

## Chapter 3

# Independent-particle model for fermions in finite systems

Very useful descriptions for finite systems comprised of fermions can be obtained by identifying a one-body potential that already generates some of the physics associated with the interaction between the particles. This one-body potential together with the kinetic energy and other relevant one-body potentials, like the Coulomb attraction to the nucleus for electrons in atoms, forms a useful starting point to discuss the physics for such systems. In particular, it leads to a shell-model description which is relevant for atoms, nuclei, and other localized many-fermion systems. In addition, such a Hamiltonian may be used as a starting point of the perturbation expansion of relevant physical quantities as will be discussed in Ch. 9. The general discussion of this independent-particle description where fermions do not interact but are aware of each other's identity, will be given in Sec. 3.1. The application of the independent-particle model to electrons in atoms is presented in Sec. 3.2 and for nucleons in nuclei in Sec. 3.3. An important hypothetical system entitled “nuclear matter” is introduced in Sec. 3.3.1. It represents an idealized way to represent and study the global properties of the interior of nuclei which exhibit strikingly similar features for nuclei heavier than  $^{16}\text{O}$ . In Sec. 3.4 the method of second quantization is applied to the concept of isospin as it is relevant for the description of nuclei.

### 3.1 General results and the independent-particle model

A solvable many-particle problem is obtained by considering the following decomposition of the original Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \hat{H}_0 + \hat{H}_1, \quad (3.1)$$

where

$$\hat{H}_0 = \hat{T} + \hat{U} \quad (3.2)$$

and

$$\hat{H}_1 = \hat{V} - \hat{U} \quad (3.3)$$

with  $\hat{U}$  a suitably chosen one-body operator. When only  $\hat{H}_0$  is considered the corresponding many-particle problem can be solved straightforwardly. Note that a one-body external field  $\hat{U}_{ext}$  can also be included in  $\hat{H}_0$  if appropriate.

There are various situations in which the choice of  $\hat{U}$  is very important. In general, it can be used to include the average effect of the two-body interaction  $\hat{V}$ . One may then hope that the remaining effects of  $\hat{V}$  are small as in the case of atoms. If the actual ground state of the system breaks a symmetry which the Hamiltonian respects, the choice of  $\hat{U}$  is critical. Systems with spontaneous magnetization provide an example. In such cases it can be fruitful to add to the Hamiltonian  $\hat{H}_0$  a term which includes the symmetry-breaking effect and yields a noninteracting ground state which displays this behavior. Clearly, using such a starting point in a framework based on perturbation theory suggests better convergence properties than starting from a noninteracting state with the “wrong” symmetry. A potential feature of  $\hat{U}$  is therefore that it can speed up the convergence of the perturbation expansion. In the case of nuclei, one can use  $\hat{U}$  to localize the nucleons in a well so that, as a starting point, one can use the many-particle states which are eigenstates of  $\hat{H}_0$  and therefore localized. Not doing this results in having to deal with plane-wave many-particle states which are the eigenstates of  $\hat{T}$  and thus not localized complicating the description of the nucleus substantially.

One may assume that it is not too difficult to solve the relevant sp problem especially when angular momentum is conserved in the case of spherical symmetry. Such a sp problem may however require a numerical solution. Assuming this problem to be solved, one may denote the relevant eigenstates and energies of  $H_0$  by

$$H_0 |\lambda\rangle = (T + U) |\lambda\rangle = \epsilon_\lambda |\lambda\rangle. \quad (3.4)$$

The corresponding second-quantized Hamiltonian  $\hat{H}_0$  using this  $\{|\lambda\rangle\}$  basis

can then be written as

$$\begin{aligned}\hat{H}_0 &= \sum_{\lambda\lambda'} \langle \lambda | (T + U) | \lambda' \rangle a_\lambda^\dagger a_{\lambda'} \\ &= \sum_{\lambda\lambda'} \epsilon_{\lambda'} \delta_{\lambda,\lambda'} a_\lambda^\dagger a_{\lambda'} = \sum_{\lambda} \epsilon_{\lambda} a_\lambda^\dagger a_{\lambda}\end{aligned}\quad (3.5)$$

using Eq. (3.4). All the many-particle eigenkets of  $\hat{H}_0$  for  $N$  particles are then of the form

$$|\Phi_n^N\rangle = |\lambda_1 \lambda_2 \dots \lambda_N\rangle = a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger \dots a_{\lambda_N}^\dagger |0\rangle \quad (3.6)$$

with eigenvalue

$$E_n^N = \sum_{i=1}^N \epsilon_{\lambda_i}. \quad (3.7)$$

This result can be obtained by employing Eqs. (2.34) and (2.35) for this particular case which is simplified by noting that Eq. (2.34) corresponds to

$$[\hat{H}_0, a_{\lambda_i}^\dagger] = \epsilon_{\lambda_i} a_{\lambda_i}^\dagger. \quad (3.8)$$

For obvious reasons the states  $|\Phi_n^N\rangle$  are called independent-particle states since the only correlation they include pertains to the Pauli principle preventing the particles to occupy the same sp state. The state with the lowest energy for  $N$  particles is then obtained by filling the lowest sp levels in accord with the Pauli principle. This state may be a nondegenerate state when  $N$  corresponds to a shell closure (a situation with complete occupation according to the degeneracies of the occupied levels) for the system under consideration. This state is usually written as

$$|\Phi_0^N\rangle = \prod_{\lambda_i \leq F} a_{\lambda_i}^\dagger |0\rangle, \quad (3.9)$$

where  $F$  characterizes the energy level above which all levels are empty and below which all levels are completely occupied. This state  $|\Phi_0^N\rangle$  is sometimes referred to as the Fermi sea. The present discussion completely solves the many-fermion problem in terms of generating all the eigenstates and eigenenergies for any particle number  $N$ . This result only requires the solution of the relevant sp problem given by Eq. (3.4) and the proper inclusion of the Pauli principle which is facilitated by the use of second quantization.

### 3.2 Electrons in atoms

In the description of atoms most aspects of the physics can be understood on the basis of the following Hamiltonian [Lindgren and Morrison (1982)]

$$H^N = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} - \sum_{i=1}^N \frac{Ze^2}{|\mathbf{r}_i|} + \frac{1}{2} \sum_{i \neq j}^N \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + V_{mag}, \quad (3.10)$$

where  $e^2 = 1.44 \times 10^{-9} \text{eV m}$ . Note that in [Lindgren and Morrison (1982)] atomic units are used. The various parts of this Hamiltonian for  $N$  electrons correspond, in this order, to: the kinetic energy of the electrons, the attraction to the nucleus of charge  $Z$  which is assumed to be infinitely heavy, the Coulomb repulsion between the electrons, and, finally, the magnetic interactions. The latter interactions include the spin-own-orbit interaction, the spin-other-orbit interaction, and the less important spin-spin and orbit-orbit interactions. The actual form of the magnetic interactions can be obtained systematically for a single-electron system by using a non-relativistic reduction of the Dirac equation [Cohen-Tannoudji *et al.* (1992), ]. For a many-electron system this procedure cannot be applied and this problem is still being studied. Since these magnetic interactions are rather small perturbations compared to the other three contributions to the Hamiltonian, it is conventional to lump them together in an effective one-body spin-orbit interaction which has been shown to simulate most of the magnetic interaction effects:

$$V_{mag} \Rightarrow V_{so}^{eff} = \sum_i \zeta_i \ell_i \cdot \mathbf{s}_i \quad (3.11)$$

where the sum runs only over electrons in the open shells and  $\zeta$  describes the strength of this effective sp spin-orbit interaction.

The Hamiltonian for the electrons in an atom can be considered theoretically well founded. Nevertheless, it should be clear that non-relativistic calculations must at some stage be complemented by considering relativity explicitly. This becomes more urgent for heavier atoms since the Hydrogen-like binding increases with  $Z^2$  becoming a sizable fraction of the electron's rest mass while the increased localization of the  $1s$  wave function also leads to high-momentum components.

Sensible atomic many-body calculations can be performed by neglecting the magnetic interactions altogether as will be done in the following discussion. A characteristic feature of electron shell structure is exemplified

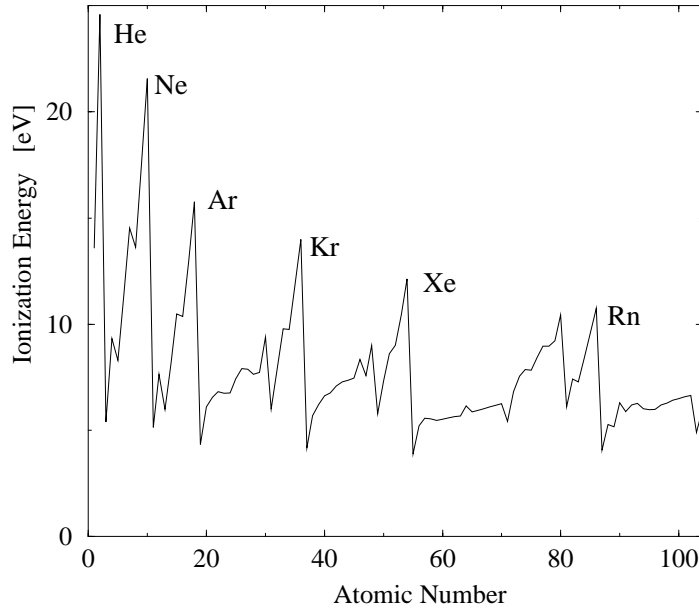


Fig. 3.1 Ionization energies for neutral atoms. At the positions of the noble gases (indicated in the figure) large jumps occur, illustrating shell closures.

by the ionization energies for neutral atoms shown in Fig. 3.1 which exhibit marked jumps at the noble gases. A simple starting point to describe features associated with shell closures for atoms is provided by the choice

$$H_0^N = \sum_{i=1}^N H_0(i) \quad (3.12)$$

with

$$H_0(i) = \frac{\mathbf{p}_i^2}{2m} - \frac{Ze^2}{r_i} + U(\mathbf{r}_i). \quad (3.13)$$

The auxiliary sp potential  $U$  must contain a large portion of the effect of the Coulomb repulsion between the electrons. The simple atomic shell model and the types of sp levels that one encounters are already generated by considering the Hydrogen-like Hamiltonian in which  $U$  is absent but a nuclear charge of  $Z$  is maintained. Clearly, the previous results for the lowest energy, non-interacting many-electron state of this  $\hat{H}_0$  problem can be immediately applied: electrons will occupy the lowest sp energy states

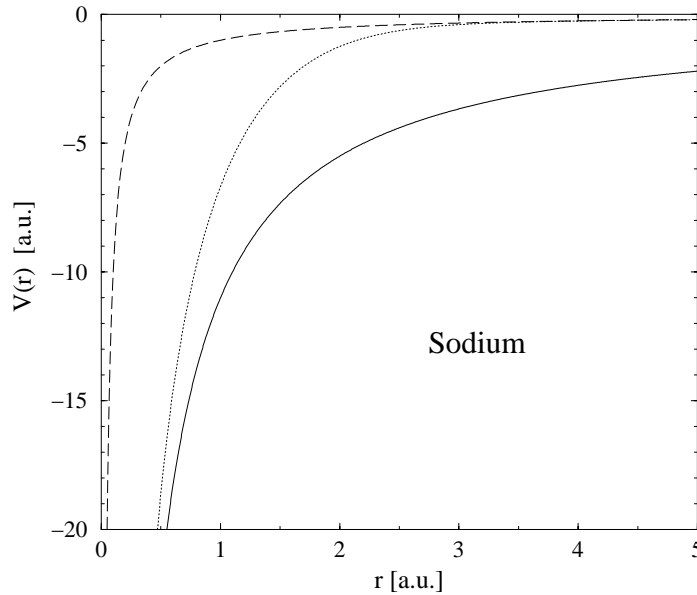


Fig. 3.2 Illustration of the effective Coulomb potential for the last electron in Na (dotted line). Close to the nucleus this potential approaches the full attraction of the nucleus ( $-Ze^2/r$ ) shown by the full line whereas at larger distances the screening of the other electrons reduces this attraction to  $-e^2/r$  shown by the dashed line.

in accordance with the Pauli principle, *i.e.* for each energy level there is a  $(2\ell + 1) * (2s + 1)$ -fold degeneracy resulting from the rotational invariance and spin-independence of the Hamiltonian. An additional, accidental degeneracy exists for this problem which results in *sp* energies which are only determined by the radial quantum number  $n$ .

This degeneracy is lifted when the effect of the closed shells is approximately included in  $U$ . Clearly this effect is an essential ingredient to explain the observed ionization energies illustrated in Fig. 3.1. A simple example, including  $U$ , is provided by considering the alkali atoms. These atoms have one electron outside a closed shell. At large distances one expects the presence of the closed electron shell(s) to screen the nuclear charge leading to an attraction of only one unit of charge. Very close to the nucleus, the electron will experience the full attraction of the nuclear charge. Both features are illustrated in Fig. 3.2. The presence of closed shells is expected to generate a spherically symmetric field due to the filling of all  $m_\ell$  and  $m_s$  substates. A smooth interpolation between these two extreme cases therefore provides

a reasonable picture of  $U$  as shown for Na in Fig. 3.2. Using this effective potential leads to the lifting of the accidental degeneracy of the Hydrogen-like Hamiltonian in such a way that the level with the highest probability to be close to the nucleus will profit most in energy. This implies a lowering of the  $s$  state with respect to the  $p$  state and so on, for a given shell with radial quantum number “ $n$ ” which now becomes a quantum number distinguishing the states with the same  $\ell$  value. For the Sodium atom this leads to the filling of the corresponding  $1s, 2s$ , and  $2p$  shells with the notation:  $(1s)^2(2s)^2(2p)^6$ . The last electron will therefore occupy the  $3s$  shown in Fig. 3.3.

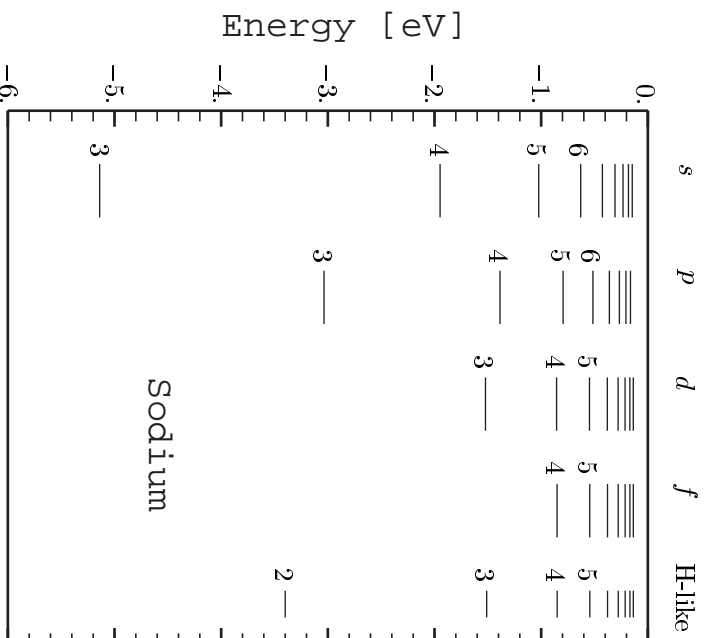


Fig. 3.3 Energy levels of the Na atom illustrating the tendency of levels with increasing “ $n$ ” and  $\ell$  to be more hydrogen-like. The latter energies are displayed in the last column. The first column corresponds to the available  $s$  states for the last electron, the second column to available  $p$  states, etc.

Excited states for this atom are then obtained by removing the last electron from the  $3s$  and placing it in one of the other  $sp$  states as illustrated in Fig. 3.3. Suppose the states  $|n\ell m_\ell m_s\rangle$  are eigenkets of  $H_0$  in Eq. (3.13)

$$H_0 |n\ell m_\ell m_s\rangle = \epsilon_{n\ell} |n\ell m_\ell m_s\rangle, \quad (3.14)$$

where  $n$  no longer refers to the Hydrogen-like quantum number but still characterizes the radial behavior of the corresponding wave functions. The ground state, *i.e.* state with the lowest energy, representing Na in this approximation is then given by

$$|300m_s, 211\frac{1}{2}, 211-\frac{1}{2}, \dots, 100\frac{1}{2}, 100-\frac{1}{2}\rangle \quad (3.15)$$

where for each occupied state the four quantum numbers  $n\ell m_\ell m_s$  are given. This state can also be written as

$$a_{300m_s}^\dagger a_{211\frac{1}{2}}^\dagger a_{211-\frac{1}{2}}^\dagger \dots a_{100\frac{1}{2}}^\dagger a_{100-\frac{1}{2}}^\dagger |0\rangle. \quad (3.16)$$

A similar interpretation of the spectra can be given for the spectra of the other alkali atoms. The fact that a simple understanding of such atoms can be obtained based on such simple considerations, indicates that it must indeed be possible to represent the effect of the interaction of the electrons among themselves by an average  $sp$  potential. The determination of this average  $sp$  potential from the electron-electron interaction will then require the explicit consideration of the two-body interaction by employing the Hartree-Fock procedure as discussed in Ch. 11.

Another simple confirmation of the atomic shell model picture is provided by considering the excited states of the Neon atom shown in Fig. 3.4. This atom has the  $(1s)^2(2s)^2(2p)^6$  configuration occupied in the ground state and corresponds to a closed-shell system. All the excited levels can be understood in terms of the promotion of the last occupied  $2p$ -electron to an unoccupied orbital starting with the  $3s$ ,  $3p$ ,  $3d$ ,  $4s$ ,  $4p$  and so on. In terms of particle addition and removal operators these states can be obtained from the closed-shell ground state which is written as  $|\Phi_0^N\rangle$  as follows

$$a_{3s}^\dagger a_{2p} |\Phi_0^N\rangle \quad (3.17)$$

represents schematically the lowest possible excited states. The presence of more than one energy level at the position of a state like Eq. (3.17) is due to the splitting that results from the inclusion of the magnetic interactions

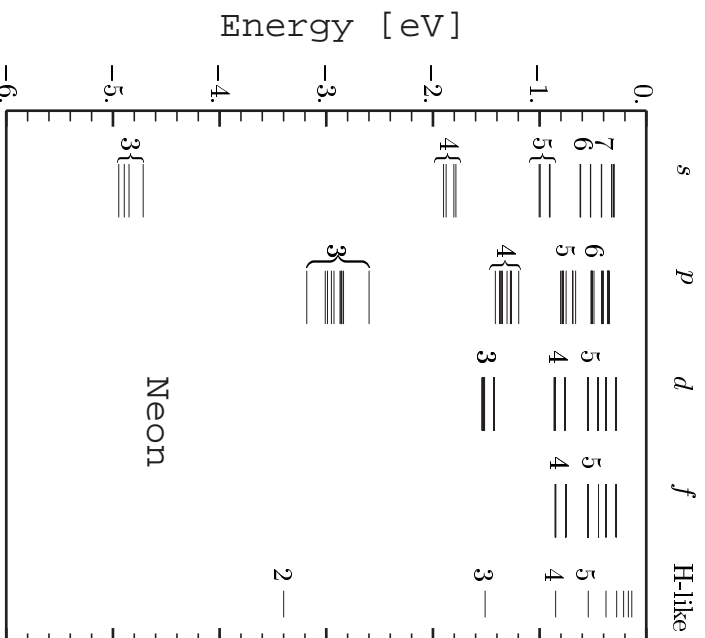


Fig. 3.4 Energy levels of the Ne atom which can be interpreted as the promotion of a  $2p$  electron to the available empty orbitals starting with  $3s$  etc. Also for this atom the energies of the states tend to become more Hydrogen-like with increasing “ $n$ ” and  $l$ .

as well as from the different action of the Coulomb interaction depending on which total angular momentum the resulting configuration has.

### 3.3 Nucleons in nuclei

The shell structure observed in atoms is also found in nuclei. The origin of shell structure in nuclei is, however, quite different. In addition, it is not as simple to understand as in the atomic case. The shell structure in atoms can be demonstrated by considering the ionization potential. Shell closures at 2, 10, 18, 36, 54, and 86 which signal the position of the noble