Quantum Mechanics II
Solution Sheet 9

Exercise 9.1 Non-interacting spin-1/2-particles in a harmonic trap

Since we are considering a system of spin-1/2-particles, we have to deal in this exercise with Fermions obeying Pauli's exclusion principle.

(i) For a system of non-interacting particles, we can write the total Hamiltonian as a sum of the single particle Hamiltonians,

$$\mathcal{H} = \sum_{i=1}^{N} \mathcal{H}_0(x_i) \tag{1}$$

where $x_i = (r_i, s_i)$ with r_i and s_i the coordinate and spin variables, respectively and

$$\mathcal{H}_0(x) = \frac{p^2}{2m} + \frac{m\omega^2 r^2}{2} \tag{2}$$

is the (spin-independent, single-particle) Hamiltonian for the harmonic trap with eigenenergies $\varepsilon_n = \hbar\omega(n + 1/2)$. In addition, we can write any many-particle state as an anti-symmetrized sum of product-wave-functions ('Slater determinant'),

$$\Psi_a = \frac{1}{\sqrt{N!}} \sum_{p \in S_N} (-1)^p \varphi_{\varepsilon_1\sigma_1}(x_{p(1)}) \dots \varphi_{\varepsilon_N\sigma_N}(x_{p(N)}) \tag{3}$$

where S_N is the symmetric group of N elements and $\varphi_{\varepsilon_i\sigma_i}(x_i)$ is the single-particle wave-function of the harmonic trap,

$$\mathcal{H}\varphi_{\varepsilon_i\sigma_i}(x_i) = \varepsilon_i \varphi_{\varepsilon_i\sigma_i}(x_i) \tag{4}$$

(coordinate and spin part).
The total energy of this non-interacting system factorizes such that it is simply given by the sum of the single-particle energies of all the occupied states,

$$E = \sum_{n \in \{\text{States occupied}\}} \varepsilon_n. \tag{5}$$

In the ground state, the particles occupy the N lowest lying levels and since we have a spin degeneracy, every energy-level of the harmonic trap can be occupied twice. It is therefore necessary to distinguish between even and odd numbers of particles:

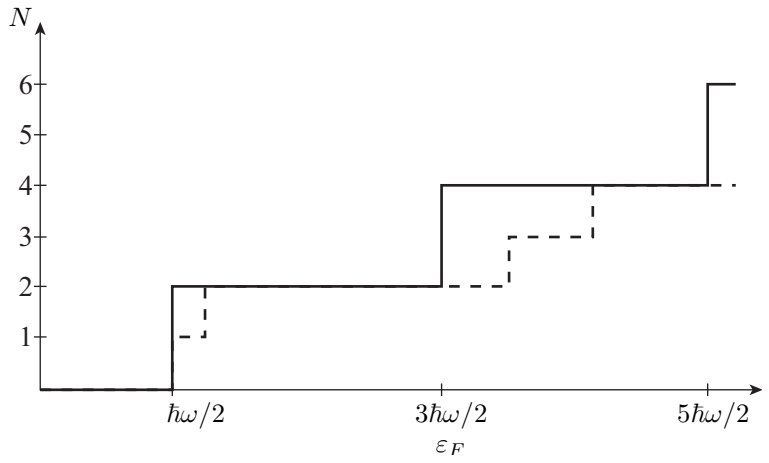
α) If N is even, the first $N/2$ states are occupied and thus, the Fermi energy is $\varepsilon_F = \hbar\omega(N-1)/2$. For the ground-state energy, we find

$$E_{gs} = 2\sum_{n=0}^{N/2-1} \varepsilon_n = 2\sum_{n=0}^{N/2-1} \hbar\omega(n + 1/2) = \frac{N^2}{4}\hbar\omega. \tag{6}$$

β) For N odd, we fill the first $(N-1)/2$ states doubly and the $(N+1)/2$th state is filled only with one particle. Therefore, the Fermi energy is $\varepsilon_F = \hbar\omega N/2$ and the ground-state energy is

$$E_{gs} = 2\sum_{n=0}^{(N-3)/2} \varepsilon_n + \varepsilon_{(N-1)/2} = \frac{N^2+1}{4}\hbar\omega. \tag{7}$$

(ii) If we fix the maximal energy and ask for the number of particles, we see that we always find an even number of particles in the trap. The first two enter as soon as an energy of $\hbar\omega/2$ is reached, the next two at $3\hbar\omega/2$ and so on (solid line of Fig.). The picture changes qualitatively when we introduce a weak Coulomb repulsion (e.g. through a charging term $\sim N^2e^2/2C$ with C the capacitance of the trap): Now, the levels are not degenerate anymore but after a first particle an additional energy is needed to add another one. Therefore, the step-size reduces to one (dashed line).



Note: This picture is of course overly simplified, since when introducing an interaction, the single-particle picture breaks down and we actually would have to deal with real many-particle wave-functions. For a qualitative picture, however, the single-particle treatment suffices.

Exercise 9.2 Non-interacting spin-1/2-particles in a box

(i) Again we are dealing with non-interacting fermions and therefore need to find the single-particle energies of the Hamiltonian. Since we have basically free particles with the constraint of a box, the eigenenergies are

$$\varepsilon_{\vec{k}} = \frac{\hbar^2}{2m}\vec{k}^2 \qquad \vec{k} = \frac{2\pi}{L}\vec{n}, \quad \vec{n} \in \mathbb{Z}^d. \tag{8}$$

(ii) To start, we first want to calculate the density of particles in our box. Since the energies only depend monotonically on the absolute value of $\vec{k}$, there is a maximal value k_F until which all the states are filled, i.e. $|\vec{k}| < k_F$ for all the single-particle states in the ground-state. Thus, the density can be written as

$$n = \frac{N}{V} = \frac{2}{L^d}\sum_{|\vec{k}|<k_F} 1 = \frac{2}{(2\pi)^d}\sum_{|\vec{k}|<k_F}\left(\frac{2\pi}{L}\right)^d \tag{9}$$

(the factor of 2 in the above equation comes from the spin summation).
For $L \to \infty$, $dk = (2\pi)/L$ gets infinitesimal and thus Eq. (9) yields a Riemann sum and can be transformed to a d dimensional integral,

$$n = \frac{2}{(2\pi)^d} \int d\Omega \int_0^{k_F} k^{d-1} dk = 2\frac{S_d(1)}{(2\pi)^d} \int_0^{\varepsilon_F} \Big(\frac{\partial \varepsilon}{\partial k}\Big)^{-1} \Big(\frac{2m\varepsilon}{\hbar^2}\Big)^{(d-1)/2} d\varepsilon. \tag{10}$$

In the first step, we have already used the spherical symmetry in k-space to separate the angular from the radial integration. In the second step, we introduced $S_d(1)$, the surface of a d-dimensional sphere with radius 1 and $\varepsilon_F = \hbar^2 k_F^2/2m$ is the Fermi energy. This is already the result we were looking for with

$$\rho(\varepsilon) = \frac{2}{(2\pi)^d} \Big(\frac{\partial \varepsilon}{\partial k}\Big)^{-1} \Big(\frac{2m\varepsilon}{\hbar^2}\Big)^{(d-1)/2} S_d(1) = \frac{2}{(2\pi)^d} \sqrt{\frac{m}{2\hbar^2\varepsilon}} \Big(\frac{2m\varepsilon}{\hbar^2}\Big)^{(d-1)/2} S_d(1). \tag{11}$$

Note: In this formulation, the spin-degeneracy is already in the density of states. This is sometimes not the case and can lead to confusion.

α) For $d = 3$, $S_d(1) = 4\pi$ and we find for the density of states

$$\rho(\varepsilon) = \frac{2}{8\pi^3} \sqrt{\frac{m}{2\hbar^2\varepsilon}} \Big(\frac{2m\varepsilon}{\hbar^2}\Big) 4\pi = \frac{m}{\pi^2\hbar^3} \sqrt{2m\varepsilon}. \tag{12}$$

The density of electrons now reads

$$n = \int_0^{\varepsilon_F} \rho(\varepsilon) d\varepsilon = \frac{m}{\pi^2\hbar^3} \int_0^{\varepsilon_F} \sqrt{2m\varepsilon} d\varepsilon = \frac{2}{3} \frac{m}{\pi^2\hbar^3} \sqrt{2m} \varepsilon_F^{3/2} \tag{13}$$

and the Fermi energy can be written as

$$\varepsilon_F = \Big(\frac{3}{2} \frac{\pi^2\hbar^3}{\sqrt{2} m^{3/2}} n\Big)^{2/3}. \tag{14}$$

Eventually, we can calculate the total energy of the system,

$$E_{gs} = \int_0^{\varepsilon_F} \rho(\varepsilon) \varepsilon d\varepsilon = \frac{2}{5} \frac{\sqrt{2} m^{3/2}}{\pi^2\hbar^3} \varepsilon_F^{5/2} = \frac{3}{5} n \varepsilon_F. \tag{15}$$

β) For $d = 2$, we find

$$\begin{aligned} \rho(\epsilon) &= \frac{2}{4\pi^2} \sqrt{\frac{m}{2\hbar^2\varepsilon}} \Big(\frac{2m\varepsilon}{\hbar^2}\Big)^{1/2} 2\pi = \frac{m}{\hbar^2\pi} && (16) \\ \Rightarrow n &= \int_0^{\varepsilon_F} \rho(\varepsilon) d\varepsilon = \frac{m\varepsilon_F}{\hbar^2\pi} && (17) \\ \Rightarrow \varepsilon_F &= \frac{\hbar^2\pi n}{m} && (18) \\ \Rightarrow E_{gs} &= \int_0^{\varepsilon_F} \rho(\varepsilon) \varepsilon d\varepsilon = \frac{1}{2} n \varepsilon_F. && (19) \end{aligned}$$

γ) Eventually, the $d = 1$ case yields

$$\begin{aligned} \rho(\epsilon) &= \frac{2}{2\pi} \sqrt{\frac{m}{2\hbar^2\varepsilon}} 2 = \sqrt{\frac{2m}{\hbar^2\pi^2\varepsilon}} && (20) \\ \Rightarrow n &= \int_0^{\varepsilon_F} \rho(\varepsilon) d\varepsilon = 2\frac{\sqrt{2m\varepsilon_F}}{\hbar\pi} && (21) \\ \Rightarrow \varepsilon_F &= \frac{\hbar^2\pi^2 n^2}{8m} && (22) \\ \Rightarrow E_{gs} &= \int_0^{\varepsilon_F} \rho(\varepsilon) \varepsilon d\varepsilon = \frac{1}{3} n \varepsilon_F. && (23) \end{aligned}$$

In the first line, the factor of 2 comes from the fact that we have to integrate along the positive and the negative k-axis in one dimension.

Note: The three cases differ most prominently in the densities of states which have $\sqrt{\varepsilon}$, 1 and $1/\sqrt{\varepsilon}$ dependences, respectively. This has important consequences for many physical properties, such as response functions of materials.
Finally, if we consider a three-dimensional box with $L = 1\text{cm}$, and $N = 10^{23}$ particles, we find a Fermi energy of

$$\varepsilon_F = \Big(\frac{3}{2}\frac{\pi^2\hbar^3}{\sqrt{2}m^{3/2}}\Big)^{2/3} n^{2/3} \approx 3.8 \cdot 10^{-15} n^{2/3}[cm^{-3}] \approx 8.2eV \tag{24}$$

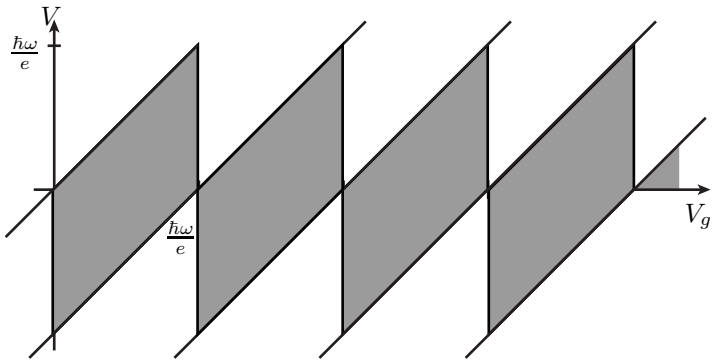
which corresponds to a temperature of approximately $T_F \approx 9 \cdot 10^4\text{K}$.

(iii) In a classical gas where the particles have a certain energy distribution depending on the temperature, every particle can be excited with an energy however small. Now, if we consider Fermions, particles with energies deep below the Fermi energy, can not be excited, since all the states above are already occupied. Thus, only states in a shell of thickness $\sim k_B T$ can be thermally excited and the specific heat is roughly

$$c_V \sim k_B n\Big(\frac{T}{T_F}\Big) \ll k_B n. \tag{25}$$

Exercise 9.3 Tunneling through a quantum dot

For an electron to hop from the left reservoir to the right, there needs to be a state available in the quantum dot or else it blocks and no current flows(gray areas in the figure). This means, that an energy level has to lie between ε_F and $\varepsilon_F + eV$. If we don't apply an external potential V, this is only the case when an energy level is exactly at ε_F which can be tuned by V_g and happens in intervals of $\hbar\omega/e$ with e the charge of the electrons. If we apply a potential V, we can also apply a gate voltage V_g up to the same value and still have a current. Eventually, when the potential is big enough, i.e. $V > \hbar\omega/e$, there will always be a current, no matter the gate voltage.



A very similar pattern has actually also been measured (see e.g. J. Weiss *et.al.*, Phys. Rev. Lett. **71**, 4019 (1993)), however, there is some more physics involved: the level splitting in a quantum dot is much smaller than the corresponding temperature at which such measurements are done. Therefore, thermally activated tunneling will occur and it should actually be impossible to detect these 'diamonds'. However, as was introduced in Ex. 9.1, there should also be Coulomb repulsion, which, for the case of a very small system, is rather large compared to the level splitting ($\Delta E_{\text{level}} \approx 0.5\text{K} \ll 10\text{K} \approx E_{\text{coulomb}}$).

This leads to the so-called Coulomb blockade (as compared to a pure Pauli blockade in the system above) and one refers to this characteristic pattern as 'Coulomb diamonds'. (Note also that usually the applied voltage is divided equally between both reservoirs, i.e. we have $\varepsilon_F + eV/2$ and $\varepsilon_F - eV/2$ for the two reservoirs which leads to a more symmetric pattern.)