

Chapter 5

Noninteracting Fermi gas

The consequences of the Pauli principle for an assembly of fermions that is localized in space has been discussed in Ch. 3. The resulting shell model or independent-particle model of an atom or a nucleus provides an appropriate starting point for further study of these systems that will be taken up in Chs. 11 and 13. When dealing with a large homogeneous system it is practical to take advantage of translation invariance in choosing a sp basis. The special role of the momentum or wave vector basis is therefore clear. The corresponding “shell model” of such an infinite system is referred to as the Fermi gas. Relevant details for the description of this system are presented in Sec. 5.1. An important idealization of a system of electrons in a metal, the electron gas, is introduced in Sec. 5.2. Fermi gas considerations are relevant for several other infinite systems and are briefly reviewed in Secs. 5.3 for nuclear and neutron matter, and in Sec. 5.4 for the ${}^3\text{He}$ liquid.

5.1 The Fermi gas at zero temperature

For an important class of systems the Fermi gas is a good starting point. It is instructive to consider this system first at zero temperature. Later applications involving fermions at finite T will be presented in Chs. 6 and 18. A Fermi gas is an idealized system that contains fermions with no mutual interaction. Each particle therefore only contributes its kinetic energy

$$H_0 = T = \frac{\mathbf{p}^2}{2m}. \quad (5.1)$$

Eigenstates of Eq. (5.1) are momentum eigentates. If we assume spin- $\frac{1}{2}$ fermions, one has

$$\frac{\mathbf{p}^2}{2m} |\mathbf{p}' m_s\rangle = \frac{\mathbf{p}'^2}{2m} |\mathbf{p}' m_s\rangle. \quad (5.2)$$

In general, one can label the discrete spin and/or isospin quantum numbers with an index μ . This includes the possibility that only one (spin/isospin) species of fermions is contained in the system. If we consider the momentum states in a box with sides L and volume $V = L^3$ one can write the sp wave function as

$$\langle \mathbf{r} | \mathbf{p} m_s \rangle = \frac{1}{\sqrt{V}} \exp \left\{ \frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r} \right\} |m_s\rangle. \quad (5.3)$$

Normalization can be chosen as follows

$$\langle \mathbf{p}' m'_s | \mathbf{p} m_s \rangle = \delta_{\mathbf{p}', \mathbf{p}} \delta_{m'_s, m_s}. \quad (5.4)$$

Suppressing spin and using the wave function from Eq. (5.3) this translates into

$$\langle \mathbf{p}' | \mathbf{p} \rangle = \int_{box} d\mathbf{r} \langle \mathbf{p}' | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{p} \rangle = \frac{1}{V} \int_{box} d\mathbf{r} \exp \left\{ \frac{i}{\hbar} (\mathbf{p} - \mathbf{p}') \cdot \mathbf{r} \right\} = \delta_{\mathbf{p}', \mathbf{p}}. \quad (5.5)$$

Usually one is interested in the situation where the size of the box goes to infinity ($L \rightarrow \infty$). Before doing this, it is convenient to introduce periodic boundary conditions as suggested by translational invariance. In the x -direction, for example, one requires

$$e^{ik_x x} = e^{ik_x(x+L)} = e^{ik_x x} e^{ik_x L}, \quad (5.6)$$

where $p_x = \hbar k_x$. This result implies that

$$\cos(k_x L) + i \sin(k_x L) = 1, \quad (5.7)$$

which is fulfilled when

$$k_x = n_x \frac{2\pi}{L} \quad n_x = 0, \pm 1, \pm 2, \dots \quad (5.8)$$

and similarly for k_y and k_z . This means that each triple $\{k_x, k_y, k_z\}$ corresponds to a triple of integers $\{n_x, n_y, n_z\}$. Since the Pauli principle allows only a fixed number of fermions in each sp momentum eigenstate (depending on the spin and/or isospin degeneracy), the ground state is obtained by filling the momentum states up to a maximum value, the Fermi momentum $p_F = \hbar k_F$. The maximum wavenumber can be determined by calculating

the expectation value of the number operator (see Eq. (2.51)) in the ground state

$$|\Phi_0\rangle = \prod_{\mathbf{p}\mu, p < \hbar k_F} a_{\mathbf{p}\mu}^\dagger |0\rangle. \quad (5.9)$$

In order to obtain this result, it is now useful to consider the limit when both $N \rightarrow \infty$ and $V \rightarrow \infty$ in such a way that their ratio (the density) remains constant. This limit is sometimes referred to as the “thermodynamic limit.” Sums over states can now be replaced by integrations over continuous quantum numbers like wave vectors in the following way

$$\begin{aligned} \sum_{\mathbf{k}\mu} f(\mathbf{k}, \mu) &= \sum_{n_x n_y n_z} \sum_{\mu} f\left(\frac{2\pi\mathbf{n}}{L}, \mu\right) \\ L \rightarrow \infty &\Rightarrow \int d\mathbf{n} \sum_{\mu} f\left(\frac{2\pi\mathbf{n}}{L}, \mu\right) = \frac{V}{(2\pi)^3} \int d\mathbf{k} \sum_{\mu} f(\mathbf{k}, \mu) \end{aligned} \quad (5.10)$$

for any function f . The transition from discrete triples $\{n_x, n_y, n_z\}$ to continuous variables can be made in the case of large L since any physical quantity described by f will change slowly when one of the discrete variables changes by one unit. To obtain the Fermi wavenumber consider

$$\begin{aligned} N &= \langle \Phi_0 | \hat{N} | \Phi_0 \rangle = \sum_{\mathbf{k}\mu} \langle \Phi_0 | a_{\mathbf{k}\mu}^\dagger a_{\mathbf{k}\mu} | \Phi_0 \rangle = \sum_{\mathbf{k}\mu} \theta(k_F - k) \\ &= \frac{V}{(2\pi)^3} \sum_{\mu} \int d^3k \theta(k_F - k) = \frac{\nu V}{6\pi^2} k_F^3, \end{aligned} \quad (5.11)$$

where ν represents the spin/isospin degeneracy and θ denotes the step function. The relation between the Fermi wavenumber and the density therefore becomes

$$k_F = \left\{ \frac{6\pi^2 N}{\nu V} \right\}^{1/3} = \left\{ \frac{9\pi}{2\nu} \right\}^{1/3} \frac{1}{r_0}, \quad (5.12)$$

where in the last equality r_0 has been introduced which is obtained from the volume per particle

$$\frac{V}{N} = \frac{1}{\rho} = \frac{4}{3} \pi r_0^3. \quad (5.13)$$

Clearly r_0 also serves as a measure of the interparticle spacing. Conversely one can write the density as

$$\rho = \frac{N}{V} = \nu \frac{k_F^3}{6\pi^2}. \quad (5.14)$$

Eqs. (5.12) and (5.14) show that for a fixed density one has a smaller Fermi wavenumber when the degeneracy factor ν is larger.

The energy of the ground state of the Fermi gas is obtained by employing the kinetic energy operator

$$\hat{T} = \sum_{\mathbf{p}\mu} \sum_{\mathbf{p}'\mu'} \langle \mathbf{p}\mu | \frac{\mathbf{p}^2}{2m} | \mathbf{p}'\mu' \rangle a_{\mathbf{p}\mu}^\dagger a_{\mathbf{p}'\mu'} = \sum_{\mathbf{p}'\mu'} \frac{\mathbf{p}'^2}{2m} a_{\mathbf{p}'\mu'}^\dagger a_{\mathbf{p}'\mu'}. \quad (5.15)$$

One thus has to calculate

$$\hat{T} |\Phi_0\rangle = \left(\sum_{\mathbf{p}'\mu'} \frac{\mathbf{p}'^2}{2m} a_{\mathbf{p}'\mu'}^\dagger a_{\mathbf{p}'\mu'} \right) \prod_{\mathbf{p}\mu, p < \hbar k_F} a_{\mathbf{p}\mu}^\dagger |0\rangle. \quad (5.16)$$

Using Eq. (2.34) one obtains a kinetic energy contribution from each sp state that is occupied in $|\Phi_0\rangle$

$$\hat{T} |\Phi_0\rangle = \left(\sum_{\mathbf{p}\mu, p < \hbar k_F} \frac{\mathbf{p}^2}{2m} \right) |\Phi_0\rangle. \quad (5.17)$$

The energy of the ground state is then obtained by taking the appropriate continuum limit discussed above

$$\begin{aligned} E_0 &= \sum_{\mathbf{p}\mu, p < \hbar k_F} \frac{\mathbf{p}^2}{2m} = \frac{V}{(2\pi)^3} \sum_{\mu} \int d^3k \frac{\hbar^2 k^2}{2m} \theta(k_F - k) \\ &= V \frac{\nu}{(2\pi)^3} 4\pi \frac{\hbar^2}{2m} \frac{1}{5} k_F^5. \end{aligned} \quad (5.18)$$

One may therefore write in the thermodynamic limit for the energy per particle

$$\frac{E_0}{N} = \frac{V}{N} \frac{\nu}{2\pi^2} \frac{\hbar^2 k_F^5}{10m} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} = \frac{3}{5} \varepsilon_F = \frac{3}{5} k_B T_F, \quad (5.19)$$

where Eq. (5.14) has been used and the Fermi energy (for the Fermi gas) and temperature have been introduced by the last equalities while denoting Boltzmann's constant by k_B .

5.2 Electron gas

Various different systems qualify to be considered in terms of this simple Fermi gas model. A very important example is provided by the homogeneous electron gas which provides a first approximation to a metal or a plasma. One assumes that the positive ions yield a uniform background yielding a total system that is electrically neutral. One neglects therefore the motion of the ions which, at least in first approximation, is permissible due to their much larger mass. The uniform background assumption is less appropriate but the system is nevertheless of great importance. We note that the degeneracy factor $\nu = 2$. It is also customary to use the Bohr radius ($a_0 = \hbar^2/mc^2 = 5.29 \cdot 10^{-11} \text{ m} = 0.529 \text{ \AA}$) to introduce a dimensionless parameter for this system given by

$$r_s = \frac{r_0}{a_0}. \quad (5.20)$$

A metallic element contains N_A (Avogadro's number) atoms per mole and ρ_m/A moles per cm^3 , where ρ_m is the mass density (in grams per cm^3), and A is the atomic mass. If one assumes that each atom contributes Z electrons to conduction, the number of free electrons per cubic centimeter is

$$\rho = \frac{N}{V} = 6.02205 \times 10^{23} \frac{Z\rho_m}{A}. \quad (5.21)$$

Assuming $Z = 1$ for alkali metals yields densities (at a temperature of 5K) of 0.91 for Cs, 1.15 for Rb, 1.40 for K, and 2.65 for Na times $10^{22}/\text{cm}^3$. Corresponding values of r_s are 5.62 for Cs, 5.20 for Rb, 4.86 for K, and 3.93 for Na, respectively. This translates into Fermi wavenumbers ranging from 0.65 \AA^{-1} for Cs to 0.92 \AA^{-1} for Na. The corresponding range of Fermi energies and temperatures is given by 1.59 eV and $1.84 \times 10^4 \text{ K}$ for Cs, and 3.24 eV and $3.77 \times 10^4 \text{ K}$ for Na. The electron gas model can also be used in its relativistic version to model white dwarf stars. One typically assumes that the star contains the nuclei of He atoms (α particles) and electrons [Landau and Lifshitz (1980); Huang (1987)]. Note that for realistic conditions it is necessary to treat the electrons relativistically due to the high density of such a system.

Perhaps surprisingly, properties of the interacting (not free) electron gas are also used extensively in quantum chemistry, within the framework of modern density functional theory (DFT). In DFT the energy of any electronic system (also strongly inhomogeneous ones like atoms or molecules)

are expressed as a universal functional of the local electron density in the system. While the structure of this functional is unknown, it should become equal to the electron gas result in the limit of slowly varying electron densities. This feature is used as an important constraint in the construction of phenomenological density functionals [Dreizler and Gross (1990)].

We will now consider more details of this electron gas. This infinite Fermi system consists of a homogeneous distribution of electrons at density ρ interacting through their mutual Coulomb repulsion. To keep the system electrically neutral an inert background distribution of positive charge with the same density is added. The electrostatic energy of this positive background is simply

$$E_b = \frac{1}{2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{e^2 \rho^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{1}{2} e^2 \rho^2 V \int d\mathbf{r} \frac{1}{r}, \quad (5.22)$$

which shows that the energy per particle, (E_b/N) , diverges in the thermodynamic limit because of the long-range nature of the Coulomb potential. Note that we have assumed that the density appeared in Eq. (5.22) is the same everywhere. As the system is globally charge-neutral we expect a finite result if we add E_b to similar contributions of the electron-electron and electron-background interaction. To look at this cancellation in a controlled manner it is convenient to replace momentarily the Coulomb interaction $1/r$ with the Yukawa-type interaction $V(r) = \pm e^2 e^{-\mu r}/r$, so that e.g. the energy of the background now reads

$$E_b = \frac{1}{2} e^2 \rho^2 V \int d\mathbf{r} \frac{e^{-\mu r}}{r} = \frac{1}{2} e^2 \rho^2 V \frac{4\pi}{\mu^2}. \quad (5.23)$$

The interaction between the electrons and the background charge distribution gives rise to the following one-body potential for the electrons

$$U(r) = -e^2 \rho \int d\mathbf{r}' \frac{e^{-\mu|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = -e^2 \rho \int d\mathbf{r}' \frac{e^{-\mu r'}}{r'} = -e^2 \rho \frac{4\pi}{\mu^2}. \quad (5.24)$$

This potential is just a constant, as a consequence of translational invariance. The contribution to the total energy per electron is therefore

$$E_{e-b} = N(-e^2 \rho \frac{4\pi}{\mu^2}) = -e^2 \rho^2 V \frac{4\pi}{\mu^2}. \quad (5.25)$$

The matrix elements of Yukawa and Coulomb interactions in a plane-wave basis were already derived in Eqs. (4.33) and (4.34), respectively.

Including also the possible spin projection $m_s = \pm\frac{1}{2}$ of the electron spin states, the electron-electron interaction is therefore given by

$$(\mathbf{p}_1 m_1, \mathbf{p}_2 m_2 | V | \mathbf{p}_3 m_3, \mathbf{p}_4 m_4) = \delta_{m_1, m_3} \delta_{m_2, m_4} \delta_{\mathbf{P}, \mathbf{P}'} \frac{4\pi e^2}{V} \frac{1}{(\mathbf{p} - \mathbf{p}')^2 + \mu^2}. \quad (5.26)$$

Note that a spin-independent interaction is necessarily diagonal in the spin labels, and that we introduced center-of-mass and relative momenta,

$$\begin{aligned} \mathbf{P} &= \mathbf{p}_1 + \mathbf{p}_2, & \mathbf{p} &= \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2), \\ \mathbf{P}' &= \mathbf{p}_3 + \mathbf{p}_4, & \mathbf{p}' &= \frac{1}{2}(\mathbf{p}_3 - \mathbf{p}_4). \end{aligned} \quad (5.27)$$

For the second-quantized form of the electron-electron interaction we therefore have

$$\begin{aligned} \hat{V} &= \frac{1}{2} \sum_{\substack{\mathbf{p}_1 \mathbf{p}_2 m_1 m_2 \\ \mathbf{p}_3 \mathbf{p}_4 m_3 m_4}} (\mathbf{p}_1 m_1, \mathbf{p}_2 m_2 | V | \mathbf{p}_3 m_3, \mathbf{p}_4 m_4) a_{\mathbf{p}_1 m_1}^\dagger a_{\mathbf{p}_2 m_2}^\dagger a_{\mathbf{p}_4 m_4} a_{\mathbf{p}_3 m_3} \\ &= \frac{1}{2} \sum_{\substack{\mathbf{P} \mathbf{p} \mathbf{p}' \\ m_1 m_2}} \frac{4\pi e^2}{V} \frac{1}{(\mathbf{p} - \mathbf{p}')^2 + \mu^2} a_{\frac{1}{2}\mathbf{P}+\mathbf{p}, m_1}^\dagger a_{\frac{1}{2}\mathbf{P}-\mathbf{p}, m_2}^\dagger a_{\frac{1}{2}\mathbf{P}-\mathbf{p}', m_2} a_{\frac{1}{2}\mathbf{P}+\mathbf{p}', m_1}. \end{aligned} \quad (5.28)$$

Let's now isolate the part of \hat{V} where no relative momentum is transferred, i.e. we split $\hat{V} = \hat{V}_d + \hat{V}'$ where \hat{V}_d contains the diagonal contributions in Eq. (5.28) having $\mathbf{p} = \mathbf{p}'$, and \hat{V}' contains the remainder. Since the interaction matrix element in \hat{V}_d is a constant, the result can be expressed in terms of the number operator,

$$\hat{V}_d = \frac{1}{2} \frac{4\pi e^2}{V \mu^2} \sum_{\substack{\mathbf{p}_1 \mathbf{p}_2 \\ m_1 m_2}} a_{\mathbf{p}_1 m_1}^\dagger a_{\mathbf{p}_2 m_2}^\dagger a_{\mathbf{p}_2 m_2} a_{\mathbf{p}_1 m_1} = \frac{1}{2} \frac{4\pi e^2}{V \mu^2} \hat{N}(\hat{N} - 1). \quad (5.29)$$

The contribution of \hat{V}_d to the total energy is therefore [note that in the thermodynamic limit $N(N-1) \rightarrow N^2$],

$$E_d = \frac{1}{2} \frac{4\pi e^2}{V \mu^2} N^2 = \frac{1}{2} \frac{4\pi e^2}{\mu^2} \rho^2 V. \quad (5.30)$$

This is the classical electrostatic repulsion of the electron charge density, which nicely cancels with corresponding terms E_b and E_{e-b} arising from the positive background.

The final electron gas Hamiltonian therefore becomes

$$\hat{H} = \hat{T} + \hat{V}' + E_d + E_{e-b} + E_b = \hat{T} + \hat{V}', \quad (5.31)$$

where \hat{V}' is

$$\hat{V}' = \frac{1}{2} \sum_{\substack{\mathbf{p}, \mathbf{p}' \\ m_1 m_2}} \frac{4\pi e^2}{V} \frac{1}{(\mathbf{p} - \mathbf{p}')^2} a_{\frac{1}{2}\mathbf{p}+\mathbf{p}, m_1}^\dagger a_{\frac{1}{2}\mathbf{p}-\mathbf{p}, m_2}^\dagger a_{\frac{1}{2}\mathbf{p}-\mathbf{p}', m_2} a_{\frac{1}{2}\mathbf{p}+\mathbf{p}', m_1}. \quad (5.32)$$

Since the summation is restricted to $\mathbf{p} \neq \mathbf{p}'$ there is now no danger in setting $\mu = 0$ and going back to the genuine Coulomb force. It is useful to evaluate the expectation value of this interaction in noninteracting ground state. This is left as an exercise for the reader. We will take up the discussion of the electron gas again in Chs. 11, 13, 14, and 16.

5.3 Nuclear and neutron matter

The hypothetical infinite system with $N = Z$ and no Coulomb interaction between protons is called nuclear matter and was introduced in Sec. 3.3.1. This system should reflect two essential numbers in nuclear physics that characterize global properties of nuclei. The first number is associated with the observed density in the interior of nuclei corresponding to 0.16 nucleons per fm^3 . The corresponding wavenumber according to Eq. (5.12) using a degeneracy factor of 4 for nuclear matter is therefore $k_F = 1.33 \text{ fm}^{-1}$. In terms of the interparticle spacing one has $r_0 = 1.14 \text{ fm}$ comparable to the minimum in the interaction in the $T = 1$ channel (see Fig.). This density is referred to as the saturation or normal density of nuclear matter. According to the volume term of the empirical mass formula which survives in this limit one therefore expects a binding at this density corresponding to about 16 MeV per particle. Nuclear matter calculations starting from realistic interactions are therefore expected to explain these saturation properties. This issue will be further discussed in Ch. 16.

Additional properties of nuclear matter have been studied over the years. When electrons transfer momentum and energy to nuclei in scattering experiments, one may assume that a nuclear matter picture becomes useful

when this momentum transfer is large enough to probe the local properties of the interior of nuclei. The resulting study of the response of nuclear matter to different excitation operators is explored in Ch. 14.

Another important application of infinite nuclear systems involves the study of the interior of neutron stars. This interior of a neutron star supports itself against gravitational collapse by the pressure exerted by neutrons when electrons can no longer prevent this collapse. The physics of neutron stars is intricate but the low-density exterior of this system is well understood in terms of nuclei and free electrons. With increasing density it is energetically favorable to “remove” electrons by the process of inverse β -decay. This β -decay process turns the protons in nuclei to neutrons until the nuclei with large neutron excess begin to “drip” neutrons because they can no longer bind them. The matter density for this “neutron drip” corresponds to $4 \times 10^{11} \text{ g cm}^{-3}$. Above this density electrons, nuclei, and free neutrons coexist and determine the state of lowest energy. With increasing density the neutron proton ratio increases further and the neutron gas essentially determines the properties of the system above a density of $4 \times 10^{12} \text{ g cm}^{-3}$ where the neutrons start to provide more pressure than the electrons. This neutron gas with degeneracy factor 2 can be considered a huge nucleus with a lower density than normal nuclear matter. At higher densities the interactions between neutrons must be taken into account and other degrees of freedom like strange particles or quarks may have to be considered. Another important property of the neutron fluid is that it may exhibit superfluid properties as discussed in Ch. 18.

5.4 Liquid ^3He

Helium atoms come in two varieties ^3He and ^4He . The lighter version is a fermion, the heavier one a boson. Systems of both types of particles exhibit spectacular quantum features at low temperature and remain liquid down to the lowest temperatures. The binding forces of these atoms (to form the liquid) are van der Waals forces which arise from the polarization induced in the electronic shells when the atoms approach each other (for a simple discussion see [Sakurai (1994)]). In addition to this attractive component which is quite weak for He atoms, there is an effective repulsion between the atoms due to the Pauli principle which is almost hard-core like. Due to their light mass there is a delicate balance between the kinetic and potential energy. At zero pressure both systems remain liquid when the temperature

approaches 0 K. Both exhibit superfluidity and other remarkable properties when the temperature is lowered. For ${}^3\text{He}$ the observed density at zero pressure corresponds to $36.84 \text{ cm}^3/\text{mole}$. This translates into $0.0163 \text{ atoms}/\text{\AA}^3$ which in turn yields a wavenumber of $k_F = 0.784 \text{ \AA}^{-1}$ using a degeneracy factor of 2 since the total spin of the atom is $1/2$. At this density the binding energy per atom is 2.52 K a tiny amount compared to the atomic energy scales. For this reason it makes sense to discuss such a system from the perspective of atoms interacting through (a dominant) two-body interaction which in turn may be calculated from a more microscopic starting point and (in addition) may be obtained from information obtained at higher temperature where quantum effects no longer play a role and the kinetic and potential energy separate. The boson counterpart ${}^4\text{He}$ forms a system that is more bound (not surprising since there is no Pauli principle which leads to a substantial kinetic energy contribution). At a density of $0.0218 \text{ atoms}/\text{\AA}^3$ the binding energy per atom is 7.14 K. Attempts have been underway for a long time to form fully spin-polarized ${}^3\text{He}$. Such a system would have a degeneracy of 1 with interesting consequences for the way in which the interaction is sampled (see Sec. 4.1).

5.5 Exercises

- (1) Evaluate the the ground state energy of the electron gas in first-order perturbation theory. Make a plot of the energy per particle as a function of r_s and determine the minimum.
- (2) Assume that nucleons interact by means of a two-body interaction given by

$$V = V_0(r) + V_\tau(r)\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + V_\sigma(r)\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + V_{\sigma\tau}(r)\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2,$$

where each radial dependence is governed by a Yukawa form with possible different masses and constants. Evaluate the ground state energy of nuclear matter in first-order perturbation theory using this interaction.