} = \int_0^\infty \sigma(E) dE = \frac{2\pi^2 e^2 \hbar}{mc} \frac{NZ}{A} \approx 0.06 \frac{NZ}{A} [\text{MeV} \cdot \text{barn}]. \quad (8.43)$$

This value is enlarged by 40–80% if the two-body interaction contains exchange mixtures (see, e.g., Breng [Br 65b]) and tensor forces [WKB 73], which then seems to yield roughly the right magnitude of the overall energy integrated cross section. It thus turns out that in  $^{16}\text{O}$  approximately 3% of the dipole sum lies in low-lying  $1^-$  states, whereas the giant resonance shell model  $p-h$  resonances below 20 MeV, whereas the giant resonance peak contains about 50%, clearly reflecting its collective character. The rest of the dipole sum is to be found beyond 30 MeV [ABC 63, FH 62a, b, Ha 65b, BS 64, ADW 78]. For heavy nuclei the giant dipole resonance can

exhaust up to 100% of the sum rule. The experiment therefore shows that a very large part of the dipole sum (8.43) is exhausted by the giant dipole resonance, and this means that this resonance has a large overlap with the state

$$|D\rangle = D|0\rangle = \frac{NZ}{A} \left\{ \frac{1}{Z} \sum_{pp'} \langle p | z | p' \rangle a_p^+ a_{p'} - \frac{1}{N} \sum_{nn'} \langle n | z | n' \rangle a_n^+ a_{n'} \right\} |0\rangle, \quad (8.44)$$

which has become known as the Goldhaber-Teller state [GT 48] (see Sec. 13.3.3).

The quantum numbers of the state are identical with those of the giant resonance  $J^\pi = 1^-$ . In the case of the isospin, we have to distinguish two cases.

(a) For light  $N=Z$  nuclei the Coulomb force can be neglected. The ground state  $|0\rangle$  then has  $T=0$ . The operator  $D$  is a vector in isospin space, as we see from Eq. (B.88). Angular momentum coupling rules therefore show that  $D|0\rangle$  has  $T=1$ .

(b) For heavy nuclei the isospin is again conserved. The ground state has  $T_0 = (N-Z)/2$ . Using similar arguments as in Sec. 2.6.3 we can convince ourselves that the dipole state  $|D\rangle$  has the same isospin  $T_0$  by showing that

$$T_+ |D\rangle \approx 0. \quad (8.45)$$

This does not, however, mean that there are no other  $1^-$  states with  $T=T_0+1$  in the excitation spectrum of the nucleus. We simply do not excite them by dipole  $\gamma$ -rays.

The structure of the operator  $D$  shows that the giant dipole resonance consists mainly of  $1\hbar\omega_0$  excitations. Because of the repulsive character of the residual interaction it is shifted to higher energies.

Besides this well known dipole state, in the last ten years a number of other giant resonances of higher multipolarity have been found. The *giant quadrupole resonance* is especially well established over the whole periodic table at an energy somewhat less than the giant dipole resonance [PW 71, FT 72, LB 72, HGA 74, Sa 74, KWB 75, YMR 76, Be 76]

$$E_{2+} \approx 60-65 A^{-1/3} [\text{MeV}]. \quad (8.46)$$

It exhausts 40–100% of the energy weighted sum rule of the isoscalar quadrupole operator\*

$$r^2 Y_{20}. \quad (8.47)$$

\* Unfortunately, in a direct comparison with experiment we cannot use photo-absorption, as in the dipole case, because (i) the photon field does not contain the isovector part for  $\lambda > 1$ , and (ii) in practice the photonuclear reactions proceed primarily through the dipole mode. The most important experimental tool used to excite such vibrations is inelastic scattering of electrons and heavier particles such as protons, deuterons, and alpha particles [Sa 76]. The corresponding excitation operators have a more complicated structure (see, for instance, [UE 71, Sa 72a+b, 74, HMS 75] and the sum rules are no longer model independent. Therefore, we will not go into the details of the analysis of such experiments.

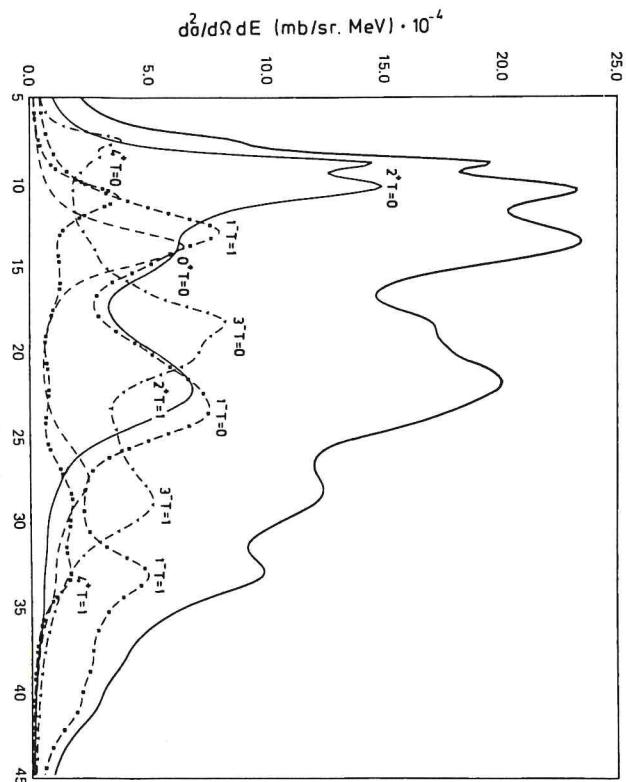
It consists, as numerical calculations show [RS 74a], mainly of  $2\hbar\omega_0$  excitations, and is shifted downwards in energy by the residual interaction to around  $1.4\hbar\omega_0$ . \* (The corresponding isovector mode is expected at  $3.3\hbar\omega_0$  [Ha 72].) The rest of the isoscalar quadrupole strength lies in the low-lying collective  $2^+$  state, which shows drastic shell effects (Fig. 1.7) and consists mainly of  $0\hbar\omega_0$  excitations.

Recently, a *breathing mode* was also observed [MMW 75, ST 77, HBI 77, YRM 77, BBL 80], a spherical density oscillation with the quantum number  $J''=0^+$ ,  $T=0$ . As we shall see in Fig. 8.14, its transition density is not only concentrated on the nuclear surface but involves changes of the nuclear density over the whole volume. Its excitation energy lies at

$$E_{0^+} \approx 80A^{-1/3} \text{ MeV.} \quad (8.48)$$

This energy is a direct measure of the nuclear incompressibility (5.95) [Wa 62a, BGG 76]. In  $^{208}\text{Pb}$  the experimental breathing mode lies at 13.8 MeV, a value corresponding to  $K \approx 200$  MeV, which is in good agreement with theoretical predictions [RS 74a, SZR 74, WMR 77].

\* In deformed regions we observe a splitting of the giant quadrupole resonance into three components with  $K=0, 1$  and  $2$  [KMY 75].



**Figure 8.6.** The electron spectrum for 90 MeV ( $e, e'$ ) at  $75^\circ$  calculated with microscopic RPA wave functions. The numbers in the figure denote the angular momentum parity and isospin of the corresponding cross-section contribution. The thick line is the sum of all the different contributions. (From [WKS 78].)

*Magnetic resonances* are excited by operators which involve the spin and the orbital angular momentum operators. They have the quantum numbers  $1^+, 2^-, 3^+, \dots$  and have been predicted by several calculations (see, for instance, [RS 74a, SWK 76, FRS 78]). Their experimental evidence, however, is still an object of discussion.

*Further giant resonances* in the spectra have been observed in various experiments (see, for instance, [PBD 74, TIS 75, Pa 75a, SEB 74]), but the spin and parity assignments are not completely established. As an illustrative picture we show in Fig. 8.6 a calculation of the  $(e, e')$  spectrum for the giant resonance region of  $^{208}\text{Pb}$ . We see clearly that the total spectrum can only be obtained by a complicated superposition of rather different resonances.

### 8.3.4 Analog Resonances

Nuclear reactions for heavy nuclei ( $N > Z$ ), like, for example,  $^{208}\text{Pb}$  ( $p, n$ )  $^{208}\text{Bi}$ , exhibit strong collective resonances called *analog states* for reasons we will learn about in a moment.\*

To explain the structure of these states we use the fact that the nuclear wave functions in heavy nuclei are, to a rather good approximation, eigenstates of the isospin operator  $\mathbf{T}^2$  (see Sec. 2.6.3). The ground state and the low-lying excited states have the quantum numbers  $T = T_3 = (N - Z)/2$ .

Starting from such a state  $|J, T_3 = T\rangle$  at an energy  $E$ , we can define its *analog state* by the application of the isospin lowering operator  $T$ .

$$T_- |J, T, T_3 = T\rangle = \sqrt{2T} |J, T, T_3 = T-1\rangle. \quad (8.49)$$

It belongs to the "daughter" nucleus ( $N-1, Z+1$ ) and is again an eigenstate of  $H$  with the energy

$$E_a = E + \Delta_r. \quad (8.50)$$

To see this we decompose the exact Hamiltonian  $H$  into the nuclear part  $H_{\text{nuc}}$  which commutes with  $T_-$  and the Coulomb interaction  $V_c$

$$HT_- = (H_{\text{nuc}} + V_c)T_- = T_- H + [V_c, T_-]. \quad (8.51)$$

The commutator  $[V_c, T_-]$  is of the form

$$\begin{aligned} [V_c, T_-] &= \sum_i V_c(i, j) \left[ \left( \frac{1}{2} - i_3^{(i)} \right) \left( \frac{1}{2} - i_3^{(j)} \right), T_- \right] \\ &= \sum_i V_c(i) T_-^{(i)} \end{aligned} \quad (8.52)$$

with the average Coulomb field

$$V_c(i) = \sum_{j \neq i} V_c(i, j) \left( \frac{1}{2} - i_3^{(j)} \right). \quad (8.53)$$

Under the assumption that this single-particle potential in the interior of the nucleus has a constant value of roughly  $\Delta_r$  (see Fig. 2.7), we obtain for each eigenstate  $|n\rangle$  of the "parent" nucleus ( $N, Z$ ) an analog state  $T_-|n\rangle$  in the

\* For the literature, see, for instance, [AHK 72].



**Figure 8.7.** Schematic representation of the spectrum of analog states.

"daughter" nucleus  $(N-1, Z+1)$

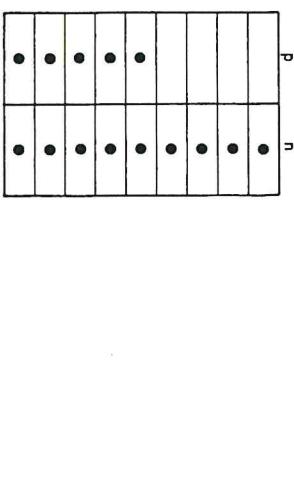
$$HT_-|n\rangle = E_n T_-|n\rangle + [H, T_-]|n\rangle \approx (E_n + \Delta_-)T_-|n\rangle. \quad (8.54)$$

This means that in the daughter nucleus there is a sequence of states with the same energy spacings as the low-lying levels of the parent nucleus itself, having isospin

$$T = \frac{N-Z}{2} = \frac{N-Z-2}{2} + 1, \quad (8.55)$$

which is one unity larger than the isospin of the daughter nucleus ground state (Fig. 8.7).

In order to learn more about the structure of the analog resonances we will forget for the moment the residual interaction used in the description of the ground state of the parent nucleus  $(N, Z)$ . This will be given by a pure shell model description, represented graphically in Fig. 8.8.



**Figure 8.8.** Schematic representation of a pure shell model determinant.

We assume that the protons and neutrons, which occupy the states with the same quantum numbers (besides  $t_3$ , of course) form an inert core and are coupled to  $T=0$ . In the following, we shall neglect this inert core, so that the ground state of the mother nucleus is given by

$$|I, T, T_3 = T\rangle = \begin{array}{|c|c|} \hline p & n \\ \hline \bullet & \bullet \\ \hline \end{array}. \quad (8.56)$$



**Figure 8.9.** Schematic representation of the analog state of the daughter nucleus.

With  $T_- = \sum_i t_3^{(i)}$ , we obtain for the analog state of the daughter nucleus:

$$|I, T, T_3 = T-1\rangle = \frac{1}{\sqrt{2T}} \left\{ \begin{array}{l} \begin{array}{|c|c|} \hline p & n \\ \hline \bullet & \bullet \\ \hline \end{array} + \begin{array}{|c|c|} \hline p & n \\ \hline \bullet & \bullet \\ \hline \end{array} + \begin{array}{|c|c|} \hline p & n \\ \hline \bullet & \bullet \\ \hline \end{array} + \begin{array}{|c|c|} \hline p & n \\ \hline \bullet & \bullet \\ \hline \end{array} \end{array} \right\} = \frac{1}{\sqrt{2T}} \sum_{\mu} |\mu\rangle. \quad (8.57)$$

The analog state in Eq. (8.57) is a coherent superposition of certain  $p\bar{n}$ -states formed by replacing, in (8.56), the neutrons by protons one by one in the corresponding states.

There are, of course, other linear combinations of the states  $|\mu\rangle$  orthogonal to the analog state  $|I, T, T_3 = T-1\rangle$ :

$$\sum_{\mu} c_{\mu} |\mu\rangle \quad \text{with} \quad \sum_{\mu} c_{\mu} = 0.$$

The operator  $T_+$  annihilates them

$$T_+ \sum_{\mu} c_{\mu} |\mu\rangle \propto \left( \sum_{\mu} c_{\mu} \right) \cdot |I, T, T_3 = T\rangle = 0. \quad (8.58)$$

Therefore, they must have isospin  $T-1$ , which is the isospin of the ground state of the daughter nucleus. Without residual interaction they lie at the same energy as the analog state and have equal spin and parity.

Experimentally, the analog states are observed as very sharp resonances at high energies [AW 61]. Their width is so small, because the isospin selection rule forbids a rapid decay into the other states which form a continuous background.

To see how they can be treated with the TDA, we start with a HF potential which is the same for protons and neutrons. Only the energy levels of protons and neutrons are shifted with respect to one another by an amount  $\Delta_t = \Delta_p - \Delta_n$  [see Eq. (2.27)]. The quantity  $\Delta_t$  has its origin in the symmetry energy. In our approximation this is the only difference in the self-consistent potential of protons and neutrons resulting from the nuclear force.

If we diagonalize the residual interaction in the space of the states  $|\mu\rangle$  we obtain a splitting between the analog resonance and the other states. Assuming a separable force we end up with the degenerate model of Section 8.2.2. Again, it concentrates all strength in the analog state and shifts its energy from the unperturbed value  $\Delta_t = \Delta_p - \Delta_n$  to its proper value  $\Delta_c$ , because it is exactly the proton-neutron interaction which causes the symmetry energy  $\Delta_c$ . For details, see the textbook of G. E. Brown [Br 64, (second edition 1967)] and other references cited in the review article [AHK 72].

### 8.3.5 Pairing Vibrations

As indicated in the treatment of the  $pp(hh)$ -TDA method, there is a great formal similarity between the  $p\bar{n}$  and  $p\bar{p}(hh)$  cases. In fact, it also turns out that there are collective  $p\bar{p}(hh)$  solutions of the corresponding TDA equation (8.24). A good example is the  $0^+$  ground state of  $^{206}\text{Pb}$ . The amplitudes  $C_{mn}^r$  according to Eq. (8.23) enter directly into the expression of, for

example, a  $^{208}\text{Pb}$  ( $p, t$ )  $^{206}\text{Pb}$  pickup or a  $^{208}\text{Pb}$  ( $t, p$ )  $^{210}\text{Pb}$  stripping cross section [GJ 65]. The fact that the  $0^+$  ground state of  $^{206}\text{Pb}$  is populated by such a reaction an order of magnitude larger than the other  $0^+$  states of  $^{208}\text{Pb}$ , clearly indicates the coherent contribution of the  $C_{ij}^{0+}$  amplitudes and therefore the collectivity of this state. Similar to this is the situation for  $^{210}\text{Pb}$ . These rather strongly bound entities of two particles in  $(0^+)$  states is due to the short-range part of the interaction and has already been discussed at the beginning of Chapter 6. Two particles form such a stable entity that they can be multiplied, added to, or removed from a nucleus (like, for example,  $^{208}\text{Pb}$ ) almost like independent particles (which behave very much like bosons because of their integer spin). The spectrum should therefore be approximately harmonic which, in fact, is the case for the lead isotopes (Fig. 8.9) [BM 75]. This harmonic spectrum is what has been termed the spectrum of "pairing vibrations." We can also produce excited  $0^+$  pairing vibrations in these nuclei. For example, let us remove from  $^{208}\text{Pb}$  a  $0^+$  pairing phonon, which leads us to  $^{206}\text{Pb}$ . At the same time, let us add a phonon leading from the  $^{208}\text{Pb}$  to the  $^{210}\text{Pb}$  ground state; this clearly gives an excitation in  $^{208}\text{Pb}$   $2\hbar\omega$  apart and indeed such a strongly excited state in  $^{208}\text{Pb}$  ( $p, t$ )  $^{208}\text{Pb}$  and  $^{208}\text{Pb}$  ( $t, p$ )  $^{208}\text{Pb}$  reactions is very well known and lies at 4.9 MeV in  $^{208}\text{Pb}$ .

The fact that particle-particle correlations lead to collective nuclear modes—now usually called pairing vibrations—was recognized by H. Schmidt [Sch 64a, b] and Bohr [Bo 64] and worked out in much detail later on by Bes and Broglia [BB 66] (for a review see [BHR 73] and the references therein).

It is a quite general concept which describes the pairing correlations on the same level as the deformations. Starting from a spherical closed shell nucleus, we can excite *quadrupole vibrations*, which have an *angular momentum* different from the ground state, and *pairing vibrations*, which belong to nuclei with a different *particle number*. Ground state correlations induced by such vibrations (see Sec. 8.4.6) give in the first case a virtual quadrupole deformation and in the second case a virtual excitation of collective  $2p - 2h$  states. As we go away from a closed shell, the nuclei get softer, that is, the correlations get larger. Finally we get a phase transition to deformed states—induced by the  $ph$ -correlations; or to superfluid states—induced by

## 8.4 Particle-Hole Theory with Ground State Correlations (RPA)

One feature of our approximate ansatz (8.5) was the fact that we could build correlations into the excited states; the ground state however, remains unchanged in the TDA method. This complete neglect of the residual interaction  $V_R$  in the ground state certainly influences the results. To remove this drawback of the TDA method, we could think of retaining also the  $(2p - 2h)$  components in Eq. (8.2). This is not practicable, since the corresponding matrices would become prohibitively large. One way out is a generalization of the TDA method in which we take, instead of the HF ground state, one in which a certain class of correlations has been summed. Although the discussion of the problem stays more or less the same as for the TDA method, we will have to pay a certain price for this refinement of our theory. Our new equations will no longer follow out of a variational principle, and thus we can generally get imaginary solutions. We will derive the new equations [random-phase approximation (RPA)]<sup>\*</sup> in close analogy to the TDA method using a different technique which will suggest quite naturally the necessary generalizations leading to the RPA.

### 8.4.1 Derivation of the RPA Equations

To get a better understanding of what is done in the random phase approximation, we will first re-derive the TDA equations using a different technique, the so-called equation of motion method [Ro 68a, 70]. We start with a set of exact eigenstates of the Hamiltonian  $H$

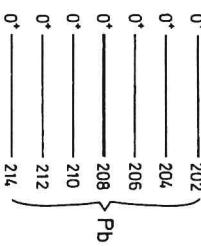
$$H|\nu\rangle = E_\nu|\nu\rangle. \quad (8.59)$$

It is possible to define operators  $Q_\nu^\dagger$  and  $Q_\nu$  in such a way that

$$|\nu\rangle = Q_\nu^\dagger |0\rangle \quad \text{and} \quad Q_\nu |0\rangle = 0. \quad (8.60)$$

\*This approximation has been introduced by Bohn and Pines [BP 53] in the theory of plasma oscillations. Other derivations have been given by several authors [GB 57, Hu 57, Sa 57, An 58].

**Figure 8.9.** Schematic representation of the ground state energies in the even Pb isotopes.



$\mathcal{Q}_\nu^+$ , for example, can be chosen as

$$\mathcal{Q}_\nu^+ = |\nu\rangle\langle\nu|.$$

From the Schrödinger equation (8.59) we get the equation of motion

$$[H, \mathcal{Q}_\nu^+]|\mathbf{0}\rangle = (E_\nu - E_0)\mathcal{Q}_\nu^+|\mathbf{0}\rangle. \quad (8.61)$$

Multiplying from the left with an arbitrary state of the form  $\langle 0|\delta Q$  we get\*

$$\langle 0|\delta Q, [H, \mathcal{Q}_\nu^+]]|\mathbf{0}\rangle = (E_\nu - E_0)\langle 0|\delta Q, \mathcal{Q}_\nu^+]]|\mathbf{0}\rangle. \quad (8.62)$$

We can use the commutator, because  $\langle 0|\mathcal{Q}_\nu^+ = \langle 0|H\mathcal{Q}_\nu^+ = 0$ . Until now we were exact and, since the variation of  $\delta Q|\mathbf{0}\rangle$  exhausts the whole Hilbert space, (8.62) corresponds to the full Schrödinger equation (8.59). First we re-derive the TDA equation (8.10) by approximating the exact ground state  $|\mathbf{0}\rangle$  by the HF state  $|\text{HF}\rangle$  and the operator  $\mathcal{Q}_\nu$  by the collective  $p\bar{h}$ -operator

$$\mathcal{Q}_\nu^+ = \sum_{mi} C_{mi}^* a_m^+ a_i. \quad (8.63)$$

By this approximation, we restrict ourselves to the space of  $1p-1h$  excitations, that is, we set,  $\delta Q|\mathbf{0}\rangle = \sum_{mi} a_m^+ a_i |\text{HF}\rangle \delta C_{mi}$  and from (8.62) get

$$\sum_{\eta j} \langle \text{HF} | [a_i^+ a_m, [H, a_n^+ a_j]] | \text{HF} \rangle C_{\eta j}^* = E_\nu^{\text{TDA}} C_{mi}^*, \quad (8.64)$$

where  $E_\nu^{\text{TDA}}$  is the excitation energy in TDA approximation. This is exactly the TDA equation we derived earlier (8.10). In deriving this equation we have not used a variational principle this time. The above procedure has, however, the advantage that it can be generalized in a straightforward way. There is no reason why we should not use, in Eq. (8.63), a more general vibration creation operator which then also implies, as we shall see, a more general ground state. If we think of a ground state containing  $2p-2h$  correlations, as indicated by Eq. (8.2), we can not only create a  $p\bar{h}$  pair but also destroy one. The most straightforward generalization of Eq. (8.63) is therefore:

$$\mathcal{Q}_\nu^+ = \sum_{mi} X_{mi}^* a_m^+ a_i - \sum_{mi} Y_{mi}^* a_i^+ a_m, \quad (8.65)$$

where the minus sign has been chosen for convenience. The RPA ground state  $|\text{RPA}\rangle$  is defined by analogy to (8.60) by†

$$\mathcal{Q}_\nu |\text{RPA}\rangle = 0. \quad (8.66)$$

We will later on deduce from this condition an explicit expression for the ground state. Instead of only one matrix  $C_{mi}^*$  we now have two matrices  $X_{mi}^*$  and  $Y_{mi}^*$ . We also have two kinds of variations  $\delta Q|\mathbf{0}\rangle$ , namely  $a_m^+ a_i |\mathbf{0}\rangle$  and

\* If we express  $\mathcal{Q}$  by the operators  $a_p^+ a_q, a_p^+ a_q^+, a_p a_q, a_q a_p$  with coefficients  $C_{pq}$  and  $C_{pqij}$ , then  $\delta Q$  is given by  $\delta Q/\delta C \cdot \delta C$  for arbitrary variations  $\delta C$ .

† One usually assumes  $|\text{RPA}\rangle$  to be the ground state of an even system with closed shells ( $I''=0^+$ ). Rowe et al. also investigated the possibility of constructing an RPA based on an open shell configuration (open shell RPA; see [RW 69, 70, NR 71, RN 75]).

$a_i^+ a_m |\mathbf{0}\rangle$ . Therefore, from (8.62) we get two sets of equations:

$$\langle \text{RPA} | [a_i^+ a_m, [H, \mathcal{Q}_\nu^+]] | \text{RPA} \rangle = \hbar\Omega_\nu \langle \text{RPA} | [a_i^+ a_m, \mathcal{Q}_\nu^+] | \text{RPA} \rangle,$$

$$\langle \text{RPA} | [a_m^+ a_i, [H, \mathcal{Q}_\nu^+]] | \text{RPA} \rangle = \hbar\Omega_\nu \langle \text{RPA} | [a_m^+ a_i, \mathcal{Q}_\nu^+] | \text{RPA} \rangle, \quad (8.67)$$

where  $\hbar\Omega_\nu$  is the excitation energy of the state  $|\nu\rangle$ . These equations contain only expectation values of four Fermion operators, which are still very complicated to calculate, because we do not as yet know the ground state  $|\text{RPA}\rangle$ .

We content ourselves with an approximation usually known as the “quasi-boson approximation” [BET 61, Br 64]. If we assume that the correlated ground state does not differ very much from the HF ground state, we can calculate all expectation values in the HF approximation, for example,

$$\begin{aligned} \langle \text{RPA} | [a_i^+ a_m, a_n^+ a_j] | \text{RPA} \rangle &= \delta_{ij} \delta_{mn} - \delta_{mn} \langle \text{RPA} | a_j a_i^+ | \text{RPA} \rangle \\ &\quad - \delta_{ij} \langle \text{RPA} | a_n^+ a_m | \text{RPA} \rangle \\ &\simeq \langle \text{HF} | [a_i^+ a_m, a_n^+ a_j] | \text{HF} \rangle = \delta_{ij} \delta_{mn}. \end{aligned} \quad (8.68)$$

The name “quasi-boson” approximation comes from the fact that Eq. (8.68) would be an exact relation if the  $p\bar{h}$  creation and annihilation operators obeyed the commutation relations for boson field operators. Equation (8.68), however, violates the Pauli principle because we have neglected terms coming from the commutator. The quality of this approximation can only be checked from realistic calculations (see also Chap. 9).

Within the quasi-boson approximation, the amplitudes  $X_{mi}^*$  and  $Y_{mi}^*$  have a very direct meaning: their absolute squares give the probability of finding the states  $a_m^+ a_i |\mathbf{0}\rangle$  and  $a_i^+ a_m |\mathbf{0}\rangle$  in the excited state  $|\nu\rangle$ , that is, the  $p\bar{h}$  and  $h\bar{p}$  matrix elements of the transition density  $\rho^{(1)}$  of equation (8.31):

$$\begin{aligned} \rho_{mi}^{(1)*} &= \langle 0 | a_i^+ a_m | \nu \rangle \simeq \langle \text{HF} | [a_i^+ a_m, \mathcal{Q}_\nu^+] | \text{HF} \rangle = X_{mi}^*, \\ \rho_{mi}^{(1)*} &= \langle 0 | a_n^+ a_i | \nu \rangle \simeq \langle \text{HF} | [a_i^+ a_n, \mathcal{Q}_\nu^+] | \text{HF} \rangle = Y_{mi}^*. \end{aligned} \quad (8.69)$$

Equations (8.67) can now be written in a very compact form:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X_{mi}^* \\ Y_{mi}^* \end{pmatrix} = \hbar\Omega_\nu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X_{mi}^* \\ Y_{mi}^* \end{pmatrix} \quad (8.70)$$

with  $(X')_{mi} = X_{mi}^*$ ;  $(Y')_{mi} = Y_{mi}^*$ ; and

$$\begin{aligned} A_{minj} &= \langle \text{HF} | [a_i^+ a_m [H, a_n^+ a_j]] | \text{HF} \rangle = (\epsilon_m - \epsilon_j) \delta_{mn} \delta_{ij} + \tilde{\tau}_{mijn}, \\ B_{minj} &= -\langle \text{HF} | [a_i^+ a_m [H, a_j^+ a_n]] | \text{HF} \rangle = \tilde{\tau}_{mijn}. \end{aligned} \quad (8.71)$$

The matrix  $A$  is Hermitian and the matrix  $B$  is symmetric.

Equation (8.70), together with (8.71), is called the *RPA equation*. We get back the TDA equation by putting all  $Y'_{mi}$  equal to zero. They are therefore a measure for the correlations in the ground state.



**Figure 8.10.** Graphical representation of the matrix elements  $B$  in Equation (8.71).

As we can see by looking at matrix  $B$  of Eq. (8.71), the RPA contains, in addition to the graphs of Fig. 8.3, the graphs shown in Fig. 8.10, which have the meaning of virtual  $2p - 2h$  excitations.

In general, we can say that the quasi-boson approximation (8.68) is valid for very collective states, that is, if we have many coefficients  $X_{mi}^\nu$  of the same order of magnitude. In such cases each single  $ph$ -component has only a small probability of being excited and the violation of the Pauli principle can be neglected. We will discuss this point again later in Chapter 9.

On the other hand, the amplitudes  $Y_{mi}^\nu$  should be small compared to the coefficients  $X_{mi}^\nu$  because they describe ground state correlations. If they are too strong, the replacement of the correlated ground state  $|RPA\rangle$  by the  $|HF\rangle$  state in Eq. (8.67) is not justified.

In cases where the coefficients  $Y_{mi}^\nu$  can be neglected completely, we get back to the TDA. This is the reason that we can describe collective states very well using the RPA, where the quasi-boson approach is justified, and also rather pure  $ph$ -states, where the coefficients  $Y_{mi}^\nu$  are negligible. The RPA equation (8.70) looks like the diagonalization of the Hamiltonian in a basis with a metric tensor  $(\underline{\underline{1}})$  which is no longer positive definite. In fact, in Section 8.4.4 we will show that the eigensolutions of Eq. (8.70) are orthogonal with respect to this metric. Another consequence of this metric is that the eigenvalues  $\hbar\Omega_\nu$  are not necessarily real.

To calculate transition probabilities (B.62) between the excited state  $|\nu\rangle$  and the ground state  $|0\rangle$  we only need matrix elements of the type  $\langle 0|F|\nu\rangle$  for a Hermitian one-body operator  $F$ .

In the RPA approximation they are given by

$$\langle 0|F|\nu\rangle = \sum_{kk'} F_{kk'} \rho_k^{(1)*} = \sum_{mi} F_{im} X_{mi}^\nu + F_{mi} Y_{mi}^\nu.$$

In the following sections we will frequently use the notation

$$\langle 0|F|\nu\rangle = f^+ \mathcal{X}^\nu \quad (8.72)$$

with the column vectors

$$f = \begin{pmatrix} F_{mi} \\ F_{mi}^* \end{pmatrix} \quad \text{and} \quad \mathcal{X}^\nu = \begin{pmatrix} X_{mi}^\nu \\ Y_{mi}^\nu \end{pmatrix}.$$

**8.4.2 Stability of the RPA**  
The matrix

$$\mathcal{S} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \quad (8.73)$$

is exactly the *stability matrix* of the HF theory derived in Eq. (7.37). It is a Hermitian matrix and its real eigenvalues characterize the nature of the HF solution. If  $\mathcal{S}$  is positive definite it corresponds to a minimum in the energy surface. In this case, we can calculate the square root of the matrix  $\mathcal{S}$  and bring the eigenvalue problem (8.70) into a more symmetric form:

$$\mathcal{S}^{1/2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathcal{S}^{1/2} \begin{pmatrix} \tilde{X} \\ \tilde{Y} \end{pmatrix} = \begin{pmatrix} \tilde{X} \\ \tilde{Y} \end{pmatrix} \hbar\Omega$$

with

$$\begin{pmatrix} \tilde{X} \\ \tilde{Y} \end{pmatrix} = \mathcal{S}^{1/2} \begin{pmatrix} X \\ Y \end{pmatrix},$$

which is a Hermitian eigenvalue problem having only real solutions. In other words, if the HF solution corresponds to a minimum in the energy surface and not to a saddle point or a maximum, then the corresponding RPA equation has only real frequencies [Th 61a]. The opposite is not necessarily true. In the following we will assume that we only have real non-vanishing eigenvalues  $\Omega_\nu$ .

### 8.4.3 Normalization and Closure Relations

Since the RPA matrix is not Hermitian, its eigenvectors cannot be orthogonal in the usual sense. We would also expect a different kind of orthogonality relations from the condition, that the excited states  $|\nu\rangle = Q_\nu^+ |RPA\rangle$  should be mutually orthogonal

$$\langle \nu | \nu' \rangle = \delta_{\nu\nu'} = \langle RPA | [Q_\nu, Q_{\nu'}^+] | RPA \rangle \approx \langle HF | [Q_\nu, Q_{\nu'}^+] | HF \rangle$$

or

$$\delta_{\nu\nu'} = \sum_{mi} (X_{mi}^{\nu*} X_{mi}^{\nu'} - Y_{mi}^{\nu*} Y_{mi}^{\nu'}). \quad (8.74)$$

In fact, we can show that the solutions of the RPA equations for  $\nu \neq \nu'$  fulfill this relation exactly. For  $\nu = \nu'$  this gives us the possibility of normalizing the vector  $(X^\nu, Y^\nu)$  if the norm is positive [Th 61a].

To show the orthogonality of the RPA solutions in the sense of (8.74) we first notice that to each eigenvector  $(X^\nu, Y^\nu)$  with eigenvalue  $\Omega_\nu$ , we have another eigenvector  $(Y^{\nu*}, X^{\nu*})$  with the eigenvalue  $-\Omega_\nu$ . Both eigenvectors have the same absolute norm in the sense of (8.74) but with different sign.

It is useful to introduce the matrices

$$\mathcal{X} = \begin{pmatrix} X & Y^* \\ Y & X^* \end{pmatrix}; \quad \mathcal{Y} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (8.75)$$

Together with (8.75), the RPA equation (8.70) has the form

$$\mathcal{S}\mathcal{X} = \mathcal{Y}\mathcal{X}\Omega, \quad (8.76)$$

where the diagonal matrix  $\Omega$  contains the real eigenvalues  $(\hbar\Omega_\mu, -\hbar\Omega_\mu)$ . Simple matrix algebra shows that

$$[\Omega, \mathcal{X}^+ \mathcal{X} \mathcal{X}] = (\mathcal{Y} \mathcal{X} \Omega)^+ \mathcal{X} - \mathcal{X}^+ (\mathcal{Y} \mathcal{X} \Omega) = \mathcal{X}^+ (\mathcal{S}^+ - \mathcal{S}) \mathcal{X} = 0 \quad (8.77)$$

that is,  $\Omega$  commutes with  $\mathcal{X}^+ \mathcal{X} \mathcal{X}$ , and thus  $\mathcal{X}^+ \mathcal{X} \mathcal{X}$  is diagonal together with  $\Omega$ . Since the norm of the vectors  $(X, Y)$  is open, we choose\*

$$\mathcal{X}^+ \mathcal{X} \mathcal{X} = \mathcal{Y}. \quad (8.78)$$

These are exactly the orthogonality conditions (8.74).

The closure condition is obtained by multiplying (8.78) with  $\mathcal{Y}$ , which shows that  $\mathcal{X} \mathcal{X} \mathcal{X}$  is the inverse matrix of  $\mathcal{X}^+$ , or

$$\mathcal{X} \mathcal{X} \mathcal{X}^+ = \mathcal{Y} \quad (8.79)$$

which gives explicitly

$$\sum_\nu X_{mi}^\nu X_{m'i'}^\nu - Y_{mi}^\nu Y_{m'i'}^\nu = \delta_{mm'} \delta_{ii'}. \quad (8.80)$$

#### 8.4.4 Numerical Solution of the RPA Equations

In many practical cases the RPA-matrices  $A$  and  $B$  are real. For real frequencies  $\Omega_\nu$  the problem can be reduced to the diagonalization of a real symmetric matrix of *half the dimension*. We define the vectors (see footnote page 301)

$$P'' = i \cdot \sqrt{\frac{\hbar\Omega_\nu}{2}} (X'' + Y''); \quad Q'' = \sqrt{\frac{\hbar}{2\Omega_\nu}} (X'' - Y''). \quad (8.81)$$

From (8.70) it is easy to deduce

$$\begin{aligned} i \cdot (A - B) Q'' &= \hbar P'', \\ -i \cdot (A + B) P'' &= \hbar \Omega_\nu^2 Q'', \end{aligned} \quad (8.82)$$

and

$$(A + B)(A - B) Q'' = \hbar^2 \Omega_\nu^2 Q''. \quad (8.83)$$

Together with the stability matrix  $\mathcal{S}$  (8.73), the matrices  $(A \pm B)$  are positive definite. We can decompose  $A - B$  into a product of two triangular matrices (Orthogonalization of Gram-Schmidt [Wi 65, Ch 70], we

\* For a positive definite stability matrix  $\mathcal{S}$  this is always possible, because  $\Omega_\nu$  then has the same sign as  $(\mathcal{X}^+ \mathcal{X} \mathcal{X})_{\nu\nu}$ .

could also search for the square root of the matrix  $(A - B)[\mathbf{U}\mathbf{R} 71]$

$$(A - B) = T^T T \quad \text{with } T_k = 0 \text{ for } i > k \quad (8.84)$$

and be left with the real symmetric eigenvalue problem

$$T(A + B)T^T R'' = \hbar^2 \Omega_\nu^2 R''. \quad (8.85)$$

Its solution gives the eigenvalues  $\Omega_\nu$  and the normalized eigenvectors  $R''$ . Finally, we get the properly normalized RPA amplitudes from

$$\begin{pmatrix} X'' \\ Y'' \end{pmatrix} = \frac{1}{2} ((\hbar\Omega_\nu)^{-1/2} T^T R'' \pm (\hbar\Omega_\nu)^{1/2} T^{-1} R''). \quad (8.86)$$

#### 8.4.5 Representation by Boson Operators

For the derivation of the RPA equations (8.70) we have used the quasi-boson approximation (8.68), that is, we have replaced the *ph* operators  $a_m^+ a_i$  by boson operators  $B_{mi}^+$

$$a_m^+ a_i \rightarrow B_{mi}^+, \quad a_i^+ a_m \rightarrow B_{mi}, \quad (8.87)$$

which fulfil exact boson commutation relations

$$[B_{mi}, B_{m'i'}] = [B_{mi}^+, B_{m'i'}^+] = 0; \quad [B_{mi}, B_{m'i'}^+] = \delta_{ii'} \delta_{mm'}. \quad (8.88)$$

This replacement is an approximation. In fact we will see in Chapter 9 that we can expand the Fermion pair operators  $a_m^+ a_i$  in a series of boson operators, in which the first term is  $B_{mi}^+$ . In the quasi-boson approximation we neglect all higher terms.

Since we use this approximation within the RPA theory it is very convenient to represent other operators, such as the Hamiltonian  $H$  or transition operators, by the  $B^+$ 's and  $B$ 's. How this can be done is discussed in Chapter 9.

Here we shall go to harmonic order only, that is, we take into account in the Hamiltonian  $H_B$  only terms quadratic in  $B$ ,  $B^+$  as  $B^+ B$ ,  $BB$ , and  $B^+ B^+$ . This is consistent with the approach (8.87) because we need only terms of the form  $[H, B^+]$ ,  $[H, B]$  (see Eq. 8.67) in the derivation of the RPA equations. In particular, we determine the coefficients of the terms  $B^+ B$ ,  $BB$ , and  $B^+ B^+$  of the Hamiltonian by the requirement\* (8.71):

$$\begin{aligned} \langle \text{HF} | [B_{mi}, [H_B, B_{nj}^+]] | \text{HF} \rangle &= \langle \text{HF} | [a_i^+ a_m, [H, a_n^+ a_j]] | \text{HF} \rangle = A_{minj}, \\ \langle \text{HF} | [B_{mi}, [H_B, B_{nj}]] | \text{HF} \rangle &= \langle \text{HF} | [a_i^+ a_m, [H, a_j^+ a_n]] | \text{HF} \rangle = -B_{mijn}. \end{aligned} \quad (8.89)$$

\* To be precise, we must remark that  $|\text{HF}\rangle$  is not exactly the ground state of the Boson operators  $B_{mi}^+$  since they coincide only approximately with the operators  $a_i^+ a_m$ . In Chapter 9, we define the ground states of Boson operators by round parenthesis  $B_{mi}| \text{HF} \rangle = 0$ . There is no difference between  $|\text{HF}\rangle$  and  $| \text{HF} \rangle$  in RPA order; we do not distinguish between these two states in the present chapter and always use  $B_{mi}| \text{HF} \rangle = 0$ .

and find\*

$$\begin{aligned} H_B &= E_{\text{HF}} + \sum_{mij} A_{mij} B_{mi}^+ B_{nj} + \frac{1}{2} \sum_{mij} (B_{mij} B_{mi}^+ B_{nj}^+ + \text{h.c.}) \\ &= E_{\text{HF}} - \frac{1}{2} \sum_{mi} A_{mmi} + \frac{1}{2} (B^+ - B) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} B \\ B^+ \end{pmatrix}. \end{aligned} \quad (8.90)$$

The constant  $E_{\text{HF}}$  corresponds to the expectation value of the Hamiltonian in the HF ground state, as can be seen by switching Eq. (8.90) between  $|HF\rangle$ . In Chapter 9, it is shown that the higher order terms in  $B$  give no contributions. There are no linear terms in the operators  $B, B^+$  because we start with a self-consistent solution [ $H^{20}=0$ , Eq. (7.36)]. A Hamiltonian of this form can also be derived in second order by the method of generator coordinates, which has been introduced in this context by Jancovici and Schiff [JS 64] (see also Chap. 10).

The diagonalization of (8.90) is straightforward if we introduce a Bogoliubov transformation [see (E.60)] amongst the Boson operators corresponding to (8.65) and replace the operators  $Q_\nu$  by pure Boson operators  $O_\nu$ .

$$O_\nu^+ = \sum_{mi} X_{mi}^\nu B_{mi}^+ - Y_{mi}^\nu B_{mi}. \quad (8.91)$$

The requirement that the operators  $O_\nu^+, O_\nu$  now fulfill exact boson commutation relations is equivalent to the unitarity of this transformation and immediately yields the orthogonality relations (8.78) and (8.79).

The Hamiltonian expressed in terms of the operators  $O_\nu^+, O_\nu$  is found to be diagonal after taking into account the RPA equation (8.76) viz:

$$\begin{aligned} H_B &= E_{\text{HF}} - \frac{1}{2} \text{Tr} A + \frac{1}{2} (O^+ - O) \mathcal{S} \mathcal{C} \begin{pmatrix} O \\ O^+ \end{pmatrix} \\ &= E_{\text{RPA}} + \sum_\nu i \hbar \Omega_\nu O_\nu^+ O_\nu \end{aligned} \quad (8.92)$$

with

$$E_{\text{RPA}} = E_{\text{HF}} - \frac{1}{2} \text{Tr} A + \frac{\hbar}{2} \sum_{\nu>0} \Omega_\nu \quad (8.93a)$$

$$= E_{\text{HF}} - \sum_\nu i \hbar \Omega_\nu \sum_m |Y_{mi}^\nu|^2. \quad (8.93b)$$

In Eq. (8.93) we have used the inverse of the RPA equation (8.76)

$$\begin{aligned} A &= X \Omega X^+ + Y^* \Omega Y^T, \\ -B &= X \Omega Y^+ + Y^* \Omega X^T. \end{aligned} \quad (8.94)$$

The Hamiltonian (8.92) corresponds to the Hamiltonian of harmonic oscillators. Therefore, the RPA is called the harmonic approximation. It

determines uncoupled eigenmodes of the system. The eigenfunctions of  $H_B$  are the ground state  $|RPA\rangle$  (it will be constructed in Section 8.4.6), one-boson states  $O_\nu^+ |RPA\rangle$ , two-boson states  $O_\nu^+ O_\nu^+ |RPA\rangle$ , and so on.

Since  $A$  is just the matrix, which is diagonalized in the TDA equation (8.10), we see from Eq. (8.93) that the RPA ground state energy  $E_{\text{RPA}}$  is lowered compared to the Hartree-Fock energy  $E_{\text{HF}}$  by the amount

$$E_{\text{HF}} - E_{\text{RPA}} = \frac{1}{2} \sum_{\nu>0} (E_\nu^{\text{TDA}} - E_\nu^{\text{RPA}}).$$

It is just half the sum of all differences in the excitation energies between the RPA and the TDA approach.

As we know from the theory of the harmonic oscillator, we may also represent the eigenmodes by generalized coordinates  $\vartheta_\nu$  and moments  $\vartheta_\nu^*$  defined by [MW 69b]

$$\vartheta_\nu = \frac{\hbar}{i} \sqrt{\frac{M_\nu \Omega_\nu}{\hbar}} \frac{1}{\sqrt{2}} (O_\nu - O_\nu^+); \quad \vartheta_\nu^* = \sqrt{\frac{\hbar}{M_\nu \Omega_\nu}} \frac{1}{\sqrt{2}} (O_\nu + O_\nu^+). \quad (8.95)$$

The numbers  $M_\nu$  are arbitrary at this point. The operators  $\vartheta_\nu, \vartheta_\nu^*$  fulfill the commutation relations of conjugate momenta and coordinates

$$[\vartheta_\nu, \vartheta_{\nu'}] = [\vartheta_\nu, \vartheta_{\nu'}^*] = 0; \quad [\vartheta_\nu, \vartheta_{\nu'}^*] = \frac{\hbar}{i} \delta_{\nu\nu'}. \quad (8.96)$$

The Hamiltonian (8.92) can be expressed in these operators:

$$H_B = E_{\text{HF}} - \frac{1}{2} \text{Tr} A + \sum_\nu \left( \frac{1}{2 M_\nu} \vartheta_\nu^2 + \frac{M_\nu \Omega_\nu^2 \vartheta_\nu^2}{2} \right). \quad (8.97)$$

The operators  $\vartheta_\nu, \vartheta_\nu^*$ , therefore, obey the equations of motion

$$[H_B, \vartheta_\nu] = i \hbar \Omega_\nu M_\nu \vartheta_\nu; \quad [H_B, \vartheta_\nu^*] = - \frac{i \hbar}{M_\nu} \vartheta_\nu^*. \quad (8.98)$$

Using the representation

$$\vartheta_\nu = \sum_{mi} P_{mi}^\nu B_{mi}^+ + P_{mi}^{\nu*} B_{mi} \quad \text{with } P_{mi}^\nu = i \hbar \sqrt{\frac{M_\nu \Omega_\nu}{2 \hbar}} (X + Y^*)_{mi}^\nu,$$

$$\vartheta_\nu^* = \sum_{mi} Q_{mi}^\nu B_{mi}^+ + Q_{mi}^{\nu*} B_{mi} \quad \text{with } Q_{mi}^\nu = \sqrt{\frac{\hbar}{2 M_\nu \Omega_\nu}} (X - Y^*)_{mi}^\nu,$$

we get an explicit form for the Eqs. (8.98):

$$\begin{aligned} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} P \\ -P^* \end{pmatrix}_\nu &= i \hbar \Omega_\nu^2 M_\nu \begin{pmatrix} \vartheta \\ \vartheta^* \end{pmatrix}_\nu; \\ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \vartheta \\ -\vartheta^* \end{pmatrix}_\nu &= \frac{\hbar}{i} \frac{1}{M_\nu} \begin{pmatrix} P \\ P^* \end{pmatrix}_\nu. \end{aligned} \quad (8.99)$$

\*We should not, in the following matrix notation, confuse the operators  $B_{mi}$  with the matrix  $B_{mij}$ .

Neither the normalization of the vectors  $P_{mi}^{\nu}$  and  $Q_{mi}^{\nu}$  nor the parameter  $M_{\nu}$  is determined from the solution of this equation. The condition (8.96),

$$(P^* \quad P)_{\nu} \left( \begin{array}{c} Q \\ -Q^* \end{array} \right)_{\nu} = \frac{\hbar}{i} \delta_{\nu\nu}, \quad (8.100)$$

can be used to determine either the parameter  $M_{\nu}$  (for fixed normalization of  $P_{mi}^{\nu}$  or  $Q_{mi}^{\nu}$ ) or the normalization of these vectors (for fixed parameter  $M_{\nu}$ ).

So far we have only treated the case of non-vanishing real RPA frequencies ( $\Omega_i^2 > 0$ ). In principle, the RPA matrix can also have complex eigenvalues. (An example is  $A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ ,  $B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ , with the eigenvalues  $\Omega_i = \pm 1 \pm i$ .) Until now such general cases have not been investigated. In the context of adiabatic time-dependent Hartree-Fock theory (see Sec. 12.3), it happens sometimes that we must diagonalize a matrix of the RPA type with a pure imaginary eigenvalue  $\Omega_i = i|\Omega_i|$ . The corresponding eigenvector  $\mathcal{R}_i$  has zero norm:

$$i|\Omega_i| \mathcal{R}_i^+ \mathcal{R}_i^- = \mathcal{R}_i^+ S \mathcal{R}_i^- = (\mathcal{R}_i^+ S \mathcal{R}_i^-)^+ = -i|\Omega_i| \mathcal{R}_i^+ \mathcal{R}_i^-.$$

In such a case there exists no boson of the form (8.91), which corresponds to this eigenvalue. Nevertheless, we can construct operators  $\mathcal{Q}_{\nu}$  and  $\mathcal{Q}_{\nu}^*$  with the properties (8.96) and (8.98). We have only to solve the system (8.99) for an arbitrary positive value of  $M_{\nu}$  and a negative value of  $\Omega_i^2$ . In order to obtain a complete set of boson operators, we can then define corresponding bosons  $O_i$ ,  $O_i^+$  by Eq. (8.95) using the absolute value  $|\Omega_i|$  instead of  $\Omega_i$  [RB 76]. The Hamiltonian  $H_B$  (8.97) is not diagonal in this basis, but “maximally” off diagonal:

$$-\frac{\hbar}{2} |\Omega_i| (O_i^+ O_i^+ + O_i O_i).$$

#### 8.4.6 Construction of the RPA Ground State

The RPA ground state was originally defined by Eq. (8.66) as the vacuum of the operators  $\mathcal{Q}_{\nu}$ . Within the quasi-boson approximation it is now equivalent to the vacuum  $|\text{RPA}\rangle$  of the boson operators  $O_{\nu}$ :

$$O_{\nu} |\text{RPA}\rangle = 0.$$

We can construct it explicitly from the vacuum  $|\text{HF}\rangle$  of the bosons  $B_{mi}^{+}$  [Eq. (8.87)] in analogy to Chapter 7, where we constructed the vacuum of quasi-particle operators, by the theorem of Thouless [Th 60] (see also Sec. E.5):

$$|\text{RPA}\rangle = N_0 e^{\hat{z}} |\text{HF}\rangle \quad (8.101)$$

where

$$\hat{Z} = \frac{1}{2} \sum_{mij} Z_{mij} B_{mi}^+ B_{\eta j}^+ \quad (8.102)$$

and  $N_0$  is a normalization (see Eqs. E.69 and E.75). In Appendix E we get, for the matrix  $Z$ , from (8.91) and the commutation relations (8.88),

$$Z = Y^* X^{-1}.$$

The inversion of the matrix  $X$  is, in principle, possible, but more practical methods have been proposed by Sanderson [Sa 65] and by da Providencia [Pr 66]. Actual calculations have been performed by Goswami and Pal [GP 63]. It turns out that the RPA ground state has to be taken with care, since the quasi-boson approximation probably overestimates the ground state correlations in many cases [IUY 65, PR 68, UR 69].

The energy of the ground state is given by Eq. (8.93). Obviously, it is always lower than the Hartree-Fock energy  $E_{\text{HF}}$ . The reason is that it takes into account higher correlations. However, we have to keep in mind that the RPA does not follow from a variational principle. It may, therefore, happen that its energy can even be deeper than the exact energy.

Since we are now able to calculate the RPA ground state, we could use it to evaluate Eq. (8.67), avoiding the quasi-boson approximation (8.68) in the calculation of the matrices  $A$  and  $B$ . Diagonalizing the new RPA equations gives a better ground state, and so on. This yields a self-consistent prescription which avoids the shortcomings of the quasi-boson approximation [Ro 70, SE 73, Ma 76a]. We will come to this method in more detail in Section 9.2.3.

Over the years, several other extensions of the RPA theory have been proposed (so-called *higher random phase approximations*; see, for instance, [Sa 62, TU 64, Ro 68a, MYM 68, GNS 70, DDK 71]). We do not want to discuss these methods in the framework of this book, since in Chapter 9 we present a systematic way of treating collective phenomena in nuclei, the so-called boson expansion technique.

#### 8.4.7 Invariances and Spurious Solutions

We assume in the following that the exact two-body Hamiltonian  $H$  is invariant under a continuous symmetry operation generated by a Hermitian one-body operator  $\hat{P}$ , as there is, for instance, the case of translation; we assume further that the HF solution violates this symmetry. This means, in particular, that the HF single-particle density  $\rho^{(0)}$  does not commute with  $\hat{P}$

$$[\rho^{(0)}, \hat{P}] \neq 0. \quad (8.103)$$

Since  $\rho^{(0)}$  is diagonal in the HF basis (0 for particles and 1 for holes) this means that not all the  $\rho h$  matrix elements  $P_{mi}^{(0)}$  vanish.

The exact Hamiltonian commutes with  $\hat{P}$ :

$$[H, \hat{P}] = 0. \quad (8.104)$$

$\hat{P}$  is therefore an exact but *spurious solution* of the RPA equation  $\langle \text{HF} | \delta \mathcal{O}, [H, \hat{P}] | \text{HF} \rangle = 0^*$  or, in matrix language,

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \left( \begin{array}{c} P \\ -P^* \end{array} \right) = 0, \quad (8.104)$$

\* The  $pp$  and  $hh$  matrix elements of  $\hat{P}$  do not contribute to this equation because of (5.35)

where  $P$  is the vector  $P_{mi}$  in particle-hole space. The corresponding state is

$$|P\rangle = \sum_{mi} (P_{mi} a_m^+ a_i + P_{mi}^* a_i^+ a_m) |RPA\rangle. \quad (8.105)$$

We realize that the RPA equation (8.70) has such a solution only for the case in which the symmetry is, in fact, broken by the HF solution. Otherwise the matrix elements  $P_{mi}$  vanish identically.

Thus, we see that to the extent that we calculate the RPA exactly and use self-consistent single-particle energies and wave functions\* the spurious excitations that correspond to a broken symmetry in the HF state—as, for example, in translation of the nucleus as a whole—separate out. They are orthogonal to the other excitations and lie at zero excitation energy.

We have derived this for density-independent interactions. However, in Section (8.5) we will see that this also holds for density-dependent interactions that obey the condition (5.71).

This fact is a major advantage of the RPA over the TDA where, as we have seen in Section 8.3.3, the spurious and physical solutions become mixed up with one another.

As we stated at the beginning of Section 8.4.3, the RPA always has two symmetric solutions,  $\Omega_p$  and  $-\Omega_p$ . For  $\hat{P}$ , however, we have no adjoint partner, since  $\hat{P}$  is Hermitian and the adjoint is simply a repetition of itself. In fact, the state  $|P\rangle$  in Eq. (8.105) is not normalizable in the sense of Eq. (8.74). There exists no corresponding boson. Since the RPA matrix has even dimensions and all non-spurious solutions are paired off, the RPA solutions are one short of forming a complete set.

To see what is going on, we follow Marshalek and Weneser [MW 69b, MW 70], and use the representation (8.95) for the spurious state. Obviously, the  $p\hbar$  and the  $h\mu$  parts of  $\hat{P}$  are now identical to the Hermitian operator  $\mathcal{P}_0$  (the canonical momentum) up to a constant  $M_0$  which, in the definition (8.95) is open in any case. In order to obtain complete sets of operators  $O_\nu^+, O_\nu^-$  ( $\nu > 0$ ) and  $\mathcal{P}_0, \mathcal{Q}_0$  we only have to determine the canonical coordinate  $\mathcal{Q}_0$ . It is given by the solution of Eq. (8.99):

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Q \\ -Q^* \end{pmatrix}_0 = -\frac{i\hbar}{M_0} \begin{pmatrix} P \\ P^* \end{pmatrix}_0, \quad (8.106)$$

which is a linear inhomogeneous problem. Since the matrix  $\mathbb{S}$  is singular, this equation only has a solution if the inhomogeneous part is perpendicular to the spurious solution. But this is exactly the case (8.104). The equations (8.106) were first derived by Thouless and Valatin in the context of nuclear rotations [TV 62].

The constant  $M_0$  is finally determined by the commutation relation (8.96):

$$\sum_{mi} (P_{mi}^* Q_{mi} - P_{mi} Q_{mi}^*)_0 = (P^* - P)_0 \begin{pmatrix} Q \\ -Q^* \end{pmatrix}_0 = \frac{\hbar}{i}. \quad (8.107)$$

Inverting (8.106), we find

$$\frac{\hbar^2}{2M_0} = \frac{1}{2}(Q^* - Q)_0 \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Q \\ -Q^* \end{pmatrix}_0 = \frac{1}{2} \langle \text{HF} | [\mathcal{Q}_0, [H, \mathcal{Q}_0]] \text{HF} \rangle \quad (8.108)$$

In practical cases it is often possible to choose the phases in such a way that  $A$  and  $B$  are real. In a case where  $Q_{mi}$  is also real,  $P_{mi}$  has to be purely imaginary and we get, for instance,

$$M_0 = 2P_0^*(A - B)^{-1}P_0. \quad (8.109)$$

We can now write down the Hamiltonian  $H_B$  in RPA order in the following way (8.97).

$$H_B = E_{\text{RPA}} + \sum_{\nu > 0} \hbar\Omega_\nu O_\nu^+ O_\nu + \frac{\mathcal{P}_0^2}{2M_0}. \quad (8.110)$$

The constant  $E_{\text{RPA}}$  no longer has the form (8.93b) because of the zero frequency mode. However, we can give it easily by constructing the HF expectation value of (8.110):

$$E_{\text{RPA}} = E_{\text{HF}} - \sum_{\nu > 0} \hbar\Omega_\nu \sum_{mi} |Y_{mi}|^2 - \frac{\langle \text{HF} | \mathcal{Q}_0^2 | \text{HF} \rangle}{2M_0}. \quad (8.111)$$

The subtraction of the term  $\langle \hat{P}^2 \rangle / 2M_0$  is often used in the recipes (Chap. 11) for doing HF calculations in nuclei in order to correct for spurious translational motion of the centre of mass. We see that this correction is included automatically in the RPA.

The form of the operator (8.110) also gives us an interpretation of the constant  $M_0$ . It is the inertial parameter corresponding to the motion characterized by  $\hat{P}$ .

Let us consider two examples:

- (i) *Translation.* Here we can use the Galilean invariance for the exact Hamiltonian

$$[H, \mathbf{X}] = -\frac{i\hbar}{Am} \mathbf{P}, \quad (8.112)$$

where  $\mathbf{X}$  is the center-of-mass coordinate, and find by calculating the matrix elements  $\langle \text{HF} | [a_i^+ a_m^-] \dots | \text{HF} \rangle$  of this equation an equation identical to (8.106). This shows that in this case  $M_0 = Am$  is the total mass of the nucleus.

(ii) *Rotation.* Starting with a deformed HF calculation, a violated symmetry is a rotation perpendicular to the symmetry axis, let us say a rotation around the  $x$ -axis—the operator  $\hat{P}$  is now the angular momentum operator  $\hat{j}_x$ . Equation (8.106) determines the  $p\hbar$ -matrix element of a corresponding coordinate, an angle  $\hat{\theta}_x$ .  $M_0$  is now a moment of inertia  $J_{\text{rv}}$  corresponding to a rotation around the  $x$ -axis. We get for real matrix elements  $J_{x_{mi}}$  in analogy to Eq. (8.109)

\* In a case where this is not true, for instance, in RPA calculations based on a phenomenological Woods-Saxon potential, special methods have been developed to remove the spurious components [PS 77, Me 79].

$$J_{\text{TV}} = 2 \sum_{mi} J_{x_{mi}}^* (A + B)^{-1} J_{x_{mi}}. \quad (8.113)$$

with

$$(A + B)_{mij} = \delta_{mm} \delta_{ij} (\epsilon_m - \epsilon_i) + \bar{v}_{mijn} + \bar{v}_{nmij}.$$

Neglecting the residual interaction  $\bar{v}$  we again find the well-known cranking formula (3.89). For a discussion of the numerical application of this formula see Chap. (3.4.2).

In the next step, we would like to construct wave functions corresponding to these “spurious” excitations. We can define a ground state  $|0\rangle$  by

$$O_\nu |0\rangle = 0 \quad \text{for } \nu > 0; \quad \mathcal{G}_0 |0\rangle = 0;$$

and excited states

$$|\nu\rangle = O_\nu^+ |0\rangle \quad \text{for } \nu > 0; \quad |p\rangle = \exp\left(i \frac{P}{\hbar} \omega_0\right) |0\rangle.$$

These wave functions give the proper excitation energies  $\Omega_\nu$  and  $p^2/2M_0$ , but it turns out that they are no longer normalizable. [MW 70]. The reason for this is that the RPA is a small amplitude approximation. Therefore, we describe the wave function of a rotational state, for instance, properly only for small angles. We can deduce therefore, energies, but not the full wave function. In particular, we do not recover the quantization of the angular momentum.

Summarizing, we can say that the RPA theory treats the inherent symmetries of the problem consistently. It separates the so-called spurious motions from the vibrations. In fact, these excitations are not really spurious, but they represent a different type of motion which has to be treated separately. At least their energies (which are not given by  $\Omega_0 = 0$  but by  $p^2/2M_0$ ) are reproduced properly, since they are characterized by the right mass parameters.

## 8.5 Linear Response Theory

In calculating collective excitations of the nuclear system, we have so far used the stationary Schrödinger equation (8.59) and tried to diagonalize the Hamiltonian at least in some approximation.

We shall now begin from quite a different starting point. We investigate the influence of an external time-dependent field

$$F(t) = F e^{-i\omega t} + F^+ e^{i\omega t} \quad (8.114)$$

on the system. We assume that  $F$  is a one-body operator, that is,

$$F(t) = \sum_{kl} f_{kl}(t) a_k^+ a_l,$$

and that the field is weak, that is, it introduces only small changes of the nuclear density, which we can treat in linear order.

As we will see, the nuclear density oscillates with this external field and we obtain resonances whenever the frequency  $\omega$  is close to an excitation energy of the system. In this way:

- (i) We get information about the excited states of the system. In particular, we find an equation for the amplitudes  $\langle 0 | a_l^+ a_m | \nu \rangle$ , which corresponds precisely to the RPA equations.
- (ii) We are able to calculate the response of the system to the external field, that is, changes in its density, energy, and so on.
- (iii) We find a method to derive the RPA equations for density-dependent forces.

### 8.5.1 Derivation of the Linear Response Equations

The wave function  $|\Phi(t)\rangle$  of a nuclear system in an external, time-dependent field is no longer stationary. It is a wave packet, and its one-body density

$$\rho_{kl}(t) = \langle \Phi(t) | a_l^+ a_k | \Phi(t) \rangle \quad (8.115)$$

is now time dependent. We want to calculate this density explicitly under the following approximations.

- (i) We assume that at any time  $\rho(t)$  corresponds to a *Slater determinant*\* (i.e.,  $\rho^2 = \rho$ ). Then  $\rho$  obeys the following equation of motion.

$$i\hbar \dot{\rho} = [\hbar[\rho] + f(t), \rho]. \quad (8.116)$$

This is the *time-dependent Hartree-Fock (TDHF) equation*. It will be derived in Section 12.2. Here  $\hbar[\rho]$  is the single-particle Hartree-Fock (HF) field as defined in Eq. (5.33) and  $f(t)$  is the time-dependent external field of Eq. (8.114).

- (ii) We assume that the external field  $f(t)$  is weak, that is, it introduces only oscillations with *small amplitudes* around the stationary density  $\rho^{(0)}$ , which is itself a solution of the stationary Hartree-Fock equation (5.36)  $[\hbar[\rho^{(0)}], \rho^{(0)}] = 0$ . Therefore, the density has the form

$$\rho(t) = \rho^{(0)} + \delta\rho(t), \quad (8.117)$$

where

$$\delta\rho = \rho^{(1)} e^{-i\omega t} + \rho^{(1)*} e^{i\omega t} \quad (8.118)$$

is linear in the field  $f$ . In the following we work in the basis in which  $\rho^{(0)}$  and  $\hbar[\rho^{(0)}]$  are diagonal, that is, in the HF-basis:

$$\rho_{kl}^{(0)} = \delta_{kl}, \quad \rho_k^{(0)} = \begin{cases} 0 & \text{for particles,} \\ 1 & \text{for holes,} \end{cases} \quad (8.119)$$

and

$$(h_0)_{kl} = (\hbar[\rho^{(0)}])_{kl} = \delta_{kl} \cdot \epsilon_k. \quad (8.120)$$

\*In this sense, the following derivation of the RPA shows that it is just a time dependent generalization of the independent particle picture (see Chap. 12).

In Section 5.3.3 we saw that the condition  $\rho^2 = \rho$  implies that the only non-vanishing matrix elements of  $\rho^{(1)}$  are  $\rho^{ph}$  and  $\rho^{hp}$  matrix elements  $\rho_{mi}^{(1)}$  and  $\rho_{im}^{(1)}$ . They are determined by the solution of the TDHF equation (8.116). We insert Eq. (8.117) and expand up to linear order in the external field  $f$ ,

$$i\hbar\delta\dot{\rho} = [\hbar_0, \delta\rho] + \left[ \frac{\partial h}{\partial\rho} \cdot \delta\rho, \rho^{(0)} \right] + [f, \rho^{(0)}], \quad (8.121)$$

where  $\delta h/\delta\rho \cdot \delta\rho$  is a shorthand notation for

$$\sum_{im} \left( \frac{\partial h}{\partial\rho_{mi}} \Big|_{\rho=\rho^{(0)}} \cdot \delta\rho_{mi} + \frac{\partial h}{\partial\rho_{im}} \Big|_{\rho=\rho^{(0)}} \cdot \delta\rho_{im} \right). \quad (8.122)$$

Using the rules for the calculation with HF densities, as given in Appendix D, [Eq. (D.30)(f)] we find that the  $pp$  and the  $hh$  matrix elements of Eq. (8.121) vanish identically. From (8.118) we obtain for the  $p_h$  and  $h_p$  elements the *linear response equation*

$$\left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} \rho^{(1)ph} \\ \rho^{(1)hp} \end{pmatrix} = - \begin{pmatrix} f^{ph} \\ f^{hp} \end{pmatrix} \quad (8.123)$$

with

$$A_{minj} = (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \frac{\partial h_{ni}}{\partial\rho_{nj}}, \quad B_{minj} = \frac{\partial h_{ni}}{\partial\rho_{jn}}.$$

These matrices correspond exactly to the matrices  $A$  and  $B$  of the RPA method, if we use as a residual interaction [see Eq. (5.32)]

$$\tilde{v}_{pqrs} = \frac{\partial h_{pq}}{\partial\rho_{rs}} = \frac{\partial^2 E}{\partial\rho_{pq}\partial\rho_{rs}}. \quad (8.124)$$

In the case of HF theory without density dependent forces, we can use the expression (5.28) for the energy and thus we get back the RPA matrices (8.71). However, the above derivation is more general. It can also be applied to theories with *density-dependent forces* (see Sec. 5.6). In this case, for the calculation of excited states we have to use the force defined by Eq. (8.124) as the second derivative of the ground state energy with respect to the density. In particular, this force is no longer necessarily antisymmetric in the indices  $q$  and  $r$ .

The linear response equation (8.123) is an inhomogeneous equation and can be solved by inverting the matrix on the left-hand side. We then find a linear connection between the external field  $f$  and the change in the nuclear density (i.e., the response of the system):

$$\rho_{kl}^{(1)} = \sum_{pq} R_{kplq}(\omega) f_{pq}. \quad (8.125)$$

The function  $R_{kplq}(\omega)$  is called the *response function* [see Eqs. (F.51) and (F.68)]. We have calculated it here only in the mean field approach (i.e., in “RPA order”), because we restrict ourselves to product wave functions

with  $\rho^2 = \rho$ . Therefore, the indices  $k/l$  and  $p/q$  run only over  $ph$  and  $hp$  indices. This is no longer true in the general case.

The response function  $R$  depends on the frequency of the external field. It has poles at the eigenfrequencies of the system, where already an infinitesimal field  $f$  is sufficient to excite the corresponding eigenmode.

To find these resonances ( $\omega = \Omega_r$ ), we have to look for the solutions of the homogeneous equation (8.123) with vanishing external field. With the notation of Eqs. (8.73) and (8.75) we obtain

$$(\mathcal{S} - \hbar\Omega_r \mathcal{V})\rho^{(1)\nu} = 0. \quad (8.126)$$

This is exactly the RPA equation (8.70). Its solution gives the transition densities (8.69)

$$\rho_{pq}^{(1)}(\Omega_r) = \langle 0 | a_q^+ a_p | \nu \rangle \quad (8.127)$$

The derivation of the RPA equations is more general than the one given in Section 8.4.1, because it can also be used in the case of density-dependent forces, which is a crucial point for the validity of the mean field approach in nuclear physics.

On the other hand, the derivation shows us also very clearly the connection of the random phase approximation to the Hartree-Fock theory. We allow the average nuclear potential to oscillate around its stationary value, which corresponds to a minimum in the energy surface of all possible product wave functions (see Sec. 7.3.1). In the limit of small amplitudes we thus get a linear eigenvalue problem for the determination of the normal modes of the system (see also Sec. 12.3.2). The *RPA approximation* is therefore nothing but the *small amplitude limit* of the *time-dependent mean field approach*.

The energy surface in the vicinity of the stationary point  $\rho_0$  can be obtained by expanding the HF energy  $E[\rho]$ , up to second order in  $\delta\rho^*$  [BG 77]:

$$\begin{aligned} E[\rho] &= E[\rho^{(0)}] + \text{Tr} \left( \frac{\delta E}{\delta\rho} \delta\rho \right) + \frac{1}{2} \text{Tr} \text{Tr} \left( \delta\rho^* \frac{\delta^2 E}{\delta\rho \delta\rho} \delta\rho \right) \\ &= E[\rho^{(0)}] + \frac{1}{2} \rho^{(1)*} \mathcal{S} \rho^{(1)}. \end{aligned} \quad (8.128)$$

We find that the stability matrix  $\mathcal{S}$  has again the form (7.37), but now the matrices  $A$  and  $B$  (8.123) are also defined for density-dependent forces.

It is easy to show also for such forces that we eventually obtain *spurious solutions* at zero frequency in the case of a broken symmetry  $\hat{P}$ . We have only to use the condition (5.68), which states that

$$\bar{\rho} = e^{ia_P} \rho^{(0)} e^{-ia_P},$$

\*In deriving Eq. (8.128) we must be aware of the fact that  $\delta\rho$  has in second order also  $pp$  and  $hh$  matrix elements. They are, however, not independent variables, because any Slater determinant can be expressed by the  $ph$  and  $hp$  matrix elements of  $\delta\rho$ . We can use the relation  $\rho^2 = \rho$  to eliminate them. Thus, the term  $\text{Tr}(\delta\rho_0 \cdot \delta\rho)$  gives a quadratic contribution, namely, just the  $ph$  energies  $\epsilon_m - \epsilon_i$  in the matrix  $A$ .

as well as  $\rho^{(0)}$ , also fulfills the equation

$$[h(\bar{\rho}), \bar{\rho}] = 0.$$

Infinitesimal changes  $\bar{\rho} = \rho^{(0)} + \rho^{(1)}$ , with  $\rho^{(1)} \propto [P, \rho^{(0)}]$ , gives

$$[h_0, \rho^{(1)}] + \left[ \frac{\delta h}{\delta \rho}, \rho^{(1)}, \rho^{(0)} \right] = 0, \quad (8.129)$$

which shows that  $\rho^{(1)}$ , that is, just the  $ph$  and  $hp$  matrix elements of  $P$ , correspond to a spurious solution at zero energy analogous to Eq. (8.104) in the case of density-independent forces.

Knowing the eigenmodes of the system, that is, the frequencies  $\Omega_\nu$  and the RPA amplitudes  $X$  and  $Y$ , makes it possible to solve the linear response equation (8.123). Using (8.76ff), we find

$$\mathcal{S} - \hbar\omega\mathcal{R} = \hbar\mathcal{R}\mathcal{X}(\Omega - \omega)\mathcal{R}\mathcal{X}^* + \mathcal{R}$$

which can easily be inverted:

$$\rho^{(1)} = \frac{1}{\hbar} \mathcal{R}(\omega - \Omega)^{-1} \mathcal{R} \mathcal{X}^* f.$$

This is equivalent to Eq. (8.125)—we have now an explicit expression for the response function,\* namely its *spectral representation*:

$$R_{pq'q''}(\omega) = \frac{1}{\hbar} \sum_{\nu > 0} \left( \frac{\langle 0 | a_q^\dagger a_p | \nu \rangle \times \nu | a_{p'}^\dagger a_{q'} | 0 \rangle}{\omega - \Omega_\nu + i\eta} - \frac{\langle 0 | a_p^\dagger a_q | \nu \rangle \times \nu | a_q^\dagger a_{p'} | 0 \rangle}{\omega + \Omega_\nu + i\eta} \right). \quad (8.130)$$

Again, the index pairs  $pq$  and  $p'q'$  run only over  $ph$  and  $hp$  pairs. All other matrix elements of  $R$  vanish in RPA order. The form (8.130), however is more general. If we use exact eigenfunctions  $|\nu\rangle$  and exact energies  $\hbar\Omega_\nu$  of the system,  $R_{pq'q''}(\omega)$  in Eq. (8.130) is just the exact response function. This can easily be seen by using time-dependent perturbation theory (see [No 64a, Chap. 2]) for the calculation of the change in the exact wave function produced by the external field  $F$ :

$$|\Psi(t)\rangle = |0\rangle + \sum_{\nu > 0} |\nu\rangle \left\{ \frac{\langle \nu | F | 0 \rangle}{\hbar(\omega - \Omega_\nu) + i\eta} e^{-i\omega t} - \frac{\langle \nu | F^+ | 0 \rangle}{\hbar(\omega + \Omega_\nu) - i\eta} e^{i\omega t} \right\}.$$

The states  $|0\rangle$  and  $|\nu\rangle$  are the stationary eigenstates of the system without perturbation. The transition density corresponding to this wave function  $\rho^{(1)}$  is then given by Eq. (8.125) with the exact response function (8.130).

If we introduce the response function  $R^0$  of the free system (without residual interaction  $\tilde{\sigma}$  in (8.124)),

$$R_{pq'q''}^0(\omega) = \frac{\rho_q^{(0)} - \rho_p^{(0)}}{\hbar\omega - \epsilon_p + \epsilon_q + i\eta} \delta_{pp'} \delta_{qq''},$$

\*For the sake of completeness we have added the infinitesimal positive parameter  $\eta$ , which determines the boundary condition in the case of unbound states (see Sec. 8.5.4). In a bound state problem  $\eta$  can be set equal to zero.

we can finally, in RPA approximation, derive another equation for  $R(\omega)$ , the so-called *linearized Bethe–Salpeter* equation (F.75), viz.

$$R_{pq'p''q''} = R_{pq'p''q''}^0 + \sum_{p'q''} R_{pq'p''q''}^0 \tilde{\sigma}_{p'q''} R_{p''q''p''q''}. \quad (8.131)$$

The correctness of this equation can be verified simply by multiplying by  $(\hbar\omega - \epsilon_p + \epsilon_q)$  and using the definition of  $R^0$ , the spectral representation (8.130) for  $R$  and the RPA equation (8.126).

## 8.5.2 Calculation of Excitation Probabilities and Schematic Model

Another useful property of the linear response function lies in the fact that its imaginary part is related to the total transition probability (8.72). We define

$$R_F(\omega) := \text{Tr}(f^+ \rho^{(1)}(\omega)) = \sum_{pq'q''} f_{pq}^* R_{pq'q''}(\omega) f_{p'q''} \quad (8.132)$$

and use the relation  $1/(\omega + i\eta) = P(1/\omega) - i\eta\delta(\omega)$  in Eq. (8.130) to obtain

$$ImR_F(\omega) = -\pi \sum_{\nu > 0} |\langle \nu | F | 0 \rangle|^2 \delta(\hbar\omega - \hbar\Omega_\nu), \quad \omega > 0. \quad (8.133)$$

We get the energy-weighted sum rule (8.154) by integrating this function,

$$-\frac{\hbar^2}{\pi} \int_0^\infty \omega ImR(\omega) d\omega = \sum_{\nu} \hbar\Omega_\nu |\langle \nu | F | 0 \rangle|^2 \equiv S_I, \quad (8.134)$$

and the transition matrix element  $|\langle \nu | F | 0 \rangle|^2$  as the residue of  $R_F(\omega)$  at the pole  $\omega = \Omega_\nu$ .

The solution becomes extremely simple in the schematic model, where the separable ansatz for the ground state correlation matrix element is now:

$$\tilde{\sigma}_{mij} = \lambda D_{mi} D_{nj}^*, \quad \tilde{\sigma}_{mij} = \lambda D_{mj} D_{ni}^*,$$

where  $D$  is identical with the external field operator  $F$ . From the Bethe–Salpeter equation (8.131), we get

$$R_D(\omega) = R_D^0(\omega)[1 + \lambda R_D(\omega)]$$

with

$$R_D^0(\omega) = \sum_{pq'q''} D_{pq}^* R_{pq'q''}^0 D_{p'q''} = \sum_{mi} |D_{mi}|^2 \left( \frac{1}{\hbar\omega - \epsilon_m + \epsilon_i + i\eta} - \frac{1}{\hbar\omega + \epsilon_m - \epsilon_i + i\eta} \right).$$

Solving for  $R_D(\omega)$  yields

$$R_D(\omega) = \frac{R_D^0}{1 - \lambda R_D^0}.$$

The poles of  $R_D(\omega)$  give the excitation energies  $\Omega_\nu$ , and thus in the schematic model

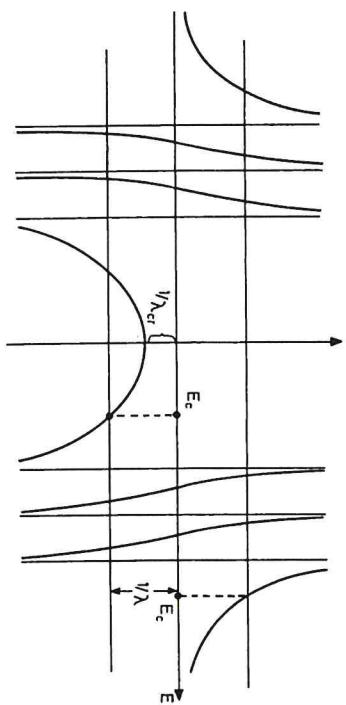


Figure 8.11. Graphical solution of the dispersion relation (8.135).

we have the following dispersion relation.

$$\frac{1}{\lambda} = R_D^0(\Omega_r) = \sum_{mi} |D_{mi}|^2 \frac{2\epsilon_{mi}}{\hbar^2 \Omega_r^2 - \epsilon_{mi}^2}; \quad \epsilon_{mi} = \epsilon_m - \epsilon_i. \quad (8.135)$$

(We can drop the infinitesimal  $\eta$  because we are only interested in bound states for which  $\Omega_r \neq \epsilon_{mi}$ .)

Equation (8.135) can be solved graphically as in the TDA case. Comparing Fig. 8.11 with Fig. 8.4, we notice two qualitative differences which are due to the RPA ground state correlations:

- (i) In the case where the residual interaction becomes stronger than the critical value (i.e.,  $\lambda < \lambda_{crit}$ ) the energy of the low-lying collective state becomes imaginary.
- (ii) The ( $T=0$ )-RPA state is shifted further down than its corresponding TDA state for a comparable interaction strength  $\lambda$ .

We can study this more closely in the degenerate case. If we put all  $\epsilon_{mi}$  equal to  $\epsilon$  we have, from Eq. (8.135),

$$E_{coll}^2 = \epsilon^2 + 2\epsilon\lambda \sum_{mi} |D_{mi}|^2.$$

In the degenerate case, therefore, we have for  $\lambda_{crit}$

$$\lambda_{crit} = -\frac{\epsilon}{2 \sum_{mi} |D_{mi}|^2}.$$

This is the point where the chosen HF-basis no longer gives the minimum for the ground state energy. The true minimum now occurs in a different HF-solution, which turns out to be deformed. We therefore often call  $\lambda_{crit}$  the point at which a phase transition from spherical state into a deformed shape of the nucleus occurs (for example,  $D \sim r^2 Y_{20}$ ). In a comparison with the TDA case, we see that

$$E_{coll}^{TDA}(\lambda_{crit}) = \frac{\epsilon}{2}$$

and

$$E_{coll}^{TDA}(2\lambda_{crit}) = 0,$$

that is, in the schematic model the “phase transition” occurs in the TDA case at only twice the interaction strength.

We now want to turn to the calculation of transition matrix elements. We have to calculate the residue of  $R_D(\omega)$  at the pole  $\omega = \Omega_r$ . In the vicinity of  $\Omega_r$ ,  $R_D(\omega)$  has the form:

$$R_D(\omega) = \frac{R_D^0(\Omega_r)}{-\lambda(dR^0/d\omega)|_{\omega=\Omega_r} \cdot (\omega - \Omega_r)}.$$

We therefore get

$$|\langle \nu | D | 0 \rangle|^2 = -\frac{\hbar}{\lambda^2} \left( \frac{dR^0}{d\omega} \right)_{\Omega_r}^{-1} = \left( \lambda^2 \sum_{mi} |D_{mi}|^2 \frac{4\epsilon_{mi}\hbar\Omega_r}{(\hbar\Omega_r^2 - \epsilon_{mi}^2)^2} \right)^{-1}.$$

In the degenerate case this yields

$$|\langle \nu | D | 0 \rangle|^2 = \frac{\epsilon}{E_{coll}} \sum_{mi} |D_{mi}|^2.$$

We see that for the low-lying states the transition probability is enhanced as compared to the TDA value (8.21) by a factor  $\epsilon/E_{coll}$ . For the collective octupole and quadrupole states this factor can be as large as two. Similar but less pronounced results are found in realistic calculations (see Sec. 8.6).

### 8.5.3 The Static Polarizability and the Moment of Inertia

We can apply linear response theory to calculate the change of the nuclear energy and the nuclear deformation in a static external field  $-\lambda F$ . This corresponds to the solution of the constrained HF equation

$$[h[\rho] - \lambda f, \rho] = 0 \quad (8.136)$$

in linear response theory. For the change of the density, we get from Eq. (8.118) and (8.125),

$$\rho^{(1)} = -\lambda R(\omega=0)f = \lambda S^{-1}f. \quad (8.137)$$

The static polarizability  $\alpha$  is defined by the change of the expectation value of  $F$ :

$$\langle \lambda | F | \lambda \rangle = \langle 0 | F | 0 \rangle + \lambda \cdot \alpha; \quad (8.138)$$

and the change in energy is given by

$$\langle \lambda | H | \lambda \rangle = \langle 0 | H | 0 \rangle + \frac{1}{2} \lambda^2 \cdot \alpha. \quad (8.139)$$

The fact that we have the same constant  $\alpha$  in both cases is called Feynman's theorem [Fe 39] and can be derived in analogy to Eq. (3.81) for density dependent forces also.

Finally, for the curvature of the energy function at the stationary point  $\lambda=0$ , which is equivalent to the static polarizability, the compression

As in Section B.6, we have to replace  $\mathbf{r}_i$  by  $\mathbf{r}_i - \mathbf{R}$  for the dipole radiation, where only the first term in an expansion of  $\exp(i\mathbf{k}(\mathbf{r}_i - \mathbf{R}))$  is kept, and get

$$\sigma_f(E) = \frac{4\pi^2 e^2}{\hbar c} (E_f - E_0) |\langle \Psi_f | D_z | \Psi_0 \rangle|^2 \delta(E - E_f + E_0). \quad (\text{B.94})$$

To get similar cross sections for higher multipolarity, we have to transform the representation (B.89) of the electromagnetic potential into the representation (B.51). This is shown in great detail in [SF 74].

## APPENDIX C Second Quantization

### C.1 Creation and Annihilation Operators

The name “second quantization” is misleading. This formalism has nothing to do with the further quantizing of quantum mechanics. It is just an alternative formulation of the usual quantum mechanics, which has turned out to be very useful for handling the many-body problem. It can be used for bosons and fermions, and we will give a short introduction and some important formulae.

We start with a complete orthogonal set of single-particle states  $|\nu\rangle$ , where  $\nu$  stands for a set of quantum numbers, for example,

- (i) space coordinate  $\mathbf{r}$ , spin  $s \equiv s_z$   $|\mathbf{r}, s\rangle$ ;
- (ii) the quantum numbers of an oscillator basis  $|nljm\rangle$ .

Orthogonality and completeness are expressed as

$$\langle \nu | \nu' \rangle = \delta_{\nu\nu'}, \quad \sum_\nu |\nu\rangle \langle \nu| = 1. \quad (\text{C.1})$$

(For continuous quantum numbers such as  $\mathbf{r}$ , the  $\delta_{\nu\nu'}$  will mean  $\delta(\mathbf{r} - \mathbf{r}')$  and the sum  $\sum_\nu$  is to be replaced by  $\int d^3 r$ .)

The coordinate representation of the state  $|\nu\rangle$  is given by

$$\varphi_\nu(1) = \varphi_\nu(\mathbf{r}_1, s_1) = \langle \mathbf{r}_1, s_1 | \nu \rangle. \quad (\text{C.2})$$

Starting with this set of single-particle states, we can construct a complete orthogonal set of totally *symmetric*  $N$ -body wave functions

$$\Phi_{\nu_1 \dots \nu_N}(1, \dots, N) = \mathcal{N} \sum_P P \{ \varphi_{\nu_1}(1) \dots \varphi_{\nu_N}(N) \}, \quad (\text{C.3})$$

where the sum runs over all permutations  $(\nu_1 \dots \nu_N)$  of the numbers  $(1 \dots N)$  and  $\mathcal{H}$  is a normalization constant.

Any arbitrary, totally *symmetric*  $N$ -body wave function can be represented in this basis:

$$\Psi(1, \dots, N) = \sum_{\nu_1 \dots \nu_N} c_{\nu_1 \dots \nu_N} \Phi_{\nu_1 \dots \nu_N}(1, \dots, N). \quad (\text{C.4})$$

We can also give to each of the single-particle states a number ( $\nu = 1, 2, \dots$ ) (in the case of continuous quantum numbers, we must first introduce a finite box) and characterize the wave function  $\Phi_{\nu_1 \dots \nu_N}$  by the “occupation numbers”  $\{\nu_\nu\}$ , which tell how often a particular number  $\nu$  is contained in the  $N$  numbers  $(\nu_1, \dots, \nu_N)$ . Obviously, we have

$$\sum_\nu n_\nu = N \quad (\text{C.5})$$

and

$$\begin{aligned} \Phi_{(\nu)}(1, \dots, N) &= \Phi_{\nu_1 \dots \nu_N}(1, \dots, N) \\ &= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \dots}} \sum_P P \{ \Phi_{\nu_1}(1) \dots \Phi_{\nu_N}(N) \}. \end{aligned} \quad (\text{C.6})$$

Such a state describes a boson system. In complete analogy, we can construct totally antisymmetric-basis wave functions

$$\Phi_{(\nu)}(1, \dots, N) = \frac{1}{\sqrt{N!}} \sum_P \text{sign}(P) P \{ \Phi_{\nu_1}(1) \dots \Phi_{\nu_N}(N) \}. \quad (\text{C.7})$$

They are called *Slater determinants* and describe fermion systems. In this case the numbers  $n_\nu$  only take the values 0 or 1, otherwise (C.7) would vanish identically.

We can now construct a Hilbert space which contains a vacuum (no particle)  $|-\rangle$ , all the one-particle states, all the symmetrized (or antisymmetrized) two-particle states, and so on...

$$\mathcal{H} = \{ \mathcal{H}_0, \mathcal{H}_1, \mathcal{H}_2, \dots \}. \quad (\text{C.8})$$

The wave functions  $\Phi_{(\nu)}$  correspond to basis states  $|n_1, n_2, \dots\rangle$  in this Hilbert space, which are characterized by the occupation numbers (occupation number representation), such that

$$\Phi_{(\nu)}(1, \dots, N) = \langle 1, \dots, N | n_1, n_2, \dots \rangle. \quad (\text{C.9})$$

These states are orthonormalized

$$\langle n'_1, n'_2, \dots | n_1, n_2, \dots \rangle = \delta_{n'_1 n_1} \delta_{n'_2 n_2} \dots \delta_{n'_\nu n_\nu} \dots. \quad (\text{C.10})$$

First we shall study boson systems and define an “annihilation operator”  $B_\nu$  by

$$B_\nu |n_1, n_2, \dots, n_\nu, \dots\rangle = \sqrt{n_\nu} |n_1, n_2, \dots, n_\nu - 1, \dots\rangle. \quad (\text{C.11})$$

The operator  $B_\nu$  lowers the occupation number in the state with the number  $\nu$  by one. An  $N$ -body state goes over into an  $(N-1)$ -body state.

$$\langle n'_1, n'_2, \dots, n'_\nu, \dots | B_\nu^+ | n'_1, n'_2, \dots, n'_\nu, \dots \rangle = \sqrt{n_\nu + 1} \delta_{n'_1 n_1} \dots \delta_{n'_\nu n_\nu + 1} \dots \quad (\text{C.12})$$

or

$$\langle n_1, n_2, \dots, n_\nu, \dots | B_\nu^+ | n'_1, n'_2, \dots, n'_\nu, \dots \rangle = \sqrt{n_\nu + 1} \delta_{n_1 n'_1} \dots \delta_{n_\nu n'_\nu} \dots \quad (\text{C.13})$$

This is valid for all basis states  $\langle n_1, n_2, \dots |$ . We therefore find

$$B_\nu^+ |n_1, n_2, \dots, n_\nu, \dots\rangle = \sqrt{n_\nu + 1} |n_1, n_2, \dots, n_\nu + 1, \dots\rangle. \quad (\text{C.14})$$

$B_\nu^+$  “creates” a particle in the state with the number  $\nu$ . Therefore, it is called a “creation operator” in the state  $\nu$ .” It is the Hermitian conjugate operator to  $B_\nu$ .

From this definition we gain the fact that

$$\begin{aligned} (B_\mu B_\nu^+ - B_\nu^+ B_\mu) |n_1, n_2, \dots, n_\mu, \dots\rangle \\ = \begin{cases} \left( \sqrt{n_\nu + 1} \sqrt{n_\mu} - \sqrt{n_\mu} \sqrt{n_\nu + 1} \right) |n_1, \dots, n_\nu + 1, \dots, n_\mu - 1, \dots\rangle = 0 & \text{for } \nu \neq \mu, \\ \left( \sqrt{n_\nu + 1} \sqrt{n_\nu + 1} - \sqrt{n_\nu} \sqrt{n_\nu} \right) |n_1, \dots, n_\nu, \dots\rangle & \text{for } \nu = \mu, \end{cases} \end{aligned} \quad (\text{C.15})$$

and hence get the commutation relations.

$$[B_\mu, B_\nu^+] = B_\mu B_\nu^+ - B_\nu^+ B_\mu = \delta_{\mu\nu}. \quad (\text{C.16})$$

In the same way, we may show that

$$[B_\mu, B_\nu] = [B_\nu^+, B_\mu^+] = 0. \quad (\text{C.17})$$

The state with the occupation numbers  $|0, 0, 0, \dots\rangle = |-\rangle$  is the *vacuum*. We thus have

$$B_\nu |-\rangle = 0 \quad \text{for all } \nu \quad (\text{C.18})$$

and

$$|n_1, n_2, \dots, n_\nu, \dots\rangle = \frac{1}{\sqrt{n_1! n_2! \dots n_\nu! \dots}} \prod_\mu (B_\mu^+)^{n_\mu} |-\rangle. \quad (\text{C.19})$$

The relation (C.11) follows from (C.16) to (C.19), which was our definition of the operators  $B_\nu$ . We can therefore also go in the opposite direction and start with a set of operators  $B_\nu, B_\nu^+$  which obey boson commutation relations and construct the many-body Hilbert space from (C.17) and (C.18).

The operator  $B_\nu^+ B_\nu$  is called the particle-number operator for the state  $\nu$ :

$$B_\nu^+ B_\nu |n_1, \dots, n_\nu, \dots\rangle = n_\nu |n_1, \dots, n_\nu, \dots\rangle. \quad (\text{C.20})$$

We now address ourselves to a fermion system. We shall use small Latin letters  $a_\nu^+, a_\nu$  for the creation and annihilation operators of fermions. Since  $n_\nu$  can only have the values 0 and 1, we may define the action of the

operators as

$$a_\nu |n_1, \dots, n_\nu = 1, \dots \rangle = |n_1, \dots, n_\nu = 0, \dots \rangle, \quad a_\nu |n_1, \dots, n_\nu = 0, \dots \rangle = 0, \quad (\text{C.21})$$

from which we get

$$a_\nu^+ |n_1, \dots, n_\nu = 0, \dots \rangle = |n_1, \dots, n_\nu = 1, \dots \rangle, \quad a_\nu^+ |n_1, \dots, n_\nu = 1, \dots \rangle = 0, \quad (\text{C.22})$$

and

$$\begin{aligned} [a_\mu, a_\nu^+]_+ &:= \{a_\mu, a_\nu^+\} := a_\mu a_\nu^+ + a_\nu^+ a_\mu = \delta_{\mu\nu}, \\ [a_\mu, a_\nu]_+ &= [a_\mu^+, a_\nu^+]_+ = 0. \end{aligned} \quad (\text{C.23})$$

The vacuum is again given by  $|-\rangle = |0, 0, \dots\rangle$  and we have

$$a_\nu |-\rangle = 0 \quad \text{for all } \nu, \quad (\text{C.24})$$

hence

$$|n_1, \dots, n_\nu, \dots \rangle = \prod_\mu (a_\mu^+)^{n_\mu} |-\rangle = a_{\nu_1}^+ \dots a_{\nu_N}^+ |-\rangle. \quad (\text{C.25})$$

## C.2 Field Operators in the Coordinate Space\*

Using the single-particle wave functions  $\varphi_\nu(\mathbf{r}, s)$  in Eq. (C.2) we can define creation and annihilation operators  $a^+(\mathbf{r}, s), a(\mathbf{r}, s)$ , which depend on the coordinates  $\mathbf{r}$  and  $s^\dagger$ :

$$a(\mathbf{r}, s) = \sum_\nu \varphi_\nu(\mathbf{r}, s) a_\nu, \quad a^+(\mathbf{r}, s) = \sum_\nu \varphi_\nu^*(\mathbf{r}, s) a_\nu^+. \quad (\text{C.26})$$

With Eq. (C.1) we can invert this relation,

$$a_\nu = \sum_s \int d^3 r \varphi_\nu^*(\mathbf{r}, s) a(\mathbf{r}, s), \quad a_\nu^+ = \sum_s \int d^3 r \varphi_\nu(\mathbf{r}, s) a^+(\mathbf{r}, s), \quad (\text{C.27})$$

and gain the commutators

$$[a(\mathbf{r}, s), a^+(\mathbf{r}', s')]_+ = \sum_{\nu\nu'} \varphi_\nu(\mathbf{r}, s) \varphi_{\nu'}^*(\mathbf{r}', s') [a_\nu, a_{\nu'}^+]_+ = \delta_{ss'} \delta(\mathbf{r} - \mathbf{r}') \quad (\text{C.28})$$

and

$$[a(\mathbf{r}, s), a(\mathbf{r}', s')]_+ = [a^+(\mathbf{r}, s), a^+(\mathbf{r}', s')]_+ = 0. \quad (\text{C.29})$$

We can express the many-body wave function (C.7) by

$$\Phi_{(n)}(1, \dots, N) = \frac{1}{\sqrt{N!}} \langle -| a(N) \dots a(1) | n_1, n_2, \dots, n_\nu, \dots \rangle \quad (\text{C.30})$$

\*In the following we investigate only the case of fermions. Analogous considerations apply for bosons.

<sup>t</sup>This definition agrees with the convention  $\Phi_r(\mathbf{r}) = \langle \mathbf{r} | \nu \rangle$ , and according to the definition (5.18) for a unitary transformation of the operators  $a_\nu^+, \varphi_\nu(\mathbf{r})$  corresponds to  $D_{rr}^*$ .

Starting from a vacuum  $|-\rangle$ , we have expressed all states in the many-body Hilbert space  $\mathcal{K}$  by creation and annihilation operators  $a_\nu^+, a_\nu$ . The same will be done for operators in the following. We have to distinguish between one- and two-body operators.

A *one-body operator* as, for example, the kinetic energy or the total momentum of an  $N$ -particle system, is given as the sum of  $N$  operators  $\hat{f}_i$  which always act on the coordinate of the particle  $i$ :

$$\hat{F} = \sum_{i=1}^N \hat{f}_i. \quad (\text{C.32})$$

Its matrix elements in the  $|v\rangle$  representation are

$$f_{\nu\nu'} = \langle v | \hat{f} | v' \rangle, \quad (\text{C.33})$$

that is,

$$\hat{f}_i \varphi_\nu(i) = \sum_\nu f_{\nu\nu} \varphi_\nu(i). \quad (\text{C.34})$$

The representation of  $\hat{F}$  in the operators  $a_\nu^+, a_\nu$  is given by

$$\hat{F} = \sum_{\nu\nu'} f_{\nu\nu'} a_\nu^+ a_\nu. \quad (\text{C.35})$$

To show this, we have to prove

$$\sum_i \hat{f}_i \Phi(1, \dots, N) = \langle 1, \dots, N | \sum_{\nu\nu'} f_{\nu\nu'} a_\nu^+ a_\nu | \Phi \rangle. \quad (\text{C.36})$$

On the l.h.s., from Eqs. (C.30), (C.26) and (C.34) up to a factor  $1/\sqrt{N!}$  we gain

$$\begin{aligned} &\sum_i \hat{f}_i \langle -| a(N) \dots a(i) \dots a(1) | \Phi \rangle \\ &= \sum_i \sum_{\nu_1 \dots \nu_N} \hat{f}_i \varphi_{\nu_N}(N) \dots \varphi_{\nu_1}(i) \dots \varphi_{\nu_1}(1) \langle -| a_{\nu_N} \dots a_{\nu_1} | \Phi \rangle \\ &= \sum_i \sum_\nu \sum_{\nu_1 \dots \nu_N} f_{\nu\nu} \varphi_{\nu_N}(N) \dots \varphi_{\nu_1}(i) \dots \varphi_{\nu_1}(1) \langle -| a_{\nu_N} \dots a_{\nu_1} | \Phi \rangle. \end{aligned}$$

This is identical to the r.h.s.:

$$\begin{aligned} &\sum_i \sum_{\nu_1 \dots \nu_N} f_{\nu\nu} \varphi_{\nu_N}(N) \dots \varphi_{\nu_1}(1) \langle -| a_{\nu_N} \dots a_{\nu_1} | \Phi \rangle \\ &= \sum_i \sum_\nu \sum_{\nu_1 \dots \nu_N} f_{\nu\nu} \varphi_{\nu_N}(N) \dots \varphi_{\nu_1}(1) \langle -| a_{\nu_N} \dots a_{\nu_1} | \Phi \rangle. \end{aligned}$$

$$|n_1, n_2, \dots, n_r, \dots \rangle = \int d^3 l \dots dN \frac{1}{\sqrt{N!}} \Phi_{(n)}(1, \dots, N) a^+(1) \dots a^+(N) |-\rangle. \quad (\text{C.31})$$

and

We give next a few examples:  
*The kinetic energy*

$$\hat{T} = \sum_i \hat{t}_i = \sum_i \frac{-\hbar^2}{2m} \Delta_i, \quad (\text{C.37})$$

$$\begin{aligned} \hat{T} &= \sum_{\nu\nu'} \sum_s \int d^3r \varphi_\nu^*(\mathbf{r}, s) \frac{-\hbar^2}{2m} \Delta \varphi_{\nu'}(\mathbf{r}, s) a_\nu^\dagger a_{\nu'} \\ &= \sum_s \int d^3r a^+(\mathbf{r}, s) \frac{-\hbar^2}{2m} \Delta a(\mathbf{r}, s). \end{aligned} \quad (\text{C.38})$$

*The single-particle density* (see Appendix D)

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \hat{\mathbf{r}}_i). \quad (\text{C.39})$$

$\hat{\mathbf{r}}_i$  is the coordinate operator of the  $i$ th particle;  $\mathbf{r}$  is a number.

$$\hat{\rho}(\mathbf{r}) = \sum_{\nu\nu'} \sum_s \int d^3r' \varphi_\nu^*(\mathbf{r}', s) \delta(\mathbf{r} - \mathbf{r}') \varphi_{\nu'}(\mathbf{r}', s) a_\nu^\dagger a_{\nu'} = \sum_s a^+(\mathbf{r}, s) a(\mathbf{r}, s). \quad (\text{C.40})$$

*The particle number*

$$\begin{aligned} \hat{N} &= \sum_\nu \sum_{ss'} \int d^3r d^3r' \varphi_\nu(\mathbf{r}, s) \varphi_\nu^*(\mathbf{r}', s') a^+(\mathbf{r}, s) a(\mathbf{r}', s') \\ &= \int \hat{\rho}(\mathbf{r}) d^3r. \end{aligned} \quad (\text{C.41})$$

In the most general case,  $\hat{f}$  will be an integral operator (a "nonlocal" one-particle operator):

$$\hat{f} \varphi(\mathbf{r}, s) = \sum_{s'} \int d^3r' f_{ss'}(\mathbf{r}, \mathbf{r}') \varphi(\mathbf{r}', s'). \quad (\text{C.42})$$

A *two-particle operator* as, for example, a two-body interaction, is given by a sum of operators  $v_{ij}$  which act on the coordinates of the particles  $i$  and  $j$ :

$$V = \sum_{i < j=1}^N v_{ij}. \quad (\text{C.43})$$

In the most general case,  $v_{ij}$  will be an integral operator in two variables, with matrix elements

$$v_{\mu\nu\mu'\nu'} = \langle \mu\nu | v | \mu'\nu' \rangle = \int d1 d2 d3 d4 \varphi_\mu^*(1) \varphi_\nu^*(2) v(1, 2, 3, 4) \varphi_{\mu'}(3) \varphi_{\nu'}(4). \quad (\text{C.44})$$

In complete analogy to Eq. (C.35), we can show that  $V$  can be written as

$$V = \frac{1}{2} \sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'} a_\mu^\dagger a_\nu^\dagger a_{\mu'} a_{\nu'} = \frac{1}{4} \sum_{\mu\nu\mu'\nu'} \bar{v}_{\mu\nu\mu'\nu'} a_\mu^\dagger a_\nu^\dagger a_{\mu'} a_{\nu'}, \quad (\text{C.45})$$

with the antisymmetrized matrix element

$$\bar{v}_{\mu\nu\mu'\nu'} = \langle \mu\nu | v | \mu'\nu' \rangle - \langle \mu\nu | v | \nu'\mu' \rangle. \quad (\text{C.46})$$

Very often we use local two-body interactions of the form (we neglect spin)

$$v_{ij} = v(\mathbf{r}_i, \mathbf{r}_j). \quad (\text{C.47})$$

In this case, we can verify Eq. (C.45) immediately with Eq. (C.40):

$$\begin{aligned} \frac{1}{2} \sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'} a_\mu^\dagger a_\nu^\dagger a_{\mu'} a_{\nu'} &= -\frac{1}{2} \int d^3r d^3r' a^+(\mathbf{r}) a^+(\mathbf{r}') v(\mathbf{r}, \mathbf{r}') a(\mathbf{r}) a(\mathbf{r}') \\ &= \frac{1}{2} \left( \int d^3r d^3r' v(\mathbf{r}, \mathbf{r}') \hat{\rho}(\mathbf{r}) \hat{\rho}(\mathbf{r}') - \int d^3r v(\mathbf{r}, \mathbf{r}) \hat{\rho}(\mathbf{r}) \right) \\ &= \frac{1}{2} \left( \sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j) - \sum_i v(\mathbf{r}_i, \mathbf{r}_i) \right) = \sum_{i < j=1}^N v(\mathbf{r}_i, \mathbf{r}_j). \end{aligned} \quad (\text{C.48})$$

#### C.4 Wick's Theorem

In practical applications of the second quantization, Wick's theorem has turned out to be very useful. It is a rule which allows a very simple reordering of a set of  $N$ -operators  $a$  or  $a^\dagger$ , which have the property that the commutator (in the case of bosons) or the anticommutator (in the case of fermions) of two arbitrarily chosen operators of this set is a number.

We first define the  $T$ -product (time ordered product) of a product of operators  $a(t_2), a(t_3), a^\dagger(t_1) \dots$  to be the one where the field operators have been reordered in such a way that the time arguments are increasing from right to left (an odd permutation gives a minus sign):

$$T \{ a(t_1) a^\dagger(t_3) a(t_2) a^\dagger(t_4) \} = -a(t_1) a(t_2) a^\dagger(t_3) a^\dagger(t_4) \quad t_1 > t_2 > t_3 > t_4.$$

In a *normal ordered* product, the field operators are ordered in such a way that all creation operators are to the left of all annihilation operators\* (again, an odd permutation gives a minus sign):

$$N \{ a_\nu a_\mu a_\rho a_\sigma^\dagger \} := a_\nu a_\mu a_\rho a_\sigma^\dagger := -a_\sigma^\dagger a_\nu a_\mu a_\rho. \quad (\text{C.50})$$

The *contraction*  $\widehat{UV}$  of two field operators  $U$  and  $V$  is defined as

$$\widehat{UV} = T \{ UV \} - N \{ UV \}. \quad (\text{C.51})$$

With these definitions, *Wick's Theorem* [Wi 50] can be stated as:

$$\begin{aligned} T \{ UVW \dots XYZ \} &= N \{ UVW \dots XYZ \} + N \{ \widehat{U} \widehat{V} W \dots XYZ \} \\ &\quad + \dots + N \{ \widehat{U} \widehat{V} \widehat{W} \dots XY \widehat{Z} \} + \dots \\ &\quad + \dots + N \{ \widehat{U} \widehat{V} \widehat{W} \dots X \widehat{Y} \widehat{Z} \} + \dots \end{aligned} \quad (\text{C.52})$$

The time ordered product of field operators is therefore equal to their normal ordered product plus the normal ordered products with one contraction (in all possible ways), plus the normal ordered product with two

\*Instead of  $N \{ \dots \}$  we also often use double dots  $\dots \dots$ .

contractions, and so on. Care has to be taken in the removal of a contraction out of a normal ordered product, as this can give a minus sign:

$$N \{ \widehat{UVXY} \} = \widehat{UV} N \{ XY \}; N \{ \widehat{U\bar{V}XY} \} = - \widehat{U\bar{X}} N \{ \bar{V}Y \}. \quad (\text{C.53})$$

(For the proof of Wick's theorem see, e.g., Thouless [Th 61b].)

Wick's theorem is especially useful for the calculation of ground state expectation values of time ordered products of field operators (e.g., the expectation value of particle operators with respect to the quasi-particle vacuum in Chap. 6). The result is equal to the r.h.s. of (C.52), where all operators have been contracted in all possible ways.

If there are time-independent field operators, as in (C.45), then the given order is to be defined as time ordered. The contraction of time-independent operators is especially simple; for example, we get:

$$\widehat{a_\mu a_\nu^+} = a_\mu a_\nu^+ - N \{ a_\mu a_\nu^+ \} = \delta_{\mu\nu}. \quad (\text{C.54})$$

## APPENDIX D

## Density Matrices

### D.1 Normal Densities

For the description of the dynamics of a many-body system, we often use *density matrices*. We distinguish between one-particle density matrices, two-body density matrices, and so on. In this book we use mostly one-particle densities. For higher densities the reader is referred to the work of [Th 61b]. We shall also restrict ourselves to the fermion case.

First we define a single-particle operator  $\hat{\rho}(\mathbf{r})$  in an  $N$ -body Hilbert space:

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \hat{\mathbf{f}}_i), \quad (\text{D.1})$$

where  $\hat{\mathbf{f}}_i$  is the space operator of particle  $i$  and  $\mathbf{r}$  is a parameter.  $\hat{\rho}(\mathbf{r})$  may be expressed in the framework of second quantization (see Appendix C):

$$\hat{\rho}(\mathbf{r}) = \sum_{pq} d_{pq} a_p^+ a_q, \quad (\text{D.2})$$

$$d_{pq} = \langle p | \delta(\mathbf{r} - \hat{\mathbf{f}}) | q \rangle = \sum_s \varphi_p^*(\mathbf{r}, s) \varphi_q(\mathbf{r}, s), \quad (\text{D.3})$$

$$\hat{\rho}(\mathbf{r}) = \sum_s a^+(\mathbf{r}, s) a(\mathbf{r}, s). \quad (\text{D.4})$$

The expectation value of this operator in an  $N$ -body state  $|\Psi\rangle$  is (see

### Appendix C

$$\langle \Psi | \hat{\rho}(\mathbf{r}) | \Psi \rangle = \sum_s \langle \Psi | a^+(\mathbf{r}, s) a(\mathbf{r}, s) | \Psi \rangle$$

$$= N \sum_{s_2, \dots, s_N} \int d^3 r_2 \dots d^3 r_N |\Psi(\mathbf{r}, s, \mathbf{r}_2, s_2, \dots, \mathbf{r}_N, s_N)|^2 = \rho(\mathbf{r}), \quad (\text{D.6})$$

which expresses the fact that the expectation value of  $\hat{\rho}(\mathbf{r})$  is just the average particle density  $\rho(\mathbf{r})$  at the point  $\mathbf{r}$  in this state. Integrating (D.6) over the whole space gives the particle number  $N$  of the system.

Equation (D.6) can also be interpreted as the diagonal element of an operator  $\hat{\rho}_\Psi$  in the coordinate space representation, which is called the *density matrix*. In general, it is defined as

$$\langle \mathbf{r}, s | \hat{\rho}_\Psi | \mathbf{r}', s' \rangle := \rho(\mathbf{r}s; \mathbf{r}'s') = \langle \Psi | a^+(\mathbf{r}', s') a(\mathbf{r}, s) | \Psi \rangle. \quad (\text{D.7})$$

From Eq. (C.26) we get

$$\begin{aligned} \rho(\mathbf{r}, s; \mathbf{r}', s') &= \sum_{pq} \varphi_p(\mathbf{r}, s) \rho_{pq} \varphi_q^*(\mathbf{r}', s') \\ &= \sum_{pq} \langle \mathbf{r}, s | p \rangle \rho_{pq} \langle q | \mathbf{r}', s' \rangle, \end{aligned} \quad (\text{D.8})$$

where

$$\rho_{pq} = \langle \Psi | c_q^\dagger c_p | \Psi \rangle \quad (\text{D.9})$$

is the matrix element of the density operator  $\hat{\rho}_\Psi$  in an arbitrary basis and  $\hat{\rho}_\Psi$  has the form

$$\hat{\rho}_\Psi = \sum_{pq} |p\rangle \rho_{pq} \langle q|. \quad (\text{D.10})$$

It is a Hermitian single-particle operator. The matrix  $\rho$  can be diagonalized by a unitary transformation of the single-particle basis

$$(D^\dagger \rho D)_{ll'} = \rho_l \delta_{ll'}, \quad a_l^\dagger = \sum_i D_{il} c_i^\dagger, \quad (\text{D.11})$$

where

$$\rho_l = \langle \Psi | c_l^\dagger c_l | \Psi \rangle, \quad 0 < \rho_l \leq 1, \quad (\text{D.12})$$

is the probability that the level  $l$  is occupied in the wave function  $\Psi$ . Here we wrote  $\rho$  down in occupation number representation (see Appendix C) in the basis where  $\rho$  is diagonal. For the particle number we get

$$N = \sum_l \rho_l = \text{Tr } \rho = \sum_l \int \rho(\mathbf{r}, s; \mathbf{r}, s) d^3 r = \int \rho(\mathbf{r}) d^3 r \quad (\text{D.13})$$

and for any other single particle operator of the form (C.32) we get

$$\langle \Psi | \hat{F} | \Psi \rangle = \sum_{ll'} f_{ll'} \langle \Psi | c_l^\dagger c_{l'} | \Psi \rangle = \text{Tr}(f \cdot \rho). \quad (\text{D.14})$$

There are two important examples of single-particle densities, which we will treat in some detail.

### D.2 Densities of Slater Determinants

In the case of product wave functions we have the following *theorem*.

*A wave function  $\Psi(1\dots N)$  is a Slater determinant if and only if the corresponding density matrix  $\rho_\Psi$  (D.10) is a projector in the single-particle Hilbert space, that is,*

$$\hat{\rho}_\Psi^2 = \hat{\rho}_\Psi. \quad (\text{D.15})$$

*There is a one-to-one correspondence between  $\hat{\rho}_\Psi$  and  $|\Psi\rangle$  in this case (of course, only up to a phase factor in  $|\Psi\rangle$ ).*

To prove this theorem we start with a Slater determinant

$$|\Psi\rangle = a_1^+ \dots a_N^+ |-\rangle \quad (\text{D.16})$$

in some single-particle basis characterized by the operators  $a_i^+$ ,  $a_i$ . From (D.9) we see that  $\rho$  is diagonal in this basis, with

$$\rho_l = \begin{cases} 0 & \text{for } l > N \quad (\text{empty levels, particles}), \\ 1 & \text{for } l \leq N \quad (\text{occupied levels, holes}). \end{cases} \quad (\text{D.17})$$

$\hat{\rho}_\Psi$  (D.10) has the form

$$\hat{\rho}_\Psi = \sum_{i=1}^N |i\rangle \langle i|. \quad (\text{D.18})$$

This is a projector onto the space of occupied states with the property (D.15).

On the other hand, we can start with a density matrix  $\rho$  with the property (D.15). It can be diagonalized [see Eq. (D.11)] and the eigenvalues  $\rho_l$  have the property

$$\rho_l^2 = \rho_l, \quad (\text{D.19})$$

that is, they are either 0 or 1. Constructing a Slater determinant from the single-particle wave functions with  $\rho_l = 1$  gives us the corresponding wave function  $\Psi$ . These single-particle wave functions  $\varphi_i$  are not uniquely determined by the diagonalization of  $\rho$ . Any unitary transformation among the occupied levels leaves  $\rho$  invariant. As we see from (D.16), however, such a unitary transformation multiplies the wave function  $|\Psi\rangle$  only by the determinant of this transformation, which is a phase.

This shows that there is a one-to-one correspondence between  $\rho$  and  $|\Psi\rangle$  in the case of Slater determinants. In particular, we can use Wick's theorem (C.52) and express the expectation value  $\langle \Psi | \hat{O} | \Psi \rangle$  of an arbitrary operator  $\hat{O}$  by the single-particle density  $\rho$ .

We next prove a *theorem due to Baranger and Veneroni* [BV 78, RS 77b], which states that any single-particle density matrix  $\rho$  that belongs to a Slater determinant ( $\rho^2 = \rho$ ) can be decomposed in the following way.

$$\rho = e^{i\chi} \rho_0 e^{-i\chi}, \quad (\text{D.20})$$

where  $\chi$  and  $\rho_0$  are Hermitian matrices that are even under time reversal. This decomposition is unique if we require

- (i) that  $\chi$  has only  $ph$  and  $hp$  matrix elements in the basis in which  $\rho_0$  is diagonal:

$$\rho_0 \chi \rho_0 = \sigma_0 \chi \sigma_0 = 0 \quad (\text{D.21})$$

- (ii) that the eigenvalues  $\chi_\mu$  of the matrix  $\chi$  have the property

$$-\frac{\pi}{4} \leq \chi_\mu < \frac{\pi}{4}. \quad (\text{D.22})$$

To prove this and to establish the uniqueness of the decomposition (D.20) we use the operator

$$\tau = 2\rho - 1 \quad \text{with} \quad \tau^2 = 1. \quad (\text{D.23})$$

The product, with its time reserved operator  $\tau_T = T\tau T^+$ , is unitary and is therefore of the form

$$\tau\tau_T = e^{4i\chi}, \quad (\text{D.24})$$

where the Hermitian operator  $\chi$  is uniquely defined by the condition (D.22). By inversion, time reversal, and Hermitian conjugation,

$$\tau_T \tau = e^{-4i\chi} = e^{-4ix} = e^{-4ix^*}, \quad (\text{D.25})$$

we see that  $\chi$  is time-reversal invariant and Hermitian. Let  $|\mu\rangle$  be a set of eigenstates of  $\tau\tau_T$  with eigenvalue  $\mu = e^{4i\chi_0}$ , then  $T|\mu\rangle$  is another eigenvector with the same eigenvalue  $\mu$  and  $\tau|T|\mu\rangle$  is an eigenvector with eigenvalue  $\mu^*$ . This implies

$$(\chi\tau + \tau\chi)|\mu\rangle = (-\chi_\mu + \chi_\mu)\tau|\mu\rangle = 0, \quad (\text{D.26})$$

and thus

$$\chi\tau + \tau\chi = 0. \quad (\text{D.27})$$

This means, in particular, that for an arbitrary real number  $\alpha$ ,

$$e^{i\alpha\chi}\tau = \tau e^{-i\alpha\chi} \quad (\text{D.28})$$

and

$$\tau_0 := e^{-2i\chi_T} = \tau e^{2ix} = \tau e^{-2ix}\tau_T = e^{2i\chi_T}\tau_T = \tau_T e^{-2ix}.$$

$\tau_0$  is therefore Hermitian and time even. The same holds for

$$\rho_0 := \frac{1}{2}(\tau_0 + 1). \quad (\text{D.29})$$

Using Eq. (D.28) again gives

$$\chi\rho_0 + \rho_0\chi = \chi, \quad (\text{D.30})$$

which is equivalent to Eq. (D.21).

Q.E.D.

In the following, we give some rules for calculating with single-particle densities  $\rho$  of Slater determinants ( $\rho^2 = \rho$ ,  $\sigma = 1 - \rho$ ). An arbitrary matrix  $A$

has the following  $pp$ ,  $ph$ ,  $hp$ , and  $hh$  parts in a basis in which  $\rho$  is diagonal:

$$A^{pp} := \sigma A \sigma; \quad A^{hh} = \rho A \rho; \quad A^{ph} = \sigma A \rho; \quad A^{hp} = \rho A \sigma. \quad (\text{D.31})$$

The three statements

$$A = A\rho + \rho A \Leftrightarrow A = \sigma A + A\sigma \Leftrightarrow A^{pp} = A^{hh} = 0 \quad (\text{D.32})$$

are equivalent. If two matrices  $A$  and  $B$  obey the relation  $B = [A, \rho]$  it follows:

$$B^{pp} = B^{hh} = 0; \quad B^{ph} = A^{ph}; \quad B^{hp} = -A^{hp}. \quad (\text{D.32})$$

If, in addition,

$$A^{pp} = A^{hh} = 0$$

we can write

$$A = [B, \rho]. \quad (\text{D.33})$$

For Hermitian matrices  $A, B$  with vanishing  $pp$  and  $hh$  matrix elements, we often define vectors

$$\begin{pmatrix} A \\ A^* \end{pmatrix} = \begin{pmatrix} A_{mi} \\ A_{mi}^* \end{pmatrix}, \quad (\text{D.34})$$

and find the relations

$$(A^* A) \begin{pmatrix} B \\ B^* \end{pmatrix} = \sum_{mi} A_{mi}^* B_{mi} + A_{mi} B_{mi}^* = \text{Tr}(A \cdot B) \quad (\text{D.35})$$

$$(A^* A) \begin{pmatrix} B \\ -B^* \end{pmatrix} = \text{Tr}(A \cdot [B, \rho]).$$

Next we investigate some properties of a family of Slater determinants  $|\Phi(q)\rangle$  depending on some parameter  $q$  (e.g. the deformation) with the densities  $\rho(q)$ . Starting from one wave function in this family,  $|\Phi(q_0)\rangle$ , we can represent the other wave functions by a Hermitian single-particle operator  $\hat{P}$ , which has only  $ph$  and  $hp$  matrix elements with respect to  $|\Phi(q_0)\rangle$ , as follows [see Eq. (E.40)].

$$|\Phi(q + q_0)\rangle = e^{-(i/\hbar)q\hat{P}} |\Phi(q_0)\rangle, \quad (\text{D.36})$$

$$\hat{P} = P^0 + \sum_{mi} P_{mi} a_m^+ a_i + P_{mi}^* a_i^+ a_m. \quad (\text{D.37})$$

The constant  $P^0$  eventually determines a phase. The operator  $\hat{P}$  generally depends on  $q$  and  $q_0$ , and only in the limit  $q \rightarrow 0$  does it become independent of  $q$  and we then gain

$$\hat{P} |\Phi(q)\rangle = i\hbar \frac{\partial}{\partial q} |\Phi(q)\rangle. \quad (\text{D.38})$$

For the density we have

$$\rho(q_0 + q) = e^{-(i/\hbar)qP} \rho(q_0) e^{(i/\hbar)qP} \quad (\text{D.39})$$