Функционал плотности энергии и приближение среднего поля

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1. ***Применение оболочечной модели к проблеме многих тел***
2. ***Метод Хартри-Фока***
3. ***Применение метода Хартри–Фока на примере модели Липкина***
4. ***Построение эффективного нуклон-нуклонного взаимодействия***
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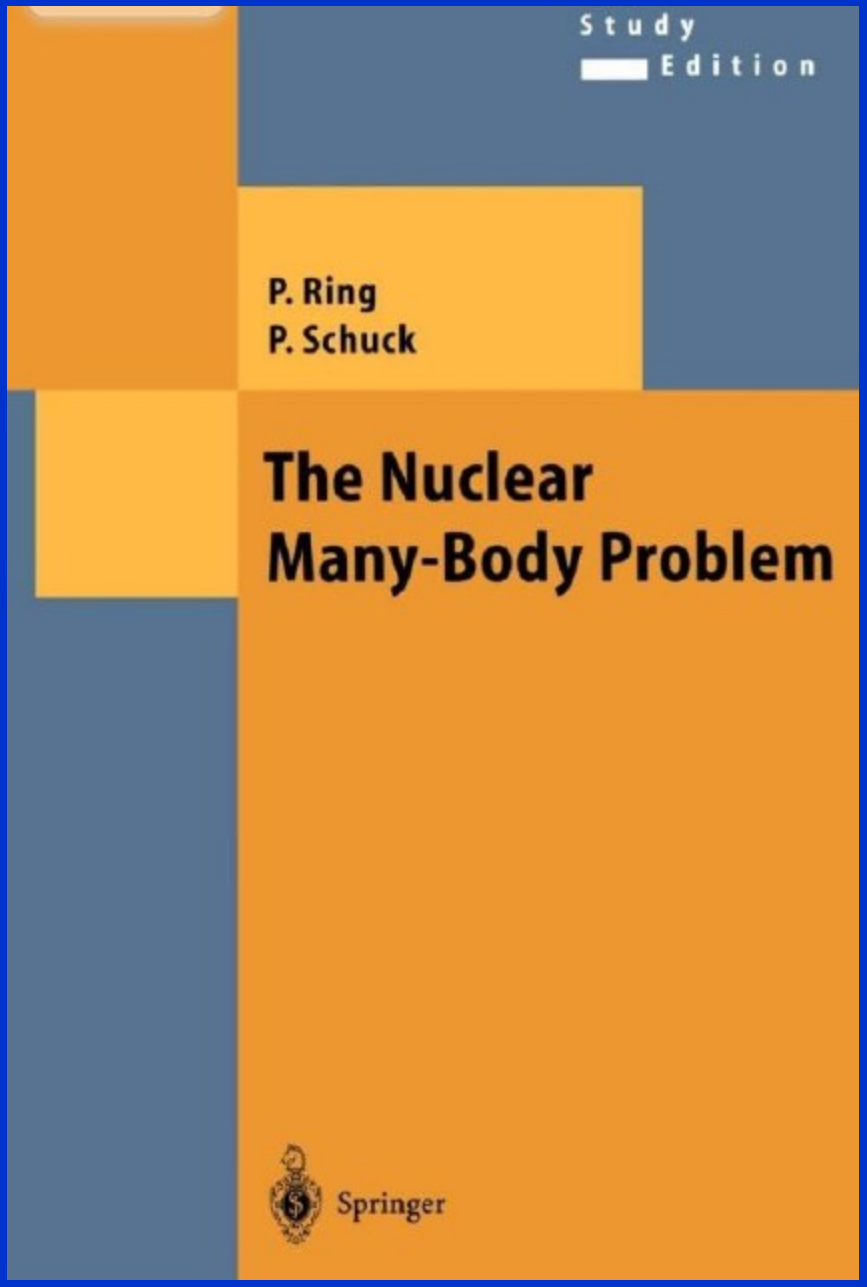
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Применение оболочечной модели к проблеме многих тел

2.5 The Shell Model Approach to the Many-Body Problem

The single-particle model takes into account the individual nucleons. It therefore provides a microscopic description of the nucleus. This is certainly only an approximation of the exact many-body problem. We will see, however, in the following, that the shell model can be used as a basis for more elaborate many-body theories, so before we talk about further details of the model, we want to discuss some general properites of the single particle model.

The microscopic theory of the nucleus is usually based on the following three properties.

(i) The nucleus is a quantum mechanical many-body system.
(ii) The velocities in the nucleus are small enough so that one can neglect relativistic effects $[(v/c)^2 \sim 1/10]$.
(iii) The interaction between the nucleons has a two-body character.

A full microscopic theory of the nucleus would then be given by the solution of the many-body Schrödinger equation

$$H\Psi = \left\{ \sum_{i=1}^{A} -\frac{\hbar^2}{2m}\Delta_i + \sum_{i<j}^{A} v(i,j) \right\} \Psi(1,\ldots,A) = E\Psi(1,\ldots,A), \quad (2.19)$$

where i represents all coordinates of the ith nucleon, for instance,

$$(i) = (\mathbf{r}_i, s_i, t_i), \quad (2.20)$$

where t_i will be $\frac{1}{2}$ for neutrons and $-\frac{1}{2}$ for protons. With the assumption of the nuclear shell model, the above equation reduces to the much simpler equation

$$H_0\Psi = \left\{ \sum_{i=1}^{A} h_i \right\} \Psi = \sum_{i=1}^{A} \left\{ -\frac{\hbar^2}{2m}\Delta_i + V(i) \right\} \Psi = E\Psi. \quad (2.21)$$

The solutions Ψ of Eq. (2.21) are anti-symmetrized products of single-particle functions, which are eigenfunctions to the single-particle Hamilto-

nian h_i:

$$h_i\phi_k(i)=\epsilon_k\phi_k(i). \tag{2.22}$$

The functions ϕ_k provide an orthogonal basis for an occupation number representation within the framework of second quantization (see Appendix C). To each level k corresponds a pair of creation and annihilation operators a_k^+, a_k which create or annihilate particles with wave function ϕ_k. Since nucleons are Fermions, each level can be occupied only once, and the operators a_k, a_k^+ obey Fermi commutation relations (C. 23).

The shell model Hamiltonian H_0 has the form

$$H_0=\sum \epsilon_k a_k^+ a_k.$$

Using the bare vacuum $|-\rangle$ its eigenfunctions can be represented as

$$|\Phi_{k_1\ldots k_A}\rangle=a_{k_1}^+\ldots a_{k_A}^+|-\rangle.$$

They are Slater determinants

$$\Phi_{k_1\ldots k_A}(1,\ldots,A)=\begin{vmatrix}\phi_{k_1}(1) & \cdots & \phi_{k_1}(A)\\ \vdots & & \vdots\\ \phi_{k_A}(1) & & \phi_{k_A}(A)\end{vmatrix} \tag{2.23}$$

with eigenvalues

$$E_{k_1\ldots k_A}=\epsilon_{k_1}+\cdots+\epsilon_{k_A}. \tag{2.24}$$

In the ground state the levels are filled successively according to their energy (see Fig. 2.6)

$$|\Phi_0\rangle=a_1^+\ldots a_A^+|-\rangle. \tag{2.25}$$

Thus we have for closed shells the following unique prescription for the construction of the A particle ground state as well as for the A particle excitation spectrum: Starting with the $(1s_{1/2})$ level, one has to occupy each level $|nsljm\rangle$ with just one particle until all A particles are used up. We thus obtain an A nucleon ground state where all different quantum states are occupied with just one particle up to the Fermi level (the highest occupied level); above the Fermi level all levels are unoccupied.

The independent particle picture of the nucleus is different from that in an atom in the sense that in a nucleus there are *two* different kinds of particles, the proton and the neutron, whereas in an atom there is only the

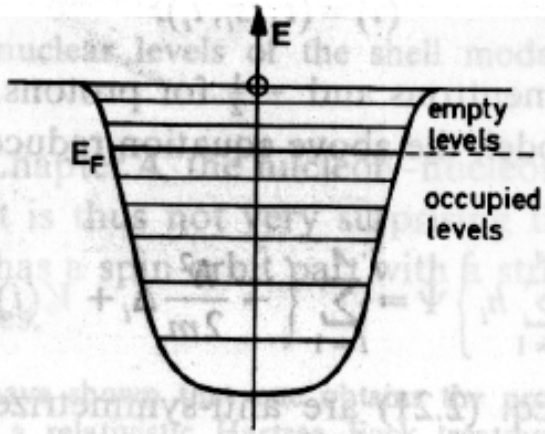
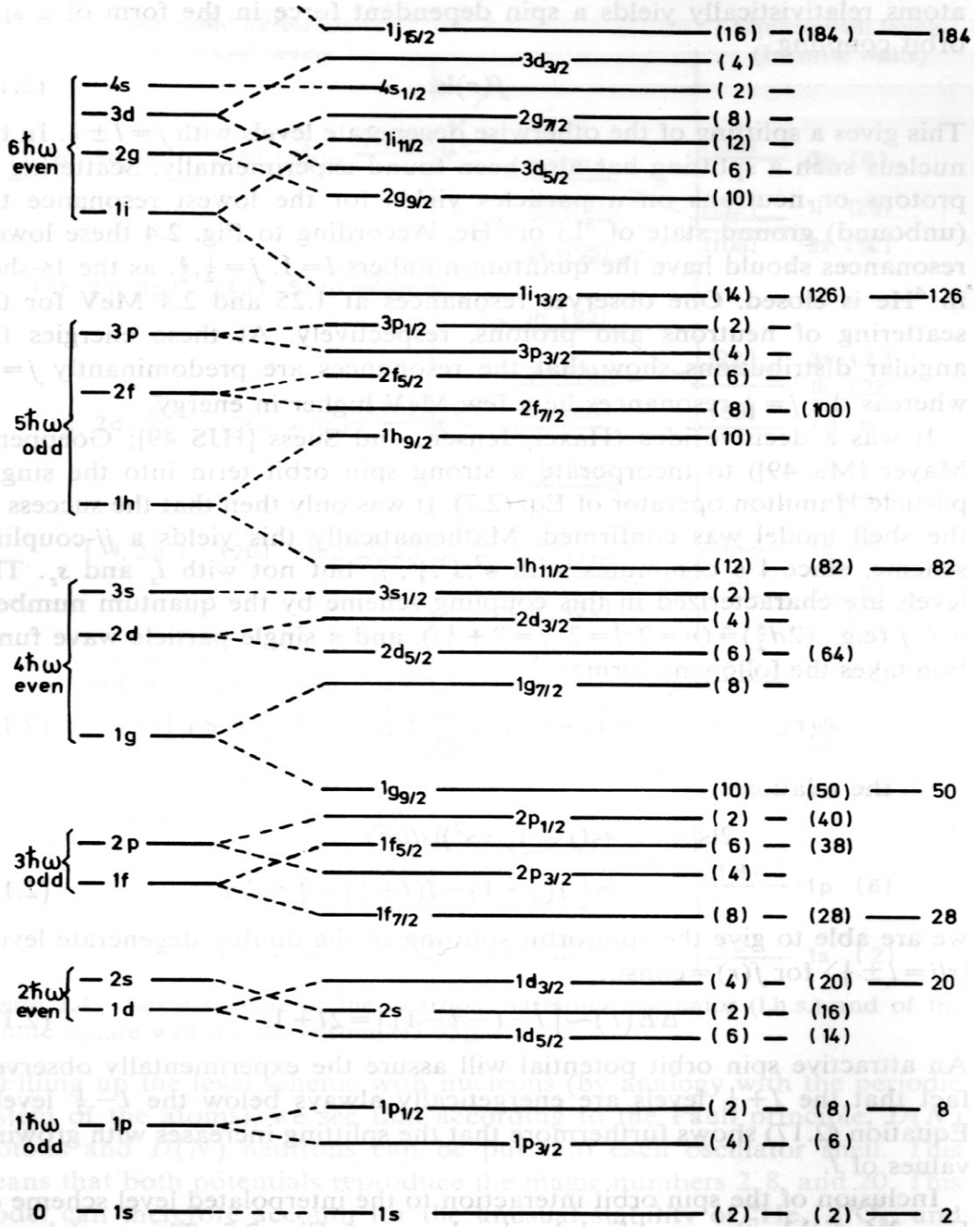


Figure 2.6. Shell model potential and Fermi level.


1j15/2 (16) (184) 184
3d3/2 (4)
4s1/2 (2)
2g7/2 (8)
1i11/2 (12)
3d5/2 (6)
2g9/2 (10)
1i13/2 (14) (126) 126
3p1/2 (2)
3p3/2 (4)
2f5/2 (6)
2f7/2 (8) (100)
1h9/2 (10)
1h11/2 (12) (82) 82
3s1/2 (2)
2d3/2 (4)
2d5/2 (6) (64)
1g7/2 (8)
1g9/2 (10) (50) 50
2p1/2 (2) (40)
1f5/2 (6) (38)
2p3/2 (4)
1f7/2 (8) (28) 28
1d3/2 (4) (20) 20
2s (2) (16)
1d5/2 (6) (14)
1p1/2 (2) (8) 8
1p3/2 (4) (6)
1s (2) (2) 2
6ħω even
4s
3d
2g
1i
5ħω odd
3p
2f
1h
4ħω even
3s
2d
1g
3ħω odd
2p
1f
2ħω even
2s
1d
1ħω odd
1p
0
1s

electron. Protons and neutrons feel different average potentials for two reasons:

(i) Protons also interact via the *Coulomb force*. One therefore usually adds the potential of a homogeneously charged sphere

$$V_C(\mathbf{r}) = \begin{cases} \dfrac{Ze^2}{R}\dfrac{1}{2}\left(3-\left(\dfrac{r}{R}\right)^2\right) & r \leqslant R, \\ \dfrac{Ze^2}{r} & r > R. \end{cases} \tag{2.26}$$

Sometimes (see Sec. 2.8), this feature is approximated by using different potential parameters for protons and neutrons.

(ii) The *symmetry energy* [see Eq. (1.4)] favors a configuration with an equal number of protons and neutrons. Because of the Coulomb repulsion for heavier nuclei, one has a neutron excess: If, in the nucleus, we replace a neutron by a proton, we gain symmetry energy and lose Coulomb energy. Since the Coulomb energy is already taken into account by Eq. (2.26), there must be an additional difference between the single-particle potential for protons and neutrons, which is caused by the symmetry energy. The *nuclear* part of the proton potential is therefore deeper (see Fig. 2.7, dashed line).

These two effects go in opposite directions, but they do not cancel. In the end, the Fermi surfaces for protons and neutrons must be equal, otherwise protons would turn into neutrons by β-decay or vice versa, whichever is energetically favored.

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In $N \neq Z$ nuclei, energy levels with the same quantum numbers for protons and neutrons are therefore shifted with respect to one another by an amount Δ_ϵ resulting from a positive contribution Δ_C from the Coulomb force and a negative contribution $-\Delta_S$ from the symmetry energy

$$\epsilon_{nlj}^{(p)} - \epsilon_{nlj}^{(n)} = \Delta_\epsilon = \Delta_C - \Delta_S. \tag{2.27}$$

In heavy nuclei, this difference is such that the protons and neutrons at the Fermi surface belong to different major shells.

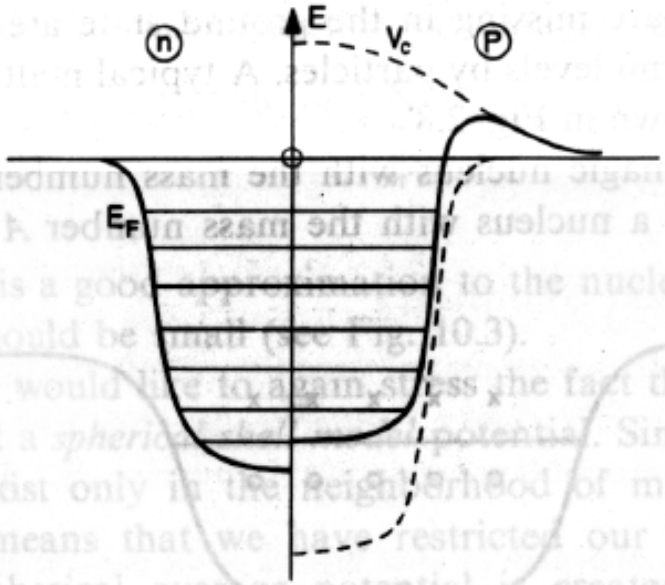

Figure 2.7. Comparison of the shell model potential for neutrons and protons in a nucleus with neutron excess.

The Fermi level coincides in this case with the $1d_{3/2}$ level (see Fig. 2.5).

If we use the indices i, j for the levels below the Fermi surface ($\epsilon_i \leqslant \epsilon_F$), and the indices m, n for the levels above the Fermi surface ($\epsilon_n > \epsilon_F$), the lowest excitations in the shell model are then *ph* excitations of the form

$$|\Phi_{mi}\rangle := a_m^+ a_i |\Phi_0\rangle = \pm a_m^+ a_1^+ \ldots a_{i-1}^+ a_{i+1}^+ \ldots a_A^+ |-\rangle \qquad (2.28)$$

with excitation energy $\epsilon_{mi} = \epsilon_m - \epsilon_i$.

In fact one has observed such states in magic nulcei. They are, however, not the lowest states. As we have already seen in Chapter 1, there are low-lying collective states which cannot be explained in the independent particle model.

The Slater determinants (2.23) form a *complete set* of states for the A nulceon system [Lö 55]. Each state of the system is characterized by the distribution of the nucleons among the levels of the single particle potential, that is, by the "occupation numbers" of the levels. It is usual to classify all excited states by taking the ground state as a reference state. The nucleons that are missing in the ground state are denoted by holes, those above the Fermi levels by particles. A typical multiparticle–multihole configuration is shown in Fig. 2.8

Starting from a magic nucleus with the mass number A, we can add a particle and obtain a nucleus with the mass number $A+1$. If we put the

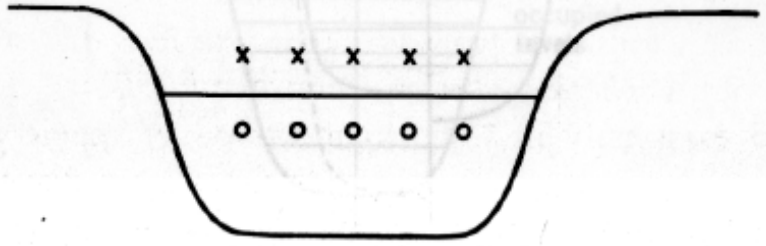

Figure 2.8. Schematic representation of a typical five-particle (crosses), five-hole (open circles) state.

Метод Хартри-Фока

5.2 The General Variational Principle

We first want to show that the exact Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \tag{5.2}$$

is equivalent to the variational equation

$$\delta E[\Psi] = 0, \tag{5.3}$$

with

$$E[\Psi] = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} . \tag{5.4}$$

Together with Eq. (5.5), we find

$$\langle \delta\Psi | H - E | \Psi \rangle = 0 \tag{5.7}$$

and the complex conjugate equation. Since $|\delta\Psi\rangle$ is arbitrary, Eq. (5.7) is equivalent to the eigenvalue problem (5.2).

The approximation of such variational methods consists of the fact that $|\Psi\rangle$ is usually restricted to a set of mathematically simple trial wave functions. As soon as the true function is not in this set, the minimal solution is no longer the exact eigenfunction, but only an approximation. The variational method is especially well suited for determining the ground state, since for any trial wave function $|\Psi\rangle$ we can show that

$$E[\Psi] \geqslant E_0, \tag{5.8}$$

and thus E_0 will always be the lower bound of a variational calculation. To prove this, we develop the trial wave function in terms of the exact eigenfunctions of the Hamiltonian:

$$|\Psi\rangle = \sum_{n=0}^{\infty} a_n |\Psi_n\rangle \tag{5.9}$$

with

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle. \tag{5.10}$$

This yields

$$E[\Psi]=\frac{\sum_{nn'} a_n^* a_n E_n \delta_{nn'}}{\sum_n |a_n|^2} \geqslant \frac{\sum_n |a_n|^2 E_0}{\sum_n |a_n|^2} = E_0, \tag{5.11}$$

which is precisely Eq. (5.8). In cases where the ground state energy is not degenerate, the equality sign in (5.11) is valid, if and only if all the coefficients a_n with $n \neq 0$ vanish, that is, $|\Psi\rangle$ is proportional to $|\Psi_0\rangle$. If we are interested in the first excited state, we then have to carry out the variation within the subspace entirely orthogonal to $|\Psi_0\rangle$, that is, over all the wave functions $|\Psi\rangle$ with $a_0=0$. Within this subspace $|\Psi_1\rangle$ has the minimal expectation value of H. To find $|\Psi_1\rangle$, we must carry out the variation with the subsidiary condition $\langle\Psi_1|\Psi_0\rangle=0$. In principle we can continue and calculate the whole spectrum using this method.

In practice, however, we do not know $|\Psi_0\rangle$ exactly. From a variation in a restricted subset of the Hilbert space, we find only an approximation $|\Phi_0\rangle$. For the calculation of an approximation $|\Phi_1\rangle$ to the first excited state $|\Psi_1\rangle$, we have to solve the variational equation (5.3) with the supplementary condition that $|\Phi_1\rangle$ is orthogonal to $|\Phi_0\rangle$:

$$\langle\Phi_1|\Phi_0\rangle=0. \tag{5.12}$$

For the second excited state, we must have two supplementary conditions, namely:

$$\langle \Phi_2 | \Phi_1 \rangle = 0; \quad \text{and} \quad \langle \Phi_2 | \Phi_0 \rangle = 0. \tag{5.13}$$

These supplementary conditions are coupled to the problem via Lagrange parameters. We thus see that for higher excited states this method quickly gets rather complicated, therefore it has been applied mainly for the calculation of the ground state. Sometimes, however, these conditions are simply fulfilled because of symmetry properties, as, for example, is the case for states with different angular momentum quantum numbers. We will see in Chapter 7 how to calculate a whole rotational band where the determination of each level is no more complicated than that of the ground state.

So far we have shown that for a certain trial wave function, the ground state energy is always larger than or equal to the exact ground state energy and corresponds to an extremum. In actual calculations, we have to make sure that this extremum actually corresponds to a *minimum*, that is, we must calculate the second derivative of the energy functional, for example, with respect to certain parameters. In the case of the Hartree–Fock or Hartree–Fock–Bogoliubov theory, we will come back to this point (in Chapter 7).

In order to decide which of two variational approaches (i.e., two sets of trial wave functions) is the better one, we have two criteria:

(i) If one set of the trial wave functions is a subset of the other, the larger set is usually the better one, because it contains the first's set minimum.

(ii) Since the exact E_0 is a lower bound, we may hope that out of two trial wave functions, the one for which the corresponding energy is closest to E_0 is better.

Both criteria are, however, not exact statements. Pathological examples can be found which contradict them.

We finish this section with the remark that the variation principle is only valid in this form for a linear eigenvalue problem of the type (5.2). In cases where the Hamiltonian itself depends on the wave function we want to determine, we have to be very careful in applying this principle.

5.3 The Derivation of the Hartree–Fock Equation

5.3.1 The Choice of the Set of Trial Wave Functions

Using the fact that the shell model has provided a suitable approximation for the qualitative explanation of many nuclear properties, we shall assume that there is an average single-particle potential (later to be called the *Hartree–Fock potential*)

$$H^{\mathrm{HF}} = \sum_{i=1}^{A} h(i) \tag{5.14}$$

whose eigenfunction having the lowest eigenvalue E_0^{HF} is an approximation to the exact ground state function. This eigenfunction $\Phi(1 \ldots A)$ is, as we have seen in Chapter 2, a *Slater determinant*

$$|\mathrm{HF}\rangle = |\Phi(1 \ldots A)\rangle = \prod_{i=1}^{A} a_i^+ |-\rangle \tag{5.15}$$

in which the Fermion operators a_k^+, a_k correspond to the single-particle wave functions φ_k, which are themselves eigenfunctions of the single-particle Hamiltonian h, viz:

$$h(i)\varphi_k(i) = \epsilon_k \varphi_k(i), \qquad i = \{\mathbf{r}_i, s_i, t_i\}. \tag{5.16}$$

As we have seen in Section 2.5, we obtain the lowest eigenvalue of H^{HF} if one occupies the A lowest levels in the state $|\mathrm{HF}\rangle$ (Eq. 5.15). In the following, we will characterize the occupied levels in $|\mathrm{HF}\rangle$ by the letters i, j (hole states) and the empty levels by m, n (particle states). If we do not distinguish, we use the letters k, l, p, q.

The wave functions $\varphi_k(\mathbf{r}, s, t)$ are a coordinate space representation of the eigenstates $|k\rangle$ of the single-particle Hamiltonian h. Very often, we work in a configuration space based on some arbitrary complete and orthogonal set of single-particle wave functions $\{\chi_l\}$ (an example is the set of spherical harmonic oscillator wave functions). The function φ_k can be

expanded on this basis:

$$\varphi_k = \sum_l D_{lk} \chi_l . \tag{5.17}$$

If, for each wave function χ_l, we define corresponding fermion creation and annihilation operators c_l^+, c_l (see Section C.1), we can similarly express the operators a_k^+ by the operators c_l^+:

$$a_k^+ = \sum_l D_{lk} c_l^+ . \tag{5.18}$$

Since both sets $\{\varphi_k\}$ and $\{\chi_l\}$ are complete and orthogonal, the transformation D has to be unitary:

$$D^+ D = D D^+ = 1. \tag{5.19}$$

This fact also guarantees that the operators (a_k^+, a_k) and (c_l^+, c_l) both obey separate Fermi commutation relations.

As discussed in Section D.2, there is no one-to-one correspondence between a Slater determinant Φ of the form (5.15) and the set of single-particle states φ_k. Any unitary transformation which does not mix particle and hole states leaves Φ unchanged (at least up to an unimportant phase).

It is therefore more convenient to represent a Slater determinant $|\Phi\rangle$ by its single-particle density matrix (D.9):

$$\rho_{ll'} = \langle \Phi | c_{l'}^{+} c_l | \Phi \rangle. \tag{5.20}$$

From Eqs. (5.18) and (5.19), we get

$$\rho_{ll'} = \sum_{kk'} D_{lk} D_{l'k'}^{*} \langle \Phi | a_{k'}^{+} a_k | \Phi \rangle = \sum_{i=1}^{A} D_{li} D_{l'i}^{*} \tag{5.21}$$

because ρ is diagonal in the basis a_k^{+}, a_k with the eigenvalues (occupation numbers) 1 for $i \leqslant A$ (holes) and 0 for $i > A$ (particles). The trace of ρ is equal to the particle number.

As we show in Appendix D.2, there is a one-to-one correspondence between the Slater determinant Φ and its single-particle density ρ. Single-particle densities ρ of Slater determinants are characterized by the fact that they have only eigenvalues 0 or 1, that is,

$$\rho^2 = \rho. \tag{5.22}$$

ρ is therefore a projector in the space of single-particle wave functions onto the subspace spanned by the hole states φ_i.

In the same way, we can define a projector σ

$$\sigma = 1 - \rho \tag{5.23}$$

onto the subspace spanned by the particle states φ_m.

The *Hartree–Fock method* [Ha 28, Fo 30] is now defined in the following way. We use the set of Slater determinants $\{\Phi\}$ of the form (5.15) consisting of A arbitrary but orthogonal single-particle wave functions φ_i as trial wave functions and minimize the energy within this set. An equivalent statement would be that we use the set of all wave functions

$\{\Phi\}$ whose single particle density (5.20) has the property $\rho^2=\rho$ and $\mathrm{Tr}\,\rho=A$.

As we will see in the following sections, this variation will give us the possibility of determining the single-particle operator H^{HF}.

5.3.2 The Hartree–Fock Energy

Before we are able to carry out the variation which allows us to determine the HF-wave function Φ, we have to calculate the HF-energy

$$E^{\mathrm{HF}}=\langle\Phi|H|\Phi\rangle. \tag{5.24}$$

We start with the many-body Hamiltonian H and represent it in second quantization by the basis operators c_l^+, c_l (see Section C.1):

$$H=\sum_{l_1 l_2} t_{l_1 l_2} c_{l_1}^+ c_{l_2}+\frac{1}{4}\sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2, l_3 l_4} c_{l_1}^+ c_{l_2}^+ c_{l_4} c_{l_3}, \tag{5.25}$$

where

$$\bar{v}_{l_1 l_2, l_3 l_4}=v_{l_1 l_2 l_3 l_4}-v_{l_1 l_2 l_4 l_3}. \tag{5.26}$$

Wick's theorem (Sec. C.4) allows us to calculate the energy (5.24) as a functional of the single-particle density

$$E^{\mathrm{HF}}[\rho] = \sum_{l_1 l_2} t_{l_1 l_2} \langle \Phi | c_{l_1}^+ c_{l_2} | \Phi \rangle + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} \langle \Phi | c_{l_1}^+ c_{l_2}^+ c_{l_4} c_{l_3} | \Phi \rangle$$

$$= \sum_{l_1 l_2} t_{l_1 l_2} \rho_{l_2 l_1} + \frac{1}{2} \sum_{l_1 l_2 l_3 l_4} \rho_{l_3 l_1} \bar{v}_{l_1 l_2 l_3 l_4} \rho_{l_4 l_2} \tag{5.27}$$

$$= \mathrm{Tr}\,(t\rho) + \frac{1}{2} \mathrm{Tr}_1 \mathrm{Tr}_1 (\rho \bar{v} \rho), \tag{5.28}$$

where $\mathrm{Tr}_1 \mathrm{Tr}_1 \ldots$ is an obvious shorthand notation. Eq. (5.28) does not depend on the basis. We can therefore use it to give an expression for the HF-energy in the HF-basis $\{\varphi_k\}$ in which ρ is diagonal with the eigenvalues 0 and 1

$$E^{\mathrm{HF}} = \sum_{i=1}^{A} t_{ii} + \frac{1}{2} \sum_{i,j=1}^{A} \bar{v}_{ij,ij}. \tag{5.29}$$

5.3.3 Variation of the Energy

To determine the HF-basis, we have to minimize the energy (5.28) for all product wave functions $|\Phi\rangle$ or for all densities ρ with the property $\rho^2 = \rho$. Since a small variation $\rho + \delta\rho$ has to be a projector again, we get

$$(\rho + \delta\rho)^2 = \rho + \delta\rho$$

or, up to linear terms in $\delta\rho$,

$$\delta\rho = \rho\,\delta\rho + \delta\rho\,\rho.$$

In the HF-basis, where ρ is diagonal, this means that the particle–particle (*pp*) and hole–hole (*hh*) matrix elements of $\delta\rho$ have to vanish, that is,

$$\rho\,\delta\rho\,\rho=\sigma\,\delta\rho\,\sigma=0. \tag{5.30}$$

To make sure that we stay within the set of Slater determinants, therefore, we can only allow for variations $\delta\rho_{mi}$ and $\delta\rho_{im}$ of the *ph* and *hp* matrix elements of ρ in the HF-basis.

The variation of the energy (5.27) is then given by

$$\delta E=E[\rho+\delta\rho]-E[\rho]=\sum_{kk'}h_{kk'}\delta\rho_{k'k}=\sum_{mi}h_{mi}\delta\rho_{im}+c.c., \tag{5.31}$$

where the Hermitian matrix h is defined as

$$h_{kk'}=\frac{\partial E^{\mathrm{HF}}[\rho]}{\partial\rho_{k'k}}. \tag{5.32}$$

From Eq. (5.27), we obtain

$$h=t+\Gamma \tag{5.33}$$

with the *self-consistent field*

$$\Gamma_{kk'}=\sum_{ll'}\bar{v}_{kl'k'l}\rho_{ll'}. \tag{5.34}$$

Since arbitrary values of $\delta\rho_{mi}$ are allowed, we see from Eq. (5.31), that the condition $\delta E = 0$ for the HF-solution means that the *ph* matrix elements of h have to vanish,

$$h_{mi} = t_{mi} + \sum_{j=1}^{A} \bar{v}_{mjij} = 0 \qquad (\text{for } i \leqslant A, m > A), \tag{5.35}$$

in the basis where ρ is diagonal, that is, h does not mix particle and hole states of ρ and Eq. (5.35) is equivalent to

$$[h, \rho] = [t + \Gamma[\rho], \rho] = 0. \tag{5.36}$$

This is a nonlinear equation, and not easy to solve. It also states that h and ρ can be diagonalized simultaneously. Since the basis in which ρ is diagonal is determined only up to unitary transformations among the occupied levels or among the empty levels, we use this freedom and require that h shall be diagonal. This defines the *Hartree–Fock basis* and converts (5.36) into an eigenvalue problem.

$$h_{kk'} = t_{kk'} + \sum_{i=1}^{A} \bar{v}_{kik'i} = \epsilon_k \delta_{kk'}. \tag{5.37}$$

Considering the fact that this basis is given by the transformation D (5.18), we obtain the set of *Hartree–Fock equations*

$$\sum_{l'} h_{ll'} D_{l'k} = \sum_{l'} \left(t_{ll'} + \sum_{i=1}^{A} \sum_{pp'} \bar{v}_{lp'l'p} D_{pi} D^{*}_{p'i} \right) D_{l'k} = \epsilon_k D_{lk}, \tag{5.38}$$

which represent a Hermitian eigenvalue problem. It is nonlinear because the matrix h depends on the density ρ, that is, on the solution of the

problem. The coefficients D_{lk} found by the solution of these equations determine the single-particle wave functions φ_k [Eq. (5.17)].

We have thus derived a single-particle Hamiltonian

$$H^{\mathrm{HF}} = \sum_{kk'} h_{kk'} a_k^+ a_{k'} = \sum_{kk'} (t+\Gamma)_{kk'} a_k^+ a_{k'}$$

$$= \sum_{kk'} \left(t_{kk'} + \sum_{j=1}^{A} \bar{v}_{kjk'j} \right) a_k^+ a_{k'} = \sum_k \epsilon_k a_k^+ a_k \tag{5.39}$$

with the properties required in Section (5.3.1): The Slater determinant $|\mathrm{HF}\rangle$, where the lowest A levels are occupied, corresponds to an energy E which is stationary against small variations of the wave function.

The single-particle Hamiltonian h contains, besides the kinetic energy t, a self-consistent field Γ (Eq. (5.34)), which depends on the density of the nucleus. It is a one-body field and averages over all two-body interactions. This point will become even clearer in the coordinate representation (Sec. 5.3.4). The energy expectation value of the HF-wave function $|\mathrm{HF}\rangle$ is given by Eqs. (5.29) and (5.37):

$$E_0^{\mathrm{HF}} = \sum_{i=1}^{A} \epsilon_i - \frac{1}{2} \sum_{ij=1}^{A} \bar{v}_{ijij}. \tag{5.40}$$

It is therefore not equal to the sum of single-particle energies [compare the discussion of this point in Sec. (2.8.6)].

5.3.4 The Hartree–Fock Equations in Coordinate Space

To give a better interpretation of the structure of Eq. (5.38), we write it down in the coordinate space. Assuming a local two-body potential which does not depend on spin or isospin, that is, a pure Wigner force (see Sec. 4.2), we find instead of Eq. (5.38):

$$-\frac{\hbar^2}{2m}\Delta\varphi_k(\mathbf{r})+\sum_{j=1}^{A}\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\cdot\varphi_j^*(\mathbf{r}')\{\varphi_j(\mathbf{r}')\varphi_k(\mathbf{r})-\varphi_j(\mathbf{r})\varphi_k(\mathbf{r}')\}$$
$$=\epsilon_k\varphi_k(\mathbf{r}). \tag{5.41}$$

Defining the local Hartree potential

$$\Gamma_H(\mathbf{r})=\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\sum_{j=1}^{A}|\varphi_j(\mathbf{r}')|^2=\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}') \tag{5.42}$$

and the nonlocal or exchange potential

$$\Gamma_{Ex}(\mathbf{r},\mathbf{r}')=-v(\mathbf{r},\mathbf{r}')\sum_{j=1}^{A}\varphi_j^*(\mathbf{r}')\varphi_j(\mathbf{r})=-v(\mathbf{r},\mathbf{r}')\rho(\mathbf{r},\mathbf{r}'), \tag{5.43}$$

we find that $\varphi_k(\mathbf{r})$ is the solution of a nonlocal Schrödinger equation

$$\left\{-\frac{\hbar^2}{2m}\Delta+\Gamma_H(\mathbf{r})\right\}\varphi_k(\mathbf{r})+\int d\mathbf{r}'\,\Gamma_{Ex}(\mathbf{r},\mathbf{r}')\varphi_k(\mathbf{r}')=\epsilon_k\varphi_k(\mathbf{r}). \tag{5.44}$$

Применение метода Хартри–Фока на примере модели Липкина

A. P. SEVERYUKHIN, M. BENDER, AND P.-H. HEENEN

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A. The model

Lipkin, Meshkov, and Glick introduced an exactly solvable model [8], usually called "Lipkin model" or "LMG model" in the literature, that has been widely used to test methods of approximation for the nuclear many-body problem.

The model consists of N fermions distributed in two N-fold degenerate shells separated by an energy ε. In their original paper, two different Hamiltonians were proposed. The one which is the most usually studied contains a monopole-monopole interaction and is given by

$$\hat{H} = \varepsilon \hat{J}_0 - \tfrac{1}{2} V (\hat{J}_+ \hat{J}_+ + \hat{J}_- \hat{J}_-), \tag{1}$$

where V is the interaction strength and $\hat{J}_0$, $\hat{J}_\pm$ are quasispin operators [8–10]

$$\hat{J}_0 = \frac{1}{2}\sum_{p=1}^{N}(\hat{c}^{\dagger}_{+p}\hat{c}_{+p} - \hat{c}^{\dagger}_{-p}\hat{c}_{-p}),$$

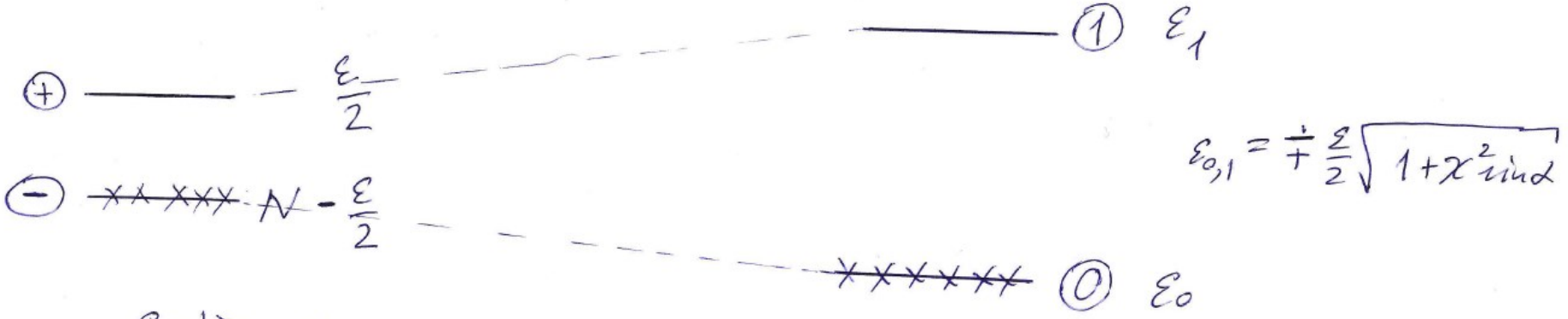
$$\hat{J}_+ = \sum_{p=1}^{N}\hat{c}^{\dagger}_{+p}\hat{c}_{-p}, \tag{2}$$

$$\hat{J}_- = \hat{J}^{\dagger}_+$$

with the algebra

$$[\hat{J}_+, \hat{J}_-] = 2\hat{J}_0, \qquad [\hat{J}_0, \hat{J}_\pm] = \pm\hat{J}_\pm. \tag{3}$$

The operators $\hat{c}^{\dagger}_{+p}$ and $\hat{c}^{\dagger}_{-p}$ create a particle in the upper or lower shells, respectively, where p labels the N degenerate levels within the shells. The operator $\hat{J}_0$ measures half of the difference between the number of particles in the upper and the lower levels.



$$\varepsilon_{0,1} = \frac{\varepsilon}{2}\sqrt{1+x^2 \sin\alpha}$$

$$c_{+p}|>=0 \qquad c^{+}_{-p}|>=0$$

$$a_{1p}|0>=0 \qquad a^{+}_{0p}|0>=0$$

$$\hat{H} = \varepsilon \hat{J}_0 - \frac{1}{2} V(\hat{J}_+ \hat{J}_+ + \hat{J}_- \hat{J}_-)$$

$$\hat{J}_0 = \frac{1}{2}\sum_{p=1}^{N}(\hat{c}^{+}_{+p}\hat{c}_{+p} - \hat{c}^{+}_{-p}\hat{c}_{-p})$$

$$\hat{J}_+ = \sum_{p=1}^{N}\hat{c}^{+}_{+p}\,\hat{c}_{-p}$$

$$\hat{J}_- = (\hat{J}_+)^{+}$$

B. Mean-field approximation

In mean-field, or Hartree-Fock (HF), approximation, the many-body wave function $|\alpha, \varphi\rangle$ is given by a Slater determinant

$$|\alpha, \varphi\rangle = \prod_{p=1}^{N} \hat{a}_{0p}^{\dagger} |-\rangle, \tag{4}$$

characterized by two real degrees of freedom α and φ, that will be specified below. The particle- and hole-creation operators of the corresponding HF single particle basis are given by a unitary transformation among the operators corresponding to the noninteracting basis [9,10]:

$$\begin{pmatrix} \hat{a}_{1p}^{\dagger} \\ \hat{a}_{0p}^{\dagger} \end{pmatrix} = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) e^{-i\varphi} \\ \sin(\alpha) e^{i\varphi} & \cos(\alpha) \end{pmatrix} \begin{pmatrix} \hat{c}_{+p}^{\dagger} \\ \hat{c}_{-p}^{\dagger} \end{pmatrix}. \tag{5}$$

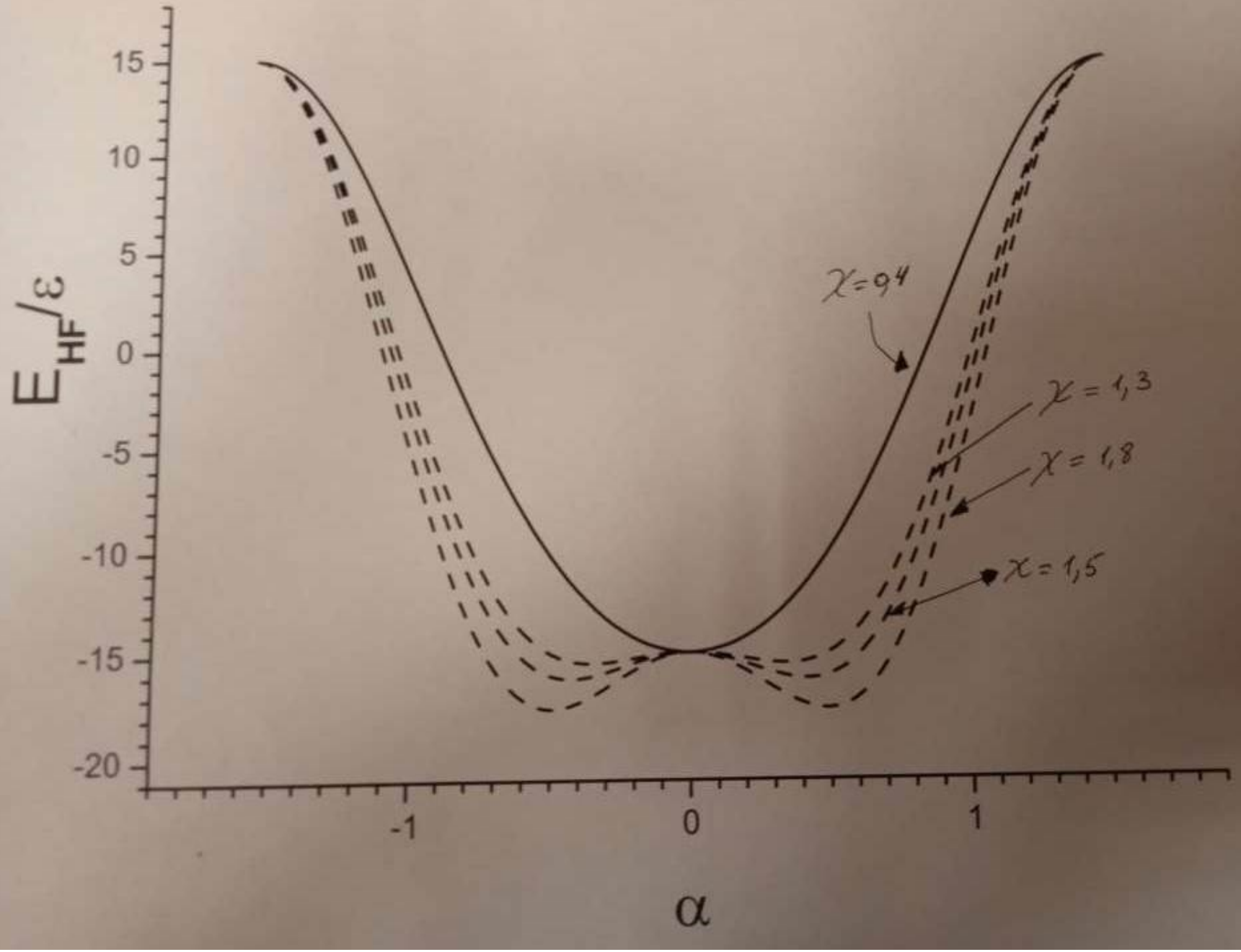
The constrained HF ground-state energy is a function of the variables α and φ:

$$E_{gs}^{\mathrm{HF}}(\alpha, \varphi) = -\frac{\varepsilon N}{2}\left[\cos(2\alpha) + \frac{1}{2}\chi \sin^2(2\alpha)\cos(2\varphi)\right], \quad (7)$$

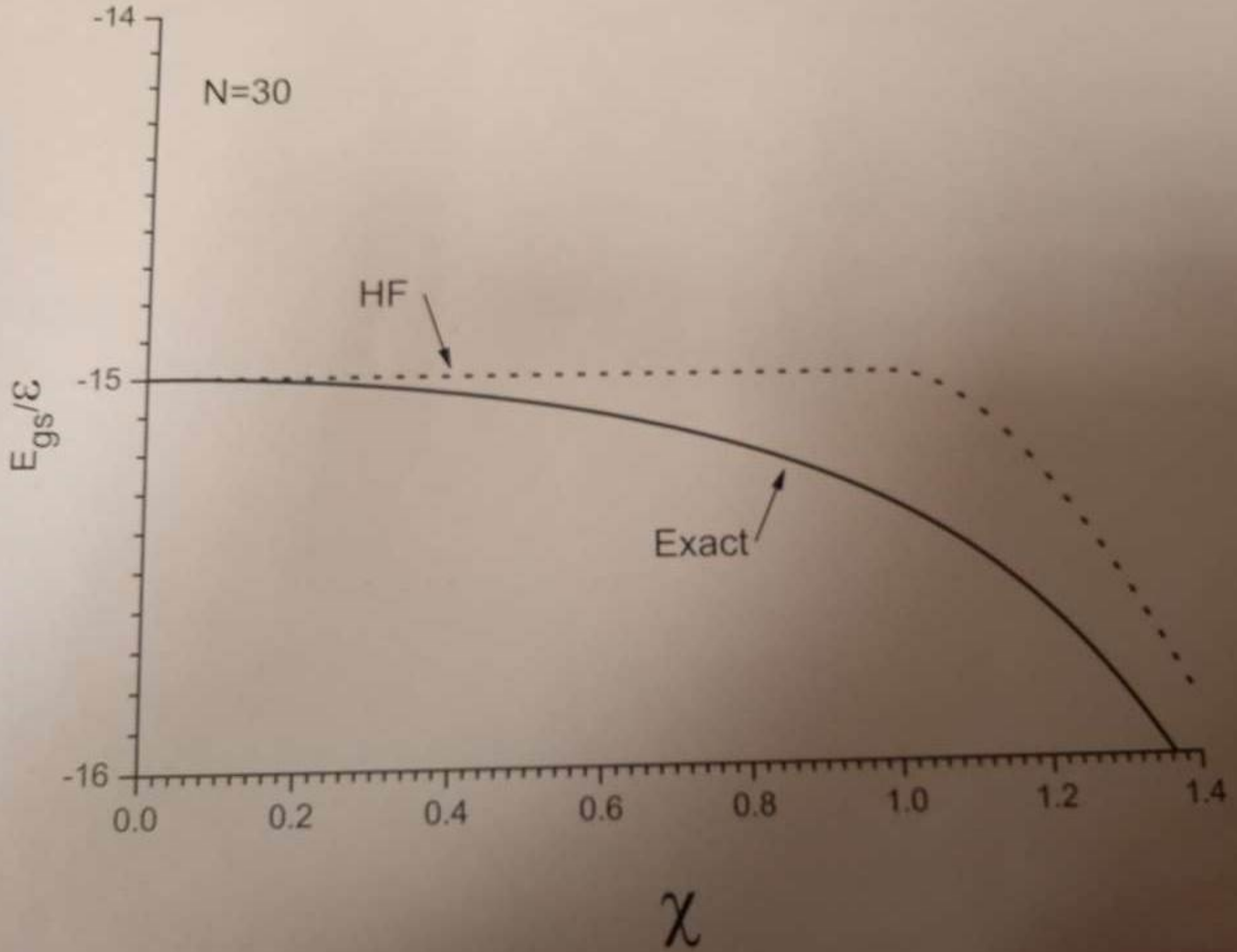
where

$$\chi = \frac{(N-1)\,V}{\varepsilon}. \quad (8)$$

Note that, for a given value of α, the lowest HF state always corresponds to $\varphi = 0$. The eigenvalues of the single-particle Hamiltonian, usually called single-particle energies, depend on α only for any mean-field state $|\alpha, \varphi\rangle$.


15
10
5
0
-5
-10
-15
-20
-1
0
1
E_{HF}/ε
α
χ=0,4
χ = 1,3
χ = 1,8
χ = 1,5

One can identify the variable α as a deformation parameter. There is a phase transition at $\chi = 1$ from a spherical ($\alpha = \varphi = 0$) to a "deformed" ground state. In the latter case, the value of α is obtained by solving the equation $\chi \cos(2\alpha) = 1$. The phase transition and the properties of exact and approximated ground states in this regime were first discussed by Agassi *et al*. [15].


-14
N=30
HF
-15
E_{gs}/ε
Exact
-16
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
χ

Lipkin model on a quantum computer

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Atomic nuclei are important laboratories for exploring and testing new insights into the universe, such as experiments to directly detect dark matter or explore properties of neutrinos. The targets of interest are often heavy, complex nuclei that challenge our ability to reliably model them (as well as quantify the uncertainty of those models) with classical computers. Hence there is great interest in applying quantum computation to nuclear structure for these applications. As an early step in this direction, especially with regards to the uncertainties in the relevant quantum calculations, we develop circuits to implement variational quantum eigensolver (VQE) algorithms for the Lipkin-Meshkov-Glick model, which is often used in the nuclear physics community as a testbed for many-body methods. We present quantum circuits for VQE for two and three particles and discuss the construction of circuits for more particles. Implementing the VQE for a two-particle system on the IBM Quantum Experience, we identify initialization and two-qubit gates as the largest sources of error. We find that error mitigation procedures reduce the errors in the results significantly, but additional quantum hardware improvements are needed for quantum calculations to be sufficiently accurate to be competitive with the best current classical methods.

Построение эффективного нуклон-нуклонного взаимодействия

The starting point for all these considerations is obviously the two-body interaction between nucleons. There are three basic assumptions in this concept:

(i) Dynamical mesonic degrees of freedom can be neglected and the nucleus can be described as a system of A nucleons whose interaction can be represented by a potential.
(ii) Relativistic effects are negligible.
(iii) Only two-body forces are important.

Even with these rather drastic assumptions, we immediately run into two difficulties when we try to proceed in the way we have discussed:

(i). There exists no derivation of the *nucleon–nucleon force* from first principles. Though this should be possible in principle with the modern theory of gauge fields for quarks and gluons, attempts in this direction are only in their infancy [De 78]. On the other hand, theories that start out from an effective Lagrangian for interacting mesons and nucleons have recently proved quite successful (see, for example, [CLL 73, LLR 75, DSB 77, Vi 78, Ho 80]). The basic ingredient is the pion–nucleon coupling constant, which is known from experiment. The nucleon–nucleon force is obtained without a free parameter for particle distances greater than 0.8 fm. The part from 0 to 0.8 fm is represented by a phenomenological potential containing six parameters in each isospin channel. Excellent fits to the measured nucleon–nucleon phase shifts are achieved.

The potentials used until now have been almost entirely phenomenological (besides the Yukawa part resulting from the one-pion exchange; see below) and contain up to about 50 parameters. The experimental phase

(ii). There is, however, a second difficulty in nuclear theory. These bare nuclear forces are, from a numerical point of view, very ill behaved. They show strong repulsion at short distances (hard core) and cannot be treated straightforwardly by the usual many-body techniques. For instance, they are too strong to be treated by perturbation theory and the hard core makes a direct self-consistent field approach (see Chap. 5), for example, impossible. In fact, the nucleons within a nucleus do not feel the bare nucleon–nucleon interaction. Taking into account that they interact with one another in the presence of many other nucleons permits one to introduce an *effective nucleon–nucleon interaction*, which is rather well behaved and allows application of the usual many-body methods, such as Hartree–Fock theory (Chap. 5). Much work has been done to derive this

In most of the so-called microscopic descriptions of the nucleus one uses *phenomenological effective forces*, which are constructed on the basis of these considerations, but depend on some parameters that are adjusted to fit experimental data.

In this chapter we do not want to go into such attempts to derive the bare nucleon–nucleon force [BJ 76a]. In the second section we will discuss

4.2.1 General Properties of a Two-Body Force

The most general quantum mechanical two-body potential V is completely specified by its matrix elements between two-body states (in a coordinate representation $|\mathbf{r}_1, s_1, t_1; \mathbf{r}_2, s_2, t_2\rangle$; where $s_i = \pm\frac{1}{2}$ and $t_i = \pm\frac{1}{2}$ are spin and isospin coordinates) as:

$$\langle \mathbf{r}_1' s_1' t_1' \mathbf{r}_2' s_2' t_2' | V | \mathbf{r}_1 s_1 t_1 \mathbf{r}_2 s_2 t_2 \rangle. \tag{4.1}$$

The space of two-particle states $|\mathbf{r}_1, s_1, t_1; \mathbf{r}_2, s_2, t_2\rangle$ is a product space of the coordinate wave functions $|\mathbf{r}_1\rangle$ and $|\mathbf{r}_2\rangle$ and the spin and isospin vectors $|s_1\rangle$, $|s_2\rangle$ and $|t_1\rangle$, $|t_2\rangle$. Since any operator in the spin space of one particle can be represented as a linear combination of the spin matrices $\sigma_1, \sigma_2, \sigma_3$ and the unity matrix $\sigma_0 = 1$, the most general form of the operator V is

$$V = \sum_{i,k=0}^{3} V_{ik} \sigma_i^{(1)} \sigma_k^{(2)}. \tag{4.2}$$

The function V_{ik} also depends analogously on the isospin operators $\boldsymbol{\tau}^{(1)}$ and $\boldsymbol{\tau}^{(2)}$. In addition to this isospin dependence, the V_{ik} are, in general, integral operators in coordinate space

$$V|\mathbf{r}_1 \mathbf{r}_2\rangle = \int V(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2) |\mathbf{r}_1' \mathbf{r}_2'\rangle \, d^3 r_1' \, d^3 r_2'. \tag{4.3}$$

In the special case in which $V(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2)$ has the form

$$V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2') = \delta(\mathbf{r}_1 - \mathbf{r}_1')\delta(\mathbf{r}_2 - \mathbf{r}_2')V(\mathbf{r}_1, \mathbf{r}_2) \tag{4.4}$$

V is called a *local potential*, and we have

$$V|\mathbf{r}_1\mathbf{r}_2\rangle = V(\mathbf{r}_1, \mathbf{r}_2)|\mathbf{r}_1\mathbf{r}_2\rangle. \tag{4.5}$$

In this case the interaction between the two particles depends only on the points $\mathbf{r}_1$ and $\mathbf{r}_2$ (and eventually on the spin and isospin). It does not, for instance, depend on the velocity of the particles.

We shall show that, in general, nonlocal potentials correspond to a velocity dependence. We therefore expand*

$$\begin{aligned} |\mathbf{r}_1', \mathbf{r}_2'\rangle &= |\mathbf{r}_1\mathbf{r}_2\rangle + (\mathbf{r}_1' - \mathbf{r}_1)\frac{\partial}{\partial \mathbf{r}_1}|\mathbf{r}_1\mathbf{r}_2\rangle + (\mathbf{r}_2' - \mathbf{r}_2)\frac{\partial}{\partial \mathbf{r}_2}|\mathbf{r}_1\mathbf{r}_2\rangle + \cdots \\ &=: \exp\left\{(\mathbf{r}_1' - \mathbf{r}_1)\frac{\partial}{\partial \mathbf{r}_1} + (\mathbf{r}_2' - \mathbf{r}_2)\frac{\partial}{\partial \mathbf{r}_2}\right\} : |\mathbf{r}_1\mathbf{r}_2\rangle \end{aligned} \tag{4.6}$$

and get, from (4.3),

$$\begin{aligned} V|\mathbf{r}_1\mathbf{r}_2\rangle &= \int V(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2)\exp\left\{\frac{i}{\hbar}(\mathbf{r}_1' - \mathbf{r}_1)\mathbf{p}_1 + \frac{i}{\hbar}(\mathbf{r}_2' - \mathbf{r}_2)\mathbf{p}_2\right\}|\mathbf{r}_1\mathbf{r}_2\rangle\, d^3r_1'\, d^3r_2' \\ &= \tilde{V}(\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2)|\mathbf{r}_1\mathbf{r}_2\rangle. \end{aligned} \tag{4.7}$$

*: : means *normal ordering*, i.e., the derivatives $\partial/\partial \mathbf{r}_i$ should not act on the coordinates $\mathbf{r}_i$ in the expansion of the exponent.

This means that the most general potential can be represented by Eq. (4.2) where the V_{ik} are operators in coordinate space of the form (4.7) (for reasons of simplicity we neglected the isospin dependence).

In the following we investigate the symmetry properties of such potentials $V(1,2)=V(\mathbf{r}_1, \mathbf{p}_1, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, \mathbf{r}_2, \mathbf{p}_2, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)})$. The form of this general function can, however, be restricted by requiring the imposition of a number of symmetries.

In particular, we require the following eight symmetries:

(i) Hermeticity

(ii) Invariance under an exchange of the coordinates

$$V(1,2)=V(2,1). \tag{4.8}$$

This property is strongly connected with the symmetry of the two-particle wave function $|1\,2\rangle$. Since nucleons are fermions, they have to be totally antisymmetric. For example, if we take a product wave function built out of ordinary space, a spin and an isospin part

$$\langle \mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2 \,|\, 12\rangle = \varphi(\mathbf{r}_1, \mathbf{r}_2)\chi(s_1, s_2)\zeta(t_1, t_2) \tag{4.9}$$

we have four combinations compatible with the Pauli principle, which are characterized by the symmetry of the coordinate space and spin part (Table 4.1). The isospin component is determined in each case by requiring the antisymmetry of the total wave function (4.9).

Table 4.1 Characterization of the symmetries of the two-particle state (4.9)

φ	χ	abbreviation	ζ
even	singlet	es	+
even	triplet	et	−
odd	singlet	os	−
odd	triplet	ot	+

(iii) Translational invariance. The potential depends on the relative coordinate $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ only

$$V(1,2)=V(\mathbf{r},\mathbf{p}_1,\boldsymbol{\sigma}^{(1)},\boldsymbol{\tau}^{(1)},\mathbf{p}_2,\boldsymbol{\sigma}^{(2)},\boldsymbol{\tau}^{(2)}). \tag{4.10}$$

(iv) Galilean invariance. The potential is not changed by a transformation to a system which moves with constant velocity, that is, it depends only on the relative momentum $\mathbf{p}=\frac{1}{2}(\mathbf{p}_1-\mathbf{p}_2)$:

$$V(1,2)=V(\mathbf{r},\mathbf{p},\boldsymbol{\sigma}^{(1)},\boldsymbol{\tau}^{(1)},\boldsymbol{\sigma}^{(2)},\boldsymbol{\tau}^{(2)}). \tag{4.11}$$

(v) Invariance under space reflection. Contrary to the weak interaction, there is no parity violation for strong interactions:

$$V(\mathbf{r},\mathbf{p},\boldsymbol{\sigma}^{(1)},\boldsymbol{\tau}^{(1)},\boldsymbol{\sigma}^{(2)},\boldsymbol{\tau}^{(2)})=V(-\mathbf{r},-\mathbf{p},\boldsymbol{\sigma}^{(1)},\boldsymbol{\tau}^{(1)},\boldsymbol{\sigma}^{(2)},\boldsymbol{\tau}^{(2)}). \tag{4.12}$$

(vi) Time reversal invariance guarantees that the equations of motion do not depend on the direction in which the time evolves (for details, see [Me 61])

$$V(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)}) = V(\mathbf{r}, -\mathbf{p}, -\boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, -\boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)}). \quad (4.13)$$

(vii) Rotational invariance in coordinate space. Rotations in three-dimensional coordinate space act not only on the vectors $\mathbf{r}$ and $\mathbf{p}$ but also on the spin matrices $\boldsymbol{\sigma} = 2 \cdot \mathbf{s}$. With respect to spin, the operator V has the form (4.2). It has to be a scalar under a rotation in coordinate space, which means in particular that V_{00} has to be a scalar. There exist three independent scalars which we can construct from the two vectors $\mathbf{r}$ and $\mathbf{p}$, namely $\mathbf{r}^2, \mathbf{p}^2$ and $\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}$. However, the latter expression can only appear quadratically because of time reversal invariance (vi). It is more convenient to express $(\mathbf{rp} + \mathbf{pr})^2$ through $\mathbf{r}^2, \mathbf{p}^2$ and $\mathbf{L}^2 = (\mathbf{r} \times \mathbf{p})^2$. V_{00} can then be written as a function of $\mathbf{r}^2, \mathbf{p}^2$ and $\mathbf{L}^2$. Because of invariance (ii) and (v) we find

$$V(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\sigma}^{(2)}) = V(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\sigma}^{(1)}). \quad (4.14)$$

The terms in (4.2) that are linear in $\boldsymbol{\sigma}^{(i)}$ therefore depend only on

$$\mathbf{S} = \tfrac{1}{2}(\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)}). \quad (4.15)$$

To form a scalar, $\mathbf{S}$ has to be multiplied by a vector, which is invariant under space reflection. Only $\mathbf{L}$ fulfils this requirement

$$\mathbf{L} \cdot \mathbf{S} = \tfrac{1}{2}\mathbf{L}(\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)}) \quad (4.16)$$

The quadratic terms in $\boldsymbol{\sigma}$ in Eq. (4.2) form a tensor. It can be decomposed into a scalar $\boldsymbol{\sigma}^{(1)} \cdot \boldsymbol{\sigma}^{(2)}$, a vector $\boldsymbol{\sigma}^{(1)} \times \boldsymbol{\sigma}^{(2)}$, and a symmetric tensor with vanishing trace $(\sigma_i^{(1)}\sigma_k^{(2)} + \sigma_k^{(1)}\sigma_i^{(2)})(1 - \frac{1}{3}\delta_{ik})$. Because of (4.14), $\boldsymbol{\sigma}^{(1)} \times \boldsymbol{\sigma}^{(2)}$ cannot appear. As shown by Okubo and Marshak [OM 58], the only possible independent combinations are

$$\begin{aligned} &\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}, (\mathbf{r}\boldsymbol{\sigma}^{(1)})(\mathbf{r}\boldsymbol{\sigma}^{(2)}), (\mathbf{p}\boldsymbol{\sigma}^{(1)})(\mathbf{p}\boldsymbol{\sigma}^{(2)}), \\ &(\mathbf{L}\boldsymbol{\sigma}^{(1)})(\mathbf{L}\boldsymbol{\sigma}^{(2)}) + (\mathbf{L}\boldsymbol{\sigma}^{(2)})(\mathbf{L}\boldsymbol{\sigma}^{(1)}). \end{aligned} \tag{4.17}$$

Each of these terms can be multiplied by an arbitrary function of $\mathbf{r}^2$, $\mathbf{p}^2$ and $\mathbf{L}^2$.

(viii) Rotational invariance in isospin space. Within the isospin formalism, protons and neutrons are considered as quantum states of one elementary particle that form a doublet (see Sec. 2.6.3) with isospin $\frac{1}{2}$. The two-dimensional representation of the rotational group reproduces all their transformation properties. Rotations within the isospin space (as long as they are not around the 3-axis) produce mixtures of protons and neutrons. Rotational invariance of the nuclear force therefore means the same as charge independence, that is, the proton–proton interaction has the same strength as the neutron–neutron interaction. This has been confirmed by nucleon–nucleon scattering experiments as well as by the symmetry properties of mirror nuclei (e.g., He^3 and H^3). Mathematically speaking, this means that the nucleon–nucleon interaction $V(1, 2)$ commutes with the operators of the total isospin

$$\mathbf{T} = \mathbf{t}_1 + \mathbf{t}_2. \tag{4.18}$$

Eigenstates can then be constructed of $\mathbf{T}^2, \mathbf{T}_3$ with eigenvalues $T=0$, $T_3=0$ and $T=1$, $T_3=-1, 0, +1$ (isospin singlet and isospin triplet). Charge invariance means that $\mathbf{T}^2$ commutes with the operator of the nuclear force. Therefore, the interactions in $T=1$ states have to be the same (*pp*, *nn*, or symmetric *pn* states). However, they may be different in the $T=0$ state (antisymmetric *pn* system).

The formalism of isospin matrices $\boldsymbol{\tau}=(\tau_1, \tau_2, \tau_3)$ is identical to that of regular spin. Since there is no other vector in isospin space, the only isospin invariant combination of the isospin matrices corresponding to particle 1 and 2 is

$$V_0 + V_\tau \boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}. \tag{4.19}$$

The functions V_0 and V_τ depend on the remaining coordinates such as $\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2$, as we have already discussed.

Not all of the combinations possible from the symmetric point of view have been used to describe the nuclear force. We will mention here only the most important terms:

(i). Among the local forces, which do not depend on the velocity, the *central force* is the most important. It depends only on the distance r between the nucleons:

$$V_C(1,2) = V_0(r) + V_\sigma(r)\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)} + V_\tau(r)\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)} + V_{\sigma\tau}(r)\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}. \tag{4.20}$$

(ii). The only remaining local part is the *Tensor force*

$$V_T(1,2)=\left[V_{T_0}(r)+V_{T_\tau}(r)\tau^{(1)}\tau^{(2)}\right]\cdot S_{12} \tag{4.21}$$

with

$$S_{12}=\frac{3}{r^2}(\boldsymbol{\sigma}^{(1)}\mathbf{r})(\boldsymbol{\sigma}^{(2)}\mathbf{r})-\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}.$$

The term $-\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}$ is added to make sure that an average of $V_T(1,2)$ taken over all directions of $\mathbf{r}$ vanishes:

$$\int V_T(1,2)\,d\Omega=0 \quad \text{where} \quad \mathbf{r}=(r,\Omega). \tag{4.22}$$

An experimental hint of the existence of a tensor component in the nucleon–nucleon potential is given by the quadrupole moment of the deuteron, which cannot be explained by pure central forces.

4.2.2 The Structure of the Nucleon–Nucleon Interaction

The central force (4.20) is the most important part of the nucleon–nucleon interaction. It can also be represented in terms of exchange or projection operators.

The operators

$$P^{\sigma} = \frac{1}{2}(1 + \boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}), \qquad P^{\tau} = \frac{1}{2}(1 + \boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}) \tag{4.25}$$

exchange the spin and isospin coordinates, respectively, in a wave function.

For instance, we can apply P^σ to the wave function (4.9) and obtain

$$P^\sigma \varphi(\mathbf{r}_1\mathbf{r}_2)\chi(s_1,s_2)\zeta(t_1,t_2)=\varphi(\mathbf{r}_1,\mathbf{r}_2)\chi(s_2,s_1)\zeta(t_1,t_2). \tag{4.26}$$

This is easy to understand by using the operator of the total spin $\mathbf{S}$ (4.15). The eigenstates of $\mathbf{S}^2$ are singlet and triplet states and we find:

$$P^\sigma=\frac{1}{2}\left(1+2(\mathbf{S}^2-\mathbf{s}^{(1)^2}-\mathbf{s}^{(2)^2})\right)=S(S+1)-1=\begin{cases}1 & \text{for triplet}\\ -1 & \text{for singlet.}\end{cases} \tag{4.27}$$

We can also define an operator P^r which exchanges the spacial coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ of the particles.* Since the wave function has to be antisymmetric under the exchange of all coordinates of the particles 1 and 2, the Pauli principle may be written in the form

$$P^rP^\sigma P^\tau=-1. \tag{4.28}$$

We can therefore express the operator $P^\tau=-P^rP^\sigma$ and eliminate the products $\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}$ and $\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}$ in Eq. (4.20).

*The operator P^r can be represented by a nonlocal operator in coordinate space, viz:

$$V(\mathbf{r})P^r\psi(\mathbf{r}_1,\mathbf{r}_2)=\int V(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_1'-\mathbf{r}_2)\delta(\mathbf{r}_2'-\mathbf{r}_1)\psi(\mathbf{r}_1',\mathbf{r}_2')\,d^3r_1'\,d^3r_2'.$$

In this sense only Wigner forces (4.30) are local.

Finally, we obtain

$$V_C = V_W(r) + V_M(r)P^r + V_B(r)P^\sigma + V_H(r)P^rP^\sigma \tag{4.29}$$

with the following relations

$$\begin{aligned} V_W &= V_0 - V_\sigma - V_\tau + V_{\sigma\tau} && \text{(Wigner force)} \\ V_M &= -4V_{\sigma\tau} && \text{(Majorana force)} \\ V_B &= 2V_\sigma - 2V_{\sigma\tau} && \text{(Bartlett force)} \\ V_H &= -2V_\tau + 2V_{\sigma\tau} && \text{(Heisenberg force).} \end{aligned} \tag{4.30}$$

The names of these different components of the nuclear force go back to the years following 1930, when the first models of the nucleus were introduced and the saturation property of nuclear forces was explained by exchange terms without introducing a hard core (for a historical review of this work see [Br 65a]).

A third way of representing the central force uses projection operators

$$\begin{aligned} \Pi_s^\sigma &= \frac{1}{2}(1 - P^\sigma), \quad \Pi_t^\sigma = \frac{1}{2}(1 + P^\sigma), \\ \Pi_s^\tau &= \frac{1}{2}(1 - P^\tau), \quad \Pi_t^\tau = \frac{1}{2}(1 + P^\tau), \\ \Pi_o^r &= \frac{1}{2}(1 - P^r), \quad \Pi_e^r = \frac{1}{2}(1 + P^r). \end{aligned} \tag{4.31}$$

The *radial dependence* of the functions V cannot be deduced from invariance principles. In 1937, Yukawa proposed an explanation of the nuclear force using a meson field theory. The nucleons influence each other by the exchange of one or several mesons. The simplest form is the one-pion exchange potential (OPEP). It has the radial dependence of the Yukawa potential [Yu 35]

$$V_Y(r)=\frac{e^{-\mu r}}{\mu r}, \tag{4.33}$$

where $1/\mu=\hbar/m_\pi c$ is the Compton wavelength of the pion. The asymptotic form of this potential is uniquely determined by the properties of the pion and its coupling strength to the nucleonic field $g^2/\hbar c\simeq 0.081$:

$$V^{\mathrm{OPEP}}=\frac{g^2}{3\hbar c}m_\pi c^2\frac{e^{-\mu r}}{\mu r}(\tau^{(1)}\tau^{(2)})\left\{\sigma^{(1)}\sigma^{(2)}+\left(1+3\frac{1}{\mu r}+3\left(\frac{1}{\mu r}\right)^2\right)S_{12}\right\}. \tag{4.34}$$

A phase shift analysis of the nucleon–nucleon scattering data shows that the OPEP-potential (4.34) is well able to reproduce the phase shifts for large orbital angular momenta $L\geqslant 6$ [Br 67b]. Since these high partial

waves only feel the tail of the nuclear force at large distances ($r \geqslant 2$ fm), we can assume that the OPEP potential describes the nuclear force properly at such large distances. For smaller distances we must, in addition, also introduce the two-pion exchange and the ρ- and ω-meson exchange in order to obtain the medium-range part of the force. This has been achieved very successfully [BJ 76a, CLL 73, LLR 75, DSB 77, Vi 78, Ho 80], so that only the short-range part of the force still has to be fitted by a phenomenological ansatz. Only six parameters are needed for each isospin state. As we mentioned in the introduction, this potential is not used very much as yet, therefore phenomenological counterparts have been employed until now. These phenomenological parametrizations consist of combinations of central, tensor, spin orbit, and higher terms, and more or less arbitrary radial functions containing up to 50 parameters, which are fitted to the experimental scattering phase shifts and to the deuteron data. There are attractive and repulsive components. At large distances they go over into the OPEP-potential, whereas at short distances they have an extremely repulsive core. Several authors have therefore used a *hard core* [$V(r) = \infty$ for $r < r_c \simeq 0.4$ fm]. Others use a very repulsive core which goes to infinity only for $r \to 0$. Such potentials are called *soft core* potentials.

Examples of such realistic nucleon–nucleon potentials using a hard core are the Hamada Johnston potential [HJ 62] and the Yale potential [LHR 62]. The Tabakin potential [Ta 64] is a nonlocal potential, separable in momentum space.

The Reid soft core potential [Re 68] is also widely used. It has the structure

$$V = V_C(\mu r) + V_T(\mu r) S_{12} + V_{LS}(\mu r) \mathbf{LS}. \tag{4.35}$$

$V_C(x)$ and $V_{LS}(x)$ have the simple form

$$V_C(x) = \sum_{n=1}^{\infty} a_n \frac{e^{-nx}}{x}, \qquad V_{LS} = \sum_{n=1}^{\infty} c_n \frac{e^{-nx}}{x}, \tag{4.36}$$

and $V_T(x)$ is given by

$$V_T(x) = \frac{b_1}{x}\left\{\left(\frac{1}{3} + \frac{1}{x} + \frac{1}{x^2}\right)e^{-x} - \left(\frac{k}{x} + \frac{1}{x^2}\right)e^{-kx}\right\} + \sum_{n=2}^{\infty} b_n \frac{e^{-nx}}{x}. \tag{4.37}$$

The constants are different for all values of T, S and $I \leqslant 2$. Only a_1, b_1, and c_1 are fixed in such a way that we obtain the OPEP-potential for large distances. For $I > 2$, Reid uses the OPEP-potential.

4.3 Microscopic Effective Interactions

The bare nucleon–nucleon force has—as we have already seen in the preceding section—certain features that are rather difficult to handle in practice.

There is, for instance, the hard core (or at least the very repulsive core), which would make some of the usual concepts of nuclear many-body physics extremely complicated if not inapplicable (as in the Hartree–Fock case; see Chap. 5).* This comes from the infiniteness of the matrix elements of a force with a hard core. In these theories, a way out of this situation is to use, in place of the bare interaction, a so-called effective interaction, which is itself an infinite sum of scattering processes of two nucleons in the nuclear medium. The bare interaction is then simply the Born term of this series. The object of this procedure is twofold: First, in re-summing the series one gets rid of the hard core problem, since the new interaction is well-behaved at short distances. Second, we can show that in replacing the bare interaction by its effective counterpart we have at the same time consistently summed up more of the many-body effects than if one had taken just the bare interaction.

The main fields of application are: (i) the ground state properties of nuclei, where the scattering of two nucleons within the nuclear medium has to be considered; (ii) the forces between the so-called valence nucleons; and (iii) effective forces between "particles" and "holes." There are also effective three-body forces which we will ignore in this section.

4.3.1 Brückner's G-Matrix and Bethe Goldstone Equation†

One of the most important effective interactions in nuclear physics is the so-called Brückner G-matrix [Br 55, Da 67, and references therein]. It is, for two nucleons in the nuclear medium—in a sense yet to be specified—the analogue of the scattering matrix for two nucleons in free space.

We therefore start our considerations with the Lippmann–Schwinger equation for the scattering matrix (T-matrix; see Fig. 4.1) of two particles (Messiah [Me 61] Chap. XIX, Sec. 14):

$$T^{E}_{\mathbf{k}_1\mathbf{k}_2,\,\mathbf{k}'_1\mathbf{k}'_2} = \bar{v}_{\mathbf{k}_1\mathbf{k}_2,\,\mathbf{k}'_1\mathbf{k}'_2} + \frac{1}{2}\sum_{\mathbf{p}_1\mathbf{p}_2} \bar{v}_{\mathbf{k}_1\mathbf{k}_2,\,\mathbf{p}_1\mathbf{p}_2} \frac{1}{E-(\mathbf{p}_1^2/2m)-(\mathbf{p}_2^2/2m)+i\eta}\, T^{E}_{\mathbf{p}_1\mathbf{p}_2,\,\mathbf{k}'_1\mathbf{k}'_2}, \tag{4.38}$$

where $\mathbf{k}_1, \mathbf{k}_2$ and $\mathbf{k}'_1, \mathbf{k}'_2$ are the momenta of the incoming and outgoing particles, respectively, and E is the total scattering energy.

If we consider the scattering of two nucleons within a nuclear medium we can show (this is derived in Sec. F.4) that it makes sense to define a scattering matrix G^E analogous to that for free particles. The changes to be made for nucleons in a nucleus are almost obvious: the plane wave indices have to be changed to shell model indices, the kinetic single-particle energies figuring in the denominator of the r.h.s. of Eq. (4.38) have to be replaced by the corresponding shell model energies, and the sum over the intermediate states has to be restricted so that it does not include states below the Fermi surface. This latter feature comes from the fact that two nucleons below the Fermi surface can only scatter into states above the Fermi surface, because all other levels are occupied and are thus excluded by the Pauli principle. Therefore, we get the following equation for the G-matrix, which is usually known under the name Bethe–Goldstone equation [BG 57] (for its mathematical derivation, see Sec. F.4).

$$G^E_{ab,\,cd} = \bar{v}_{ab,\,cd} + \frac{1}{2} \sum_{\substack{m,\,n \\ > \epsilon_F}} \bar{v}_{ab,\,mn} \frac{1}{E - \epsilon_m - \epsilon_n + i\eta} G^E_{mn,\,cd}, \tag{4.39}$$

where $ab, \ldots, mn$ are shell-model indices and ϵ_F is the Fermi energy. This

equation is usually represented graphically in an obvious way, as shown in Fig. 4.2. Two lines connecting two interactions represent the "propagator" $1/(E-\epsilon_n-\epsilon_m)$. (More will be explained about graphs in Chap. 8 and Appendix F.) For $E<\epsilon_F$, we can ignore the $i\eta$ in the denominator of (4.39), and in this case the G-matrix is obviously Hermitian as can be checked immediately by iterating Eq. (4.39). Equation (4.39) is also often

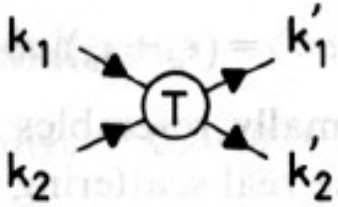

Figure 4.1. Graphical representation of the T-matrix.

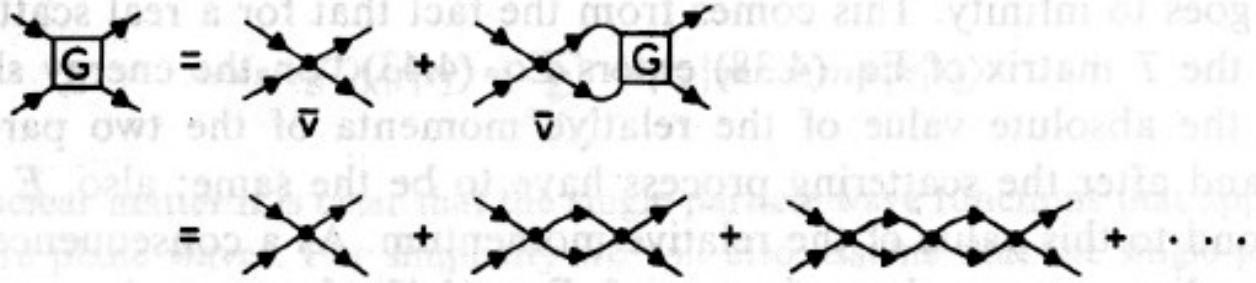

Figure 4.2. Graphical representation of the Bethe–Goldstone equation.

We have seen that the solution of the Bethe–Goldstone Equation (4.39) is far from trivial, and one can easily imagine that the task can become tremendously difficult for finite nuclei, where the wave functions are no longer plane waves and translational invariance is also lost. Several ap-

4.4 Phenomenological Effective Interactions

4.4.1 General Remarks

In Section 4.3 we saw how effective forces can be defined microscopically and how difficult it is in practice to calculate them and get quantitative agreement with experiment. Consequently, from the early days of nuclear physics the use of phenomenological forces, which contain a certain number of *fit parameters* adjusted to reproduce the experimental data has been adopted. In many cases this procedure has turned out to be extremely successful and, using only a few parameters chosen once and for all, much experimental data covering quite a large range of nuclear masses can be explained. Therefore, it is all the more disconcerting that a really satisfying microscopic theory able to explain the success of these phenomenological forces is somehow still missing.

There exists, of course, an enormous number of different phenomenological interactions that have been applied to problems in nuclear physics. Each of them has been used for a specific problem and their range of

validity and success varies very much. It lies outside the scope of this book to give a complete picture, and we will restrict our discussion to certain essential properties and the presentation of only the most successful examples. Most of them are only constructed for a special purpose, as, for example, for Hartree–Fock calculations (see Chap. 5), which calculate the nuclear self-consistent field, and bulk properties of nuclei such as binding energies and saturation densities. Others serve as effective forces between valence nucleons or between particles and holes (see Sec. 4.3). Therefore, we must be very careful in comparing these different types of interaction, even if, as we shall see, they look very similar in mathematical structure.

It is evident that we prefer to choose the analytical form of the effective interaction to be as simple as possible. For example, it is often assumed that the effective interaction obeys the same *invariance principles* as the bare nucleon–nucleon interaction (see Sec. 4.2). This is certainly not always true. For instance, we should expect the renormalization procedure which describes the transition from the bare nucleon–nucleon interaction to the effective one to depend on the actual density of the system, that is, we get a different force in the interior of the system than in the surface and outer regions. For a shell model calculation in a fixed well, we should therefore not expect a translationally invariant residual interaction.

We know that the *range of the nuclear force* is rather short. We have seen in Section 4.3 that this is true even for the range of the effective G-matrix. The simplest ansatz therefore consists in using a *zero range* force whose radial dependence is described by a δ-function. In fact, such forces turn out to be rather useful because they are simple to handle and they describe many nuclear properties quite well. More realistic forces, however, need to have a finite non-vanishing range (see [AS 71, Sch 72b]). A *finite range* can be simulated by a *momentum dependence*. To show this we transform a function $V(\mathbf{r})$ of the relative distance $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ into momentum space

$$\langle \mathbf{p}|V|\mathbf{p}'\rangle = \frac{1}{(2\pi\hbar)^3}\int e^{-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\mathbf{r}} V(\mathbf{r})d^3r. \tag{4.97}$$

We see that a δ-force is a constant and that any range represents a p-dependence in momentum space. The simplest rotationally invariant one is of the form

$$(2\pi\hbar)^3\langle \mathbf{p}|V|\mathbf{p}'\rangle = V_0 + V_1\mathbf{p}'^2 + V_1\mathbf{p}^2 + V_2\mathbf{p}\mathbf{p}', \tag{4.98}$$

which in coordinate space corresponds to the momentum dependent operator

$$V(\mathbf{r}) = V_0\delta(\mathbf{r}) + V_1(\hat{\mathbf{p}}^2\delta(\mathbf{r}) + \delta(\mathbf{r})\hat{\mathbf{p}}^2) + V_2\hat{\mathbf{p}}\delta(\mathbf{r})\hat{\mathbf{p}}. \tag{4.99}$$

Effective forces usually depend on the density $\rho(\mathbf{r})$. Such *density dependence* is easy to understand if, for example, we consider expression (4.39) for the G-matrix: The range of the summation depends on the Fermi

4.4.3 The Skyrme Interaction

In 1956 Skyrme [Sk 56, 59] proposed an effective interaction with a three-body term viz:

$$V=\sum_{i<j} V(i,j)+\sum_{i<j<k} V(i,j,k). \tag{4.104}$$

To simplify the calculations, he used a short-range expansion in the form of Eq. (4.99) for the two-body part:

$$\begin{aligned} V(1,2)=&\, t_0(1+x_0P^\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2) \\ &+\tfrac{1}{2}t_1\left[\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k}^2+\mathbf{k}^2\delta(\mathbf{r}_1-\mathbf{r}_2)\right]+t_2\mathbf{k}\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k} \\ &+iW_0(\boldsymbol{\sigma}^{(1)}+\boldsymbol{\sigma}^{(2)})\mathbf{k}\times\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k}, \end{aligned} \tag{4.105}$$

where $\mathbf{k}=(1/\hbar)\mathbf{p}$ is the operator of the relative momentum

$$\mathbf{k}=\frac{1}{2i}(\nabla_1-\nabla_2). \tag{4.106}$$

For the three-body force Skyrme also assumed a zero range force of the form

$$V(1,2,3)=t_3\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_2-\mathbf{r}_3). \tag{4.107}$$

The five constants—t_0, t_1, t_2, t_3, x_0—and W_0 were adjusted to the experimental binding energies and radii. There are several sets of parameters called Skyrme I, II, etc. (see Sec. 5.6) resulting from different fits. We present here Skyrme III [BFG 75]:

$$\begin{aligned} t_0 &= -1128.75 \text{ MeV fm}^3; & t_1 &= 395.0 \text{ MeV fm}^5; \\ t_2 &= -95.0 \text{ MeV fm}^5; & t_3 &= 14000.0 \text{ MeV fm}^6; \\ W_0 &= 120 \text{ MeV fm}^5; & x_0 &= 0.45. \end{aligned} \tag{4.108}$$

The parameter t_0 describes a pure δ-force with a spin-exchange; t_1 and t_2 simulate an effective range, as in Eq. (4.99). The fourth term in Eq. (4.105) represents a two-body spin orbit interaction. It can be obtained [BS 56] from a normal spin orbit term [see Eq. (4.23)] in the short range limit.

In Chapter 5, we shall see that this force has been used extensively in Hartree–Fock calculations. For spin saturated even–even nuclei, the three-body term (4.104) turns out to be equivalent to a density dependent two-body interaction*:

$$V_\rho(1,2) = \frac{1}{6} t_3 (1 + P^\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho\left(\tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)\right). \tag{4.109}$$

Such a density dependent term can also be regarded as the phenomenological representation of the ρ-dependence of the microscopic effective interaction. This interpretation is preferrable to the view that the Skyrme force contains a three-body interaction, since we know that three-body interactions are rather weak in nuclei.

There are essentially three reasons why this force has gained so much importance over the last ten years:

(i) Vautherin and Brink [VB 72] (see Chap. 5) were able to reproduce the nuclear binding energies over the whole periodic table with a reasonable set of parameters and, at the same time, the nuclear radii. This had not been possible with the usual non-density dependent forces.

(ii) Negele and Vautherin [NV 72] gave the connection between this force and the more fundamental G-matrix discussed in the last sections.

(iii) The mathematical form of the force is extremely simple. The δ-functions simplify all types of calculations enormously.

4.4.4 The Gogny Interaction

Despite the great success of the Skyrme interaction, it has been argued that zero range forces might not be able to simulate the long range or even the intermediate range parts of the realistic effective interaction. In particular, the present versions of the Skyrme force are not able to properly describe pairing correlations in nuclei (see Chap. 6), therefore Gogny [Go 75b] replaced the t_0, t_1 and t_2 parts of the Skyrme force by a sum of two Gaussians* with spin–isospin exchange mixtures (a force which was originally used by Brink and Booker [BB 67]) and got

$$V(1,2) = \sum_{i=1}^{2} e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/\mu_i^2}(W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau) + iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\mathbf{k}\times\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k} + t_3(1+P^\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2)\rho^{1/3}(\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)). \quad (4.110)$$

The parameters were adjusted to the properties of finite nuclei, and for nuclear matter (Table 4.4).

Table 4.4 Force parameters of the Gogny force (D1)

i	μ_i [fm]	W_i	B_i	H_i	M_i [MeV]	$W_0 = +115$ [MeV fm^5]
1	0.7	−402.4	−100.	−496.2	−23.56	$t_3 = 1350$ [MeV fm^4]
2	1.2	−21.30	−11.77	37.27	−68.81	

4.4.5 The Migdal Force

This force was proposed by Migdal [Mi 67] in his theory of finite Fermi systems. Based on the interacting quasi-particle concept of Landau's theory of a Fermi liquid [La 59], Migdal introduces this force to describe the collective excitations in nuclei.†

Starting from the ground state of an even–even system, the quasi-particles are defined as the low-lying excitations in the neighboring odd mass nuclei. The ground state of the even system contains no quasi-particles, and excited states are characterized by the quasi-particle occupation numbers n_λ. A change of these occupation numbers by the amount δn_λ causes a change in the total energy E_0 of the system by the amount

$$\delta E_0 = \sum_\lambda \epsilon_\lambda^0 \delta n_\lambda + \frac{1}{2} \sum_{\lambda\lambda'} F_{\lambda\lambda'} \delta n_\lambda \delta n_{\lambda'},$$

where ϵ_λ^0 are the energies of a quasi-particle λ in the absence of any other quasiparticle and $F_{\lambda\lambda'}$ is the so-called quasi-particle interaction. Migdal introduces an effective particle–hole interaction F^ω and an effective particle–particle (or hole–hole) interaction F^ξ.

In an infinite system with translational invariance, the quasi-particles are characterized by the momentum $\mathbf{k}$, and Landau could show that the *ph*-interaction $F(\mathbf{k}, \mathbf{k}')$ is given by the second derivative of the total energy

E_0 with respect to the quasi-particle densities $n(\mathbf{k})$:

$$F^{ph}(\mathbf{k},\mathbf{k}') = \frac{\delta^2 E_0}{\delta n(\mathbf{k})\delta n(\mathbf{k}')} . \tag{4.111}$$

At the Fermi surface this is an exact relation.

In a finite system the quasi-particle density $\bar{\rho}_{\lambda\lambda'}$ is no longer completely determined by its diagonal elements (the occupation numbers n_λ), but it also contains information about the form of the single-particle wave functions φ_λ. The effective interaction then depends on four indices, and it has been proposed to derive this quantity, in analogy to Eq. (4.111), from the exact ground state energy [Br 71]

$$F^{ph}_{psqr} = \frac{\delta E_0}{\delta\bar{\rho}_{qp}\delta\bar{\rho}_{rs}} . \tag{4.112}$$

So far it has not been shown that this is an exact relation. However, a very similar expression is obtained in a quite different (*approximate*) theory: the time dependent Hartree–Fock theory in the limit of a motion with small amplitudes (see Sec. 8.5). Starting from the assumption that the wave function is a Slater determinant (i.e., $\rho^2=\rho$; see Sec. 5.3.3) and that the total energy can be expressed by a functional $E_0[\rho]$, we obtain in this case the effective *ph*-interaction as the second derivative of $E_0[\rho]$ with respect to ρ [Eq. (8.124)], just as in Eq. (4.112).

Like the Skyrme force, the Migdal force is an expansion in momentum space. However, contrary to potentials suitable for Hartree–Fock calculations (such as the Skyrme force), the p^2-terms do not play an essential role, as the Migdal forces do not have to guarantee saturation (they are constructed to describe different physical situations anyway). In most calculations it is therefore sufficient to take into account only the constant in momentum space which gives a pure δ-force in coordinate space. On the other hand, spin and isospin exchange mixtures are now very important. They are different for the particle–particle and particle–hole forces:

$$V(1,2)=V_0\delta(\mathbf{r}_1-\mathbf{r}_2)(f+f'\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}+g\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}+g'\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}). \quad (4.113)$$

V_0 is a strength parameter which has to be adjusted to the configuration space (e.g., in the ^{208}Pb region $V_0=380$ MeV fm^3). Guman and Birbrair [GB 65] proposed to take into account the different interaction strengths inside and outside the nucleus and the diffuseness of the nuclear surface by a linear density dependence of the constants f, f',

$$f=f^{\mathrm{ex}}+(f^{\mathrm{in}}-f^{\mathrm{ex}})\rho(r), \quad (4.114)$$

where $\rho(r)$ has the form of a Fermi distribution

$$\rho(r)=\frac{1}{1+\exp[(r-R)/a]}\,. \tag{4.115}$$

The additional parameters R and a represent the radius and the diffuseness, respectively, of the nucleus. Contrary to a Hartree–Fock calculation with a density dependent interaction (see Chap. 5), the density (4.114) is not adjusted self-consistently. Therefore, the Migdal force violates translational invariance. Of course, this is no drawback, since the renormalization procedure is closely connected with the underlying single-particle potential, which also violates translational invariance. In fact, a proper choice of the effective residual interaction should restore this invariance (see Mikeska and Brenig [MB 69]). From this condition one can deduce additional relations among the parameters f, f', g, g' [NW 72, 74].

The Migdal force has been widely used to calculate low-lying collective vibrations in nuclei within the framework of the random phase approximation (see Chap. 8). The effective charges caused by such vibrations (see Chap. 9) provide an enormous amount of experimental data with which to adjust the six parameters f^{in}, f^{ex}, f'^{in}, f'^{ex}, and g, g' for the particle–hole and particle–particle forces (for details, see [RBS 73, BSK 73, BER 75]). For the particle–hole force Ring and Speth [RS 74a] found:

$$\begin{aligned} &f^{\mathrm{in}}=0.0685; \quad f'^{\mathrm{in}}=0.3315; \quad f^{\mathrm{ex}}=-2.165;\\ &f'^{\mathrm{ex}}=0.465; \quad g=0.575; \quad g'=0.725. \end{aligned} \tag{4.116}$$

It is important to note that this is an effective *ph*-force which does not have to be antisymmetrized [KMS 76]. It shows strong attraction outside the nucleus and is close to zero inside the nucleus.

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II. DESCRIPTION OF SKYRME'S INTERACTION

In its original form Skyrme's interaction can be written as a potential,

$$V = \sum_{i<j} v_{ij}^{(2)} + \sum_{i<j<k} v_{ijk}^{(3)}, \tag{1}$$

with a two-body part v_{ij} and three-body part v_{ijk}.

To simplify calculations Skyrme used a short-range expansion for the two-body interaction. The matrix elements in momentum space are

$$\langle \vec{k} \,|\, v_{12} \,|\, \vec{k}' \rangle = t_0(1 + x_0 P_\sigma) + \tfrac{1}{2} t_1 (k^2 + k'^2) + t_2 \vec{k} \cdot \vec{k}' + iW_0(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k} \times \vec{k}', \tag{2}$$

where $\vec{k}$ and $\vec{k}'$ are relative wave vectors of two nucleons. In Eq. (2) P_σ is a spin-exchange operator, and the $\vec{\sigma}$ are Pauli spin matrices. The reason why this expression corresponds to a short-range expansion can be seen in the following way. Consider, for instance, a Gaussian central force with exchange terms,

$$V = e^{-(r_{12}/\mu)^2}(W + BP_\sigma - HP_\tau - MP_\sigma P_\tau). \tag{3}$$

Only low-momentum matrix elements ($k, k' \leq 2k_F$) are important for Hartree-Fock calculations.

Now if the range μ in Eq. (3) is small compared to k_F^{-1}, then one can retain only the first few terms in the Taylor series for the matrix elements of V in momentum space, and one is left finally with an expression of the form

$$\langle \vec{k} \mid V \mid \vec{k}' \rangle = (\mu\sqrt{\pi})^3[W + M + (B + H)P_\sigma][1 - \tfrac{1}{4}(k^2 + k'^2)\mu^2]$$

$$+ \tfrac{1}{2}(\mu\sqrt{\pi})^3[W - M + (B - H)P_\sigma]\mu^2\vec{k} \cdot \vec{k}', \qquad (4)$$

which is identical to Eq. (2) except for the last term.

To see how one deals with such an interaction in practical calculations it is convenient to write it in configuration space. It can be expressed as

$$v_{12} = t_0(1 + x_0P_\sigma)\delta(\vec{r}_1 - \vec{r}_2)$$

$$+ \tfrac{1}{2}t_1[\delta(\vec{r}_1 - \vec{r}_2)k^2 + k'^2\delta(\vec{r}_1 - \vec{r}_2)]$$

$$+ t_2\vec{k}' \cdot \delta(\vec{r}_1 - \vec{r}_2)\vec{k} + iW_0(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}' \times \delta(\vec{r}_1 - \vec{r}_2)\vec{k}, \qquad (6)$$

where $\vec{k}$ now denotes the operator $(\vec{\nabla}_1 - \vec{\nabla}_2)/2i$ acting on the right; whereas, $\vec{k}'$ is the operator $-(\vec{\nabla}_1 - \vec{\nabla}_2)/2i$ acting on the left. By considering the

For the three-body force Skyrme also assumed a zero-range force

$$v_{123}^{(3)} = t_3 \delta(\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2)\delta(\vec{\mathbf{r}}_2 - \vec{\mathbf{r}}_3)\,. \tag{7}$$

In the following we will show that for Hartree-Fock calculations of even-even nuclei, this force is equivalent to a two-body density-dependent interaction:

$$v_{12} = \tfrac{1}{6} t_3 (1 + P_\sigma)\delta(\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2)\rho\left(\frac{\vec{\mathbf{r}}_1 + \vec{\mathbf{r}}_2}{2}\right). \tag{8}$$

The expectation value of the total energy is

$$E = \langle \phi, (T+V)\phi \rangle$$

$$= \sum_i \left\langle i \left| \frac{p^2}{2m} \right| i \right\rangle + \frac{1}{2} \sum_{ij} \langle ij| \bar{v}_{12} |ij\rangle$$

$$+ \frac{1}{6} \sum_{ijk} \langle ijk| \bar{v}_{123} |ijk\rangle$$

$$= \int H(\vec{\mathbf{r}})\, d^3r\,, \tag{10}$$

where the notation $\bar{v}$ denotes an antisymmetrized matrix element. For the Skyrme interaction the energy density $H(\vec{\mathbf{r}})$ is an algebraic function of the nucleon densities $\rho_n(\rho_p)$, the kinetic energy τ_n (τ_p), and spin densities $\vec{J}_n$ $(\vec{J}_p)$. These quantities depend

in turn on the single-particle states ϕ_i defining the Slater-determinant wave function ϕ,

$$\rho_q(\vec{\mathbf{r}}) = \sum_{i,\sigma} |\, \phi_i(\vec{\mathbf{r}}, \sigma, q)|^2 ,$$

$$\tau_q(\vec{\mathbf{r}}) = \sum_{i,\sigma} |\, \vec{\nabla}\phi_i(\vec{\mathbf{r}}, \sigma, q)|^2 , \tag{11}$$

$$\vec{\mathbf{J}}_q(\vec{\mathbf{r}}) = (-i) \sum_{i,\sigma,\sigma'} \phi_i^*(\vec{\mathbf{r}}, \sigma, q)[\, \vec{\nabla}\phi_i(\vec{\mathbf{r}}, \sigma', q) \times \langle \sigma |\, \vec{\sigma}\, | \sigma' \rangle\,] .$$

The sums in Eq. (11) are taken over all occupied single-particle states. The expression for $H(\vec{\mathbf{r}})$ is derived explicitly in Appendix A for the central term and in Appendix B for the spin-orbit term. Assuming that the subspace of occupied single-particle states is invariant under time reversal (which implies an even-even nucleus) one gets the following result:

$$H(\vec{\mathbf{r}}) = \frac{\hbar^2}{2m}\,\tau(\vec{\mathbf{r}}) + \tfrac{1}{2}\,t_0[(1+\tfrac{1}{2}x_0)\rho^2 - (x_0+\tfrac{1}{2})(\rho_n^{\,2}+\rho_p^{\,2})] + \tfrac{1}{4}(t_1+t_2)\,\rho\tau + \tfrac{1}{8}(t_2-t_1)(\rho_n\,\tau_n+\rho_p\,\tau_p) + \tfrac{1}{16}(t_2-3t_1)\,\rho\nabla^2\rho$$

$$+\tfrac{1}{32}(3t_1+t_2)(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p) + \tfrac{1}{16}(t_1-t_2)(\vec{\mathbf{J}}_n^{\,2}+\vec{\mathbf{J}}_p^{\,2}) + \tfrac{1}{4}\,t_3\rho_n\,\rho_p\,\rho + H_C(\vec{\mathbf{r}}) - \tfrac{1}{2}W_0(\rho\,\vec{\nabla}\cdot\vec{\mathbf{J}} + \rho_n\vec{\nabla}\cdot\vec{\mathbf{J}}_n + \rho_p\vec{\nabla}\cdot\vec{\mathbf{J}}_p) ,$$

(12)

The sums are taken over all occupied single-particle states. A lengthy but straightforward calculation [VB 72] for $N=Z$ nuclei gives

$$H(\mathbf{r})=\frac{\hbar^2}{2m}\tau(\mathbf{r})+\frac{3}{8}t_0\rho^2+\frac{1}{16}t_3\rho^3+\frac{1}{16}(3t_1+5t_2)\rho\tau$$
$$+\frac{1}{64}(9t_1-5t_2)(\nabla\rho)^2-\frac{3}{4}W_0\rho\nabla\mathbf{J}+\frac{1}{32}(t_1-t_2)\mathbf{J}^2. \quad (5.87)$$

Besides the kinetic energy τ, we also have contributions from the two-body δ-force $\sim\rho^2$ and the three-body δ-force $\sim\rho^3$. The nonlocal p^2-terms give contributions $\sim\rho\tau$ and $\sim\nabla\rho^2$. The latter has its largest contributions at the nuclear surface. The term $\frac{1}{32}(t_1-t_2)\mathbf{J}^2$ is usually neglected because it is difficult to handle in deformed nuclei and its contribution to the spin orbit part does not reproduce the experimental spin-orbit splitting.

We could also have derived the three-body term $\sim\rho^3$ from a density dependent two-body interaction

$$\frac{1}{16}t_3\rho^3=\frac{1}{2}\sum_{i,j<A}\langle ij|\frac{1}{6}t_3\delta(\mathbf{r}_1-\mathbf{r}_2)\rho(r_1)(1+P^\sigma)|ij-ji\rangle. \quad (5.88)$$

In Section (5.6.1.1) we saw that when using density dependent interactions we have first to calculate the energy and only afterwards vary with respect to the density. In that sense, the three-body contact force of Skyrme is equivalent to the two-body interaction (5.88). This equivalence, however, is only valid in even–even nuclei with time reversal symmetry.

Using (5.87), we are able to calculate the binding energy per particle in nuclear matter without Coulomb interaction. In this case we have translational invariance and the single-particle wave functions are given by plane waves normalized to a δ-function

$$\varphi_{ksl} = \frac{1}{(2\pi)^{3/2}} e^{ikr} \chi_s^{1/2} \chi_l^{1/2} \tag{5.89}$$

and in Eqs. (5.84)–(5.86) we have to replace

$$\sum_{i=1}^{A} \ldots \quad \text{by} \quad \int_{|k| < k_F} d^3k \ldots, \tag{5.90}$$

where all the levels with $|k|$ smaller than the Fermi momentum k_F are occupied. From (5.84), we get the usual relation between ρ and k_F [see also Eqs. (13.22) and (13.23)]

$$\rho = \frac{4}{(2\pi)^3} \frac{4\pi}{3} k_F^3 = \frac{2}{3\pi^2} k_F^3 \tag{5.91}$$

and from (5.85),

$$\tau = \frac{2}{3\pi^2} \frac{3}{5} k_F^5 = \frac{3}{5} \rho k_F^2 = \frac{3}{5} \left(\frac{3\pi^2}{2} \right)^{2/3} \rho^{5/3}. \tag{5.92}$$

Because of translational invariance, we have $\nabla\rho = \nabla J = 0$ and obtain for the binding energy per particle in nuclear matter

$$\frac{E_0}{A} = \frac{H}{\rho} = \frac{3}{5}\frac{\hbar^2}{2m}k_F^2 + \frac{3}{8}t_0\rho + \frac{1}{16}t_3\rho^2 + \frac{3}{80}(3t_1+5t_2)\rho k_F^2. \quad (5.93)$$

The saturation property means that there is an equilibrium density ρ_0 for which

$$\frac{\partial}{\partial\rho}\left(\frac{E_0}{A}\right)\bigg|_{\rho=\rho_0} = 0 = \frac{2}{5}\frac{\hbar^2}{2m}k_F^2\rho^{-1} + \frac{3}{8}t_0 + \frac{1}{8}t_3\rho + \frac{1}{16}(3t_1+5t_2)k_F^2. \quad (5.94)$$

The incompressibility of nuclear matter K is defined as the curvature of the binding energy E_0/A with respect to the Fermi momentum k_F at this minimum:

$$K = k_F^2\frac{\partial^2(E_0/A)}{\partial k_F^2}\bigg|_{\rho=\rho_0} = \frac{6}{5}\frac{\hbar^2}{2m}k_F^2 + \frac{9}{4}t_0\rho + \frac{15}{8}t_3\rho^2 + \frac{3}{4}(3t_1+5t_2)\rho k_F^2. \quad (5.95)$$

Equations (5.93)–(5.95) allow us to express the two constants t_0 and t_3 and the combination $3t_1+5t_2$ by the nuclear matter constants E_0/A, ρ_0, and K. From Eq. (5.95), we see that t_3 is strongly correlated with the incompressibility K.* From the Bethe–Weizsäcker Formula (1.4), we know that the value of $E_0/A = a_V = 15.9$ MeV. Less well determined is the equilibrium density $\rho_0 = 3/4\pi r_0^3 \simeq 0.14\ \text{fm}^{-3}$. Therefore, it is not possible to adjust the force parameters of a phenomenological force to nuclear matter data alone. We first have to carry out the calculation for finite nuclei.

5.6.2.3. The Derivation of the Density Dependent Hartree–Fock Equations. According to the concept of Section 5.6.1, we have to vary the functional $E_0[\rho]$ with respect to the density in order to gain the Hartree–Fock Hamiltonian. Unfortunately, (5.95) does not have the form of a functional of ρ. It also depends on τ and $\mathbf{J}$, and it is very hard to express τ and $\mathbf{J}$ in terms of ρ. In our case, however, this is no real problem, since the HF-density is uniquely defined by the single-particle wave functions φ_k (5.84), and we can also carry out the variation with respect to φ_k under the condition that they are normalized to unity. We use Lagrange multipliers ϵ_k for these subsidiary conditions and find

$$\frac{\delta}{\delta\varphi_k}\left(E_0[\rho]-\sum_l \epsilon_l \int d^3r|\varphi_l(\mathbf{r})|^2\right)=0. \tag{5.96}$$

The variation of the energy (5.83), after integrating by parts, can be written

$$\delta E=\int d^3r\left[\frac{\hbar^2}{2m^*(\mathbf{r})}\delta\tau(\mathbf{r})+U(\mathbf{r})\delta\rho(\mathbf{r})+\mathbf{W}(\mathbf{r})\delta\mathbf{J}(\mathbf{r})\right] \tag{5.97}$$

with an effective mass

$$m^*(\mathbf{r}) = m\left(1 + \frac{2m}{\hbar^2}\frac{1}{16}(3t_1 + 5t_2)\rho\right)^{-1}, \tag{5.98}$$

an average field

$$U(\mathbf{r}) = \frac{3}{4}t_0\rho + \frac{3}{16}t_3\rho^2 + \frac{1}{16}(3t_1 + 5t_2)\tau + \frac{1}{32}(5t_2 - 9t_1)\nabla^2\rho - \frac{3}{4}W_0\nabla\mathbf{J}, \tag{5.99}$$

and a one-body spin-orbit potential [we neglect the term $\frac{1}{32}(t_1 - t_2)\mathbf{J}^2$]

$$\mathbf{W}(\mathbf{r}) = \frac{3}{4}W_0\nabla\rho. \tag{5.100}$$

We now have to insert into Eq. (5.96) the variations $\delta\tau$, $\delta\rho$, and $\delta\mathbf{J}$ with respect to φ_k. From definitions (5.84)–(5.86) we get

$$\delta E = 2\sum_{i=1}^{A}\int d^3r\,\delta\varphi_i^*\left\{-\nabla\frac{\hbar^2}{2m_\tau^*}\nabla + U + \mathbf{W}\frac{1}{i}(\nabla\times\boldsymbol{\sigma})\right\}\varphi_i \tag{5.101}$$

and, using Eq. (5.96), we finally find the HF-equation in coordinate space viz:

$$\left\{-\nabla\frac{\hbar^2}{2m^*(\mathbf{r})}\nabla + U(\mathbf{r}) + \mathbf{W}\frac{1}{i}(\nabla\times\boldsymbol{\sigma})\right\}\varphi_i(\mathbf{r}) = \epsilon_i\varphi_i(\mathbf{r}). \tag{5.102}$$

Table 5.3 Experimental and calculated root mean square radii (in fm) and binding energies (in MeV) per nucleon

		Experiment	Negele [Ne 70]	Campi and Sprung [CS 72]	Nemeth et al. [NMH 73]	Skyrme III [BFG 75]
^{16}O	E	−7.98	−6.75	−7.68	−7.98	−7.96
	r_c	2.73	2.80	2.75	2.77	2.69
^{40}Ca	E	−8.55	−7.49	−8.33	−8.47	−8.54
	r_c	3.49	3.49	3.49	3.40	3.48
^{48}Ca	E	−8.67	−7.48	−8.40	−8.55	−8.71
	r_c	3.48	3.52	3.51	3.44	3.53
^{90}Zr	E	−8.71	−7.85	−8.63	−8.70	−8.71
	r_c	4.23	4.25	4.27	4.13	4.32
^{208}Pb	E	−7.87	−7.53	−7.87	−7.87	−7.87
	r_c	5.50	5.44	5.45	5.22	5.57

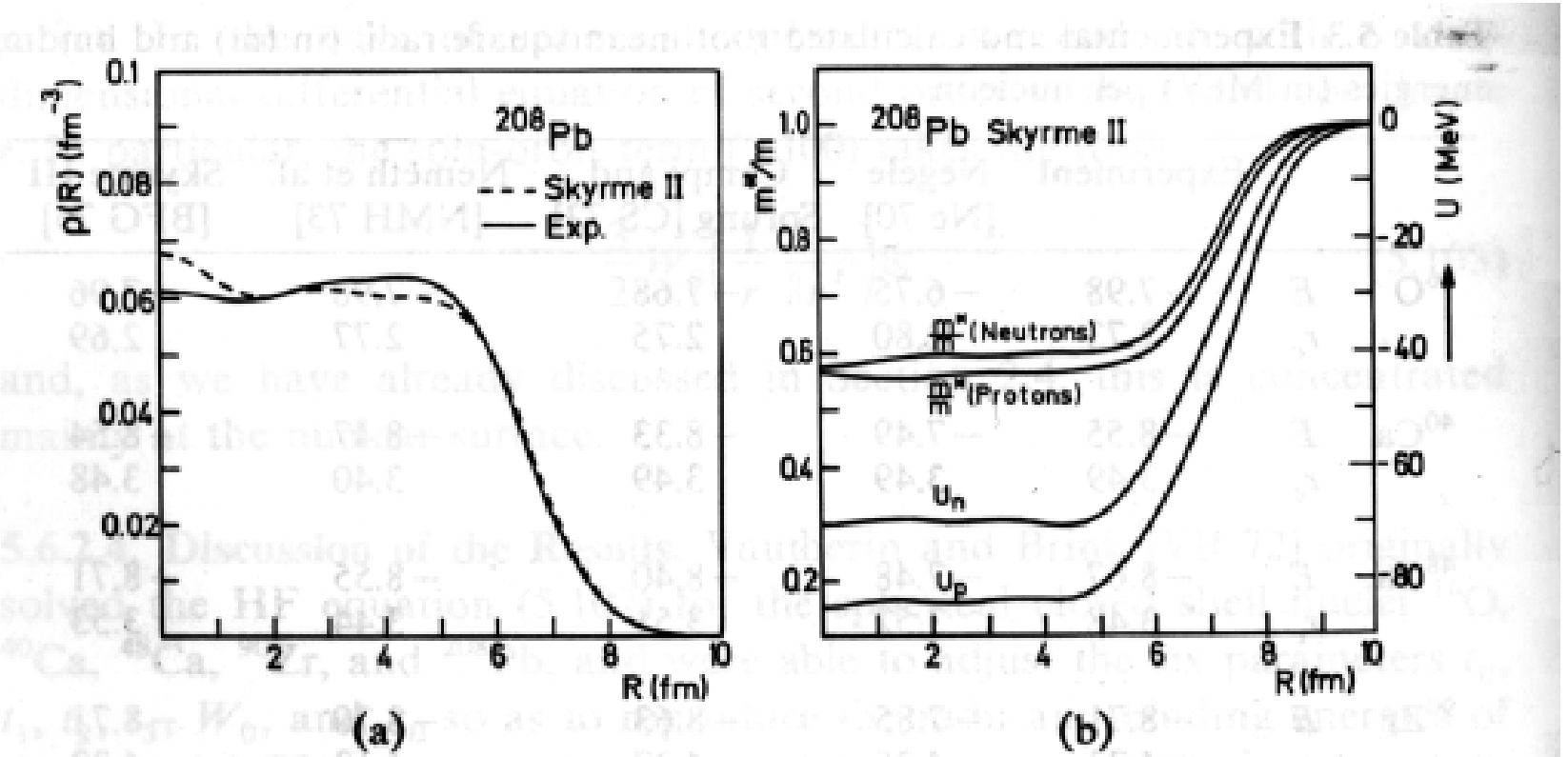

Figure 5.5. Hartree–Fock results for ^{208}Pb with the interaction Skyrme II. (a) Charge distribution. (b) Effective mass m^*/m and HF-potential $U(r)$ (the proton single-particle potential does not include the Coulomb term). (From [VB 72].)

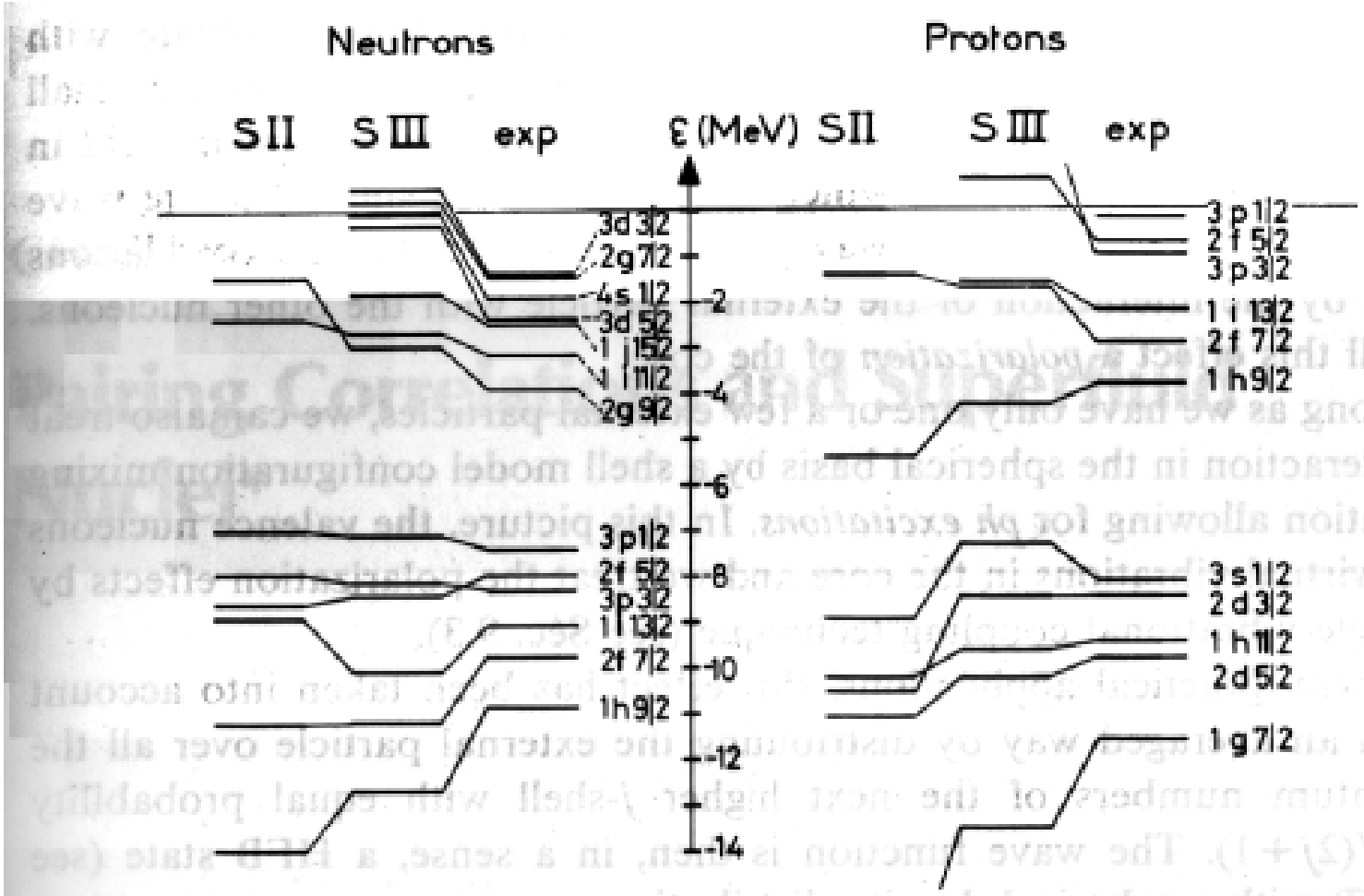

Figure 5.6. Experimental and calculated single-particle energies in the lead region. The calculated values were obtained with two different versions of the Skyrme force. With increasing effective mass, we recognize a compression of the spectrum ($m^*/m \simeq 0.6$ for SII and $\simeq 0.75$ for SIII). (From [BFG 75].)

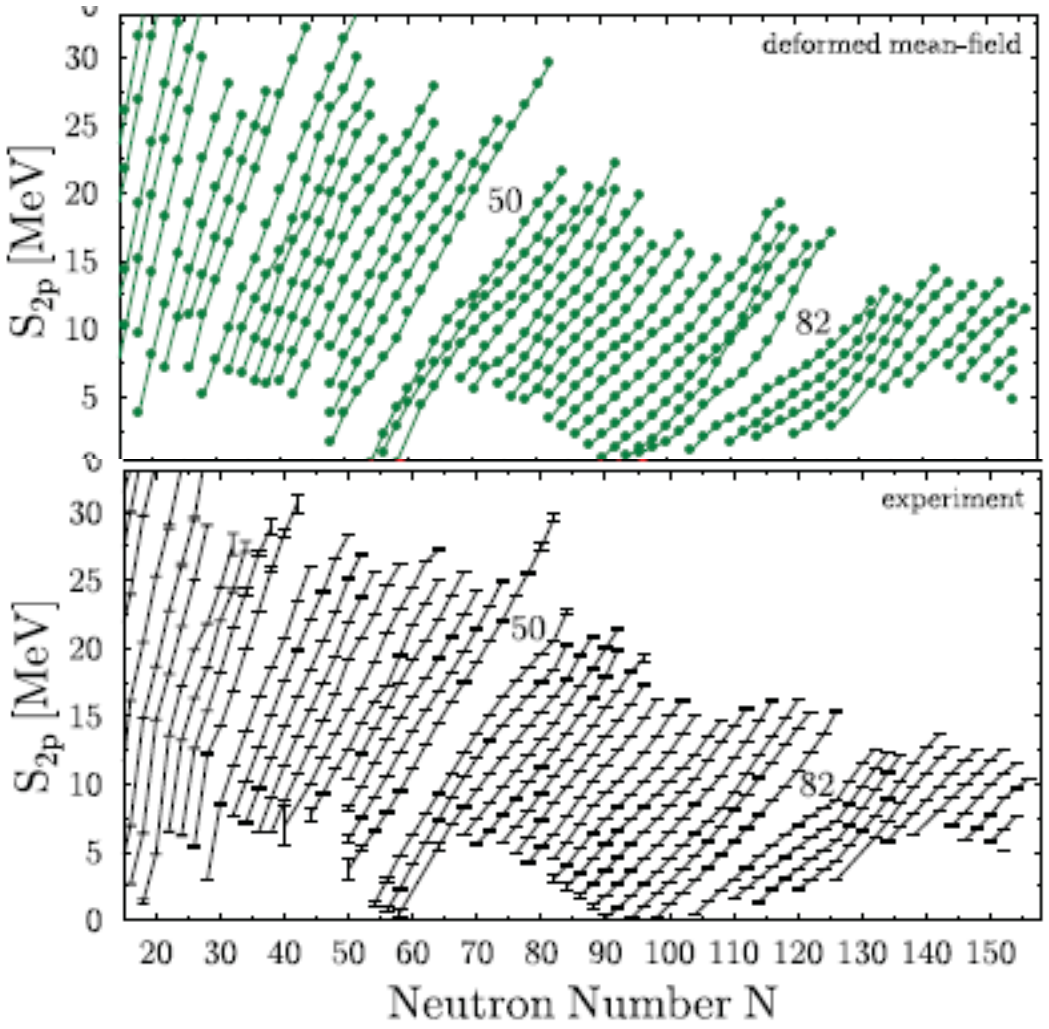

FIG. 3. (Color online) Two proton-separation energy S_{2p} for even-even nuclei. Lines connect nuclei in isotonic chains.

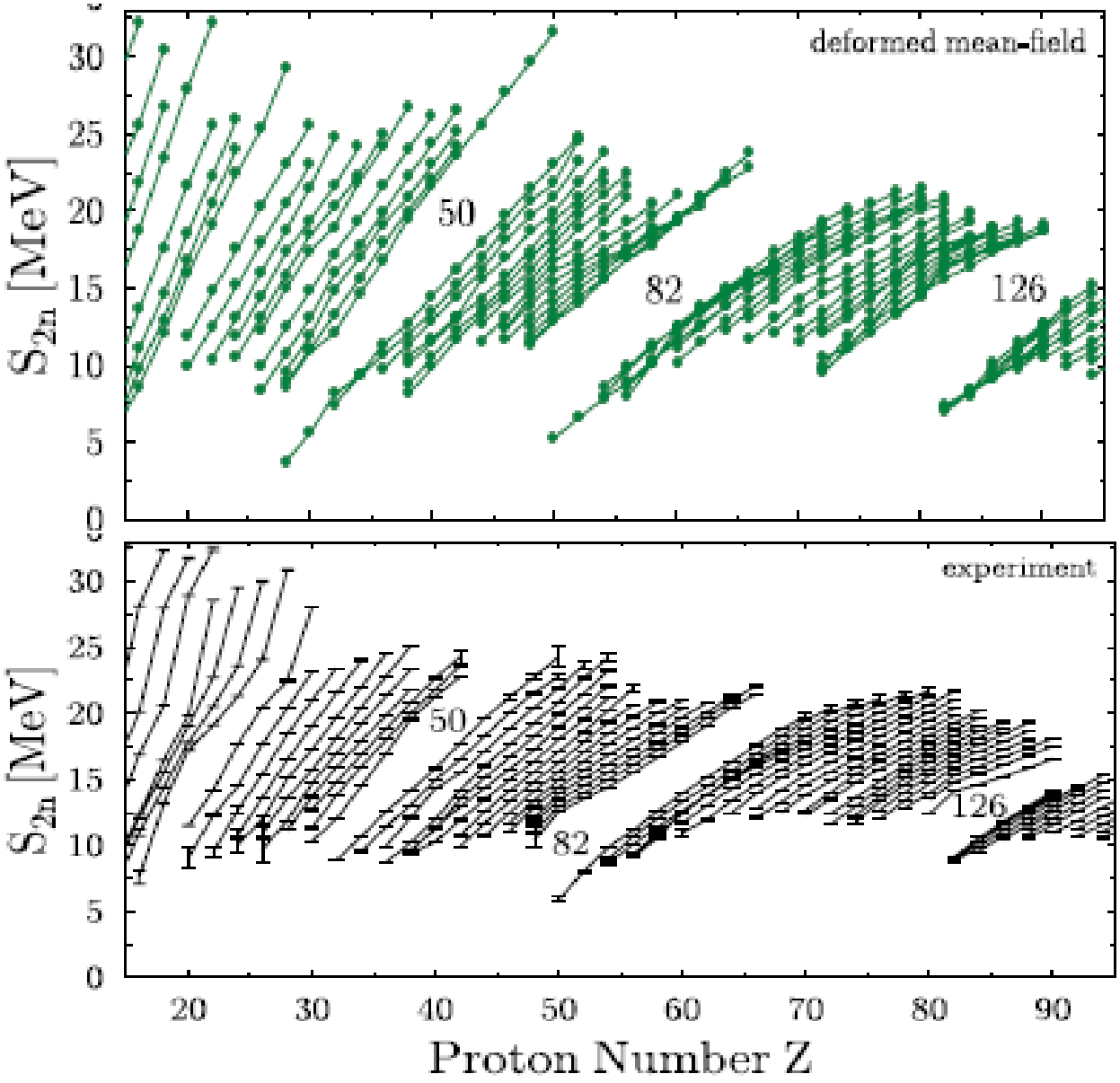

FIG. 4. (Color online) Two-neutron separation energy S_{2n} for even-even nuclei. Lines connect nuclei in isotopic chains.

Спасибо за внимание !