



UNIVERSITY OF STRASBOURG

Problem Set 1

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Exercise 1 : Particle in a box

Consider a spinless quantum particle having mass m confined in a cubic box with sides of length L .

- a) Calculate the wave-functions and the corresponding quantized energies for the cases of hard wall and periodic boundary conditions.

Because there is a separable, we can make the assumption that our wavefunction $\psi(x, y, z)$ is separable too,

$$\psi(x, y, z) = \psi_x(x)\psi_y(y)\psi_z(z)$$

Thus, we can use stationary Schrödinger's equation,

$$\hat{H}\psi(x, y, z) = E\psi(x, y, z) \iff -\frac{\hbar^2}{2m}\Delta\psi(x, y, z) = E\psi(x, y, z)$$

Which, we can write,

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi_x(x)\psi_y(y)\psi_z(z) = -\frac{2mE}{\hbar^2}\psi_x(x)\psi_y(y)\psi_z(z)$$

Which is,

$$\left(\frac{\partial_x^2\psi_x}{\psi_x} + \frac{\partial_y^2\psi_y}{\psi_y} + \frac{\partial_z^2\psi_z}{\psi_z}\right) = -\frac{2mE}{\hbar^2}$$

On the right-hand-side, we have a constant, and on the left, we have element that are only dependent on either x , y or z . The only way this is valid is that each element is a constant, which means,

$$\begin{cases} \frac{\partial^2}{\partial x^2}\psi_x = -K_x^2\psi_x \\ \frac{\partial^2}{\partial y^2}\psi_y = -K_y^2\psi_y \\ \frac{\partial^2}{\partial z^2}\psi_z = -K_z^2\psi_z \end{cases} \implies \begin{cases} \psi_x(x) = A_x e^{iK_x x} \\ \psi_y(y) = A_y e^{iK_y y} \\ \psi_z(z) = A_z e^{iK_z z} \end{cases}$$

using $K^2 = 2mE/\hbar^2$. We can also write it in an other way that is equivalent to the first one,

$$\begin{cases} \psi_x(x) = A_x \cos(K_x x) + B_x \sin(K_x x) \\ \psi_y(y) = A_y \cos(K_y y) + B_y \sin(K_y y) \\ \psi_z(z) = A_z \cos(K_z z) + B_z \sin(K_z z) \end{cases}$$

Hard-wall conditions

We will use the cos and sin expression we derived,

$$\begin{cases} \psi_x(0) = \psi_y(0) = \psi_z(0) = 0 \\ \psi_x(L) = \psi_y(L) = \psi_z(L) = 0 \end{cases} \quad (1)$$

From the first equation of (1),

$$A_x = A_y = A_z = 0$$

We can only work on the x equation here, because doing the y and z will strictly be the same. From the second one of (1),

$$B_x \sin(K_x x) = 0 \implies \sin(K_x L) = 0$$

Thus we get,

$$K_x L = n_x \pi \quad n_x \in \mathbb{N}^*$$

Thus,

$$K_x = \frac{n_x \pi}{L} \quad K_y = \frac{n_y \pi}{L} \quad K_z = \frac{n_z \pi}{L}$$

Which we can write,

$$K^2 = \left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) \quad n_i \in \mathbb{N}^*$$

Periodic boundary conditions

We will use the exp expression we derived,

$$\psi_x(x+L) = \psi_x(x) \implies A_x e^{iK_x(x+L)} = A_x e^{iK_x x}$$

Thus,

$$e^{iK_x L} = 1 \implies k_x L = 2\pi n_x \quad n_x \in \mathbb{Z}$$

Thus,

$$K_x = \frac{2n_x \pi}{L} \quad K_y = \frac{2n_y \pi}{L} \quad K_z = \frac{2n_z \pi}{L}$$

Which we can write,

$$K^2 = \left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) \quad n_i \in \mathbb{Z}$$

$$K^2 = \frac{2mE}{\hbar^2} \implies E(K) = \frac{\hbar^2 K^2}{2m}$$

- b) Estimate the number of states $N(E)$ in the box that have an energy lower than E , in the regime where the box is sufficiently large such that

$$L \gg \frac{\pi \hbar}{\sqrt{2mE}}$$

Show that in this limit, $N(E)$ is proportional to the volume $V = L^3$ of the box, and that it does not depend on the choice of the boundary conditions.

$$\frac{\hbar^2 K^2}{2m} \leq E \iff K^2 \leq \frac{2mE}{\hbar^2}$$

If we take the *hard-wall condition* here,

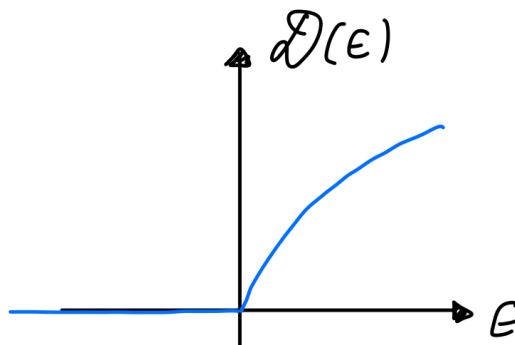
$$\left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) \leq \frac{2mE}{\hbar^2} \iff (n_x^2 + n_y^2 + n_z^2) \leq \frac{L^2}{\pi^2} \frac{2mE}{\hbar^2}$$

The condition in the text basically mean that the quantity on the right $2L^2mE/\pi^2\hbar^2 \gg 1$ is large. We recognize the equation of a sphere in the reciprocal space. Thus,

$$N = \frac{4}{3}\pi R^3 = \frac{4}{3} \frac{1}{8} \pi \left(\frac{2mEL^2}{\hbar^2 \pi^2}\right)^3 = \frac{1}{6} \pi \left(\frac{2mEL^2}{\hbar^2 \pi^2}\right)^3$$

The $1/8$ comes from we have to be in the condition that $n_i \in \mathbb{N}^*$, thus we only take effectively $1/8$ of the whole sphere. And so we can get the density of states $\mathcal{D}(E)$,

$$\begin{aligned} \mathcal{D}(E) &= \frac{1}{V} \frac{dN(E)}{dE} = \frac{1}{6} \pi \left(\frac{2mL^2}{\pi^2 \hbar^2}\right)^{3/2} \frac{3}{2} \sqrt{E} \\ &= \frac{1}{V} \frac{3}{12} \pi \left(\frac{2mL^2}{\pi^2 \hbar^2}\right)^{3/2} \sqrt{E} \\ &= K \sqrt{E} \end{aligned}$$



Here we only showed this result using hard-wall condition, but the result will be exactly the same using periodic boundary conditions.

- c) Use the result of b) to calculate the density of states $\mathcal{D}_e(E)$ (the number of quantum states per unit energy and per unit volume). How does the result change if we consider electrons (that are quantum particles with spin $1/2$).

$$\mathcal{D}_e(E) = g_s \mathcal{D}(E) = 2\mathcal{D}(E)$$

- d) Determine the density of states for free electrons in two and one dimensions.

$$\begin{cases} \mathcal{D}_{1D} \propto K'(E)^{-1/2} \\ \mathcal{D}_{2D} \propto K'' \\ \mathcal{D}_{3D} \propto K(E)^{1/2} \end{cases}$$

Exercise 2 : Three-dimensional electron gas

- a) Use the results of Exercise 1 to express the Fermi wave-vector k_F , the Fermi velocity v_F , and the Fermi energy E_F of a 3-dimensional electron gas as a function of the electron density.

We can use the condition that the system is large enough such that we have a continuum of states,

$$\bar{N} = \int_0^{+\infty} d\epsilon f(\epsilon) \mathcal{D}(\epsilon)$$

We know that Fermi-Dirac distribution $f(\epsilon)$ at temperature $T = 0$ is equal to 1 for $E < E_F$ and is equal to 0 for $E > E_F$. Thus,

$$\begin{aligned} \bar{N} &= \int_0^{E_F} d\epsilon \mathcal{D}(\epsilon) \\ &= K \int_0^{E_F} d\epsilon \sqrt{\epsilon} \\ &= \frac{2}{3} K E_F^{3/2} \end{aligned}$$

Which can be written,

$$E_F = \left(\frac{3\bar{N}}{2K} \right)^{2/3} = \left(\frac{6\pi^2 \bar{N}}{g_s} \right)^{2/3} \frac{\hbar^2}{2m}$$

Using that $g_s = 2$ for electrons, and we know that,

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

We get,

$$k_F^2 = (3\bar{N}\pi^2)^{2/3} \implies k_F = (3\bar{N}\pi^2)^{1/3}$$

We know that,

$$p_F = \hbar k_F = m v_F \implies v_F = \frac{\hbar k_F}{m}$$

which is,

$$v_F = \frac{\hbar}{m} (3\bar{N}\pi^2)^{1/3}$$

- b) Show that the total kinetic energy of a 3-dimensional electron gas containing N free electrons at zero temperature is given by

$$E_{\text{kin}} = \frac{3}{5} N E_F.$$

We will multiply by V the density of states here because it has to be in unit of quantity of electrons and not in density (but it is just a convention to follow here),

$$\begin{aligned} E_{\text{kin}} &= \int_0^{+\infty} d\epsilon f(\epsilon) \epsilon V \mathcal{D}(\epsilon) \\ &= \int_0^{E_F} d\epsilon \epsilon V \mathcal{D}(\epsilon) \\ &= KV \int_0^{E_F} d\epsilon \epsilon^{3/2} \\ &= \frac{2}{5} \times K \times V E_F^{5/2} \\ &= \frac{2}{5} \times \frac{3\bar{N}}{2V E_F^{3/2}} \times V E_F^{5/2} \\ &= \frac{3}{5} \bar{N} E_F \end{aligned}$$

We used the expression of K as a function of \bar{N} and E_F that we derived earlier in the equation.

- c) The spatial density of atoms in copper is $8.45 \times 10^{28} \text{ m}^{-3}$. Estimate the values of the quantities in a) for the conduction band of copper, assuming a free electron gas and one conduction band electron per atom. Use the bare electron mass $m_e = 9.11 \times 10^{-31} \text{ kg}$, and Planck's constant $\hbar = 1.05 \times 10^{-34} \text{ Js}$ ($1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$).

$$E_F = \frac{\hbar^2}{2m} (3\pi^2 n_{\text{Cu}})^{2/3} = 11.15 \times 10^{-19} \text{ J} = 6.97 \text{ eV}$$

in tables, the value is 7.0 eV. Means that our assumption are either not too bad, or errors do compensate. It is still the same kind of value, so it is nice.

$$k_F = (3\pi^2 n_{\text{Cu}})^{1/3} = 13.6 \times 10^9 \frac{1}{\text{m}} = \frac{13.6}{\text{nm}}$$

Thus,

$$\lambda_F = \frac{2\pi}{k_F} = 0.5 \text{ nm}$$

$$v_F = \frac{\hbar k_F}{m} = 1.57 \times 10^6 \text{ m.s}^{-1} = \frac{c}{200}$$

That is the speed of an electron at Fermi energy at zero temperature.

Exercise 3 : Frequency-dependent conductivity of a free electron gas

Consider the Drude model of metallic conductivity. It assumes a density n of free electrons with mass m that are accelerated by the force of an applied electric field, and that undergo collisions in which the electron velocity changes abruptly. Those collisions are assumed to occur in average after a relaxation time τ and result in random velocity (zero in average) right after the collision process. Such collision processes can be included in the form of a friction force

$$\vec{F}_f = -\frac{m}{\tau}\vec{v},$$

where \vec{v} is the drift (average) velocity of the electrons.

- a) A DC electric field $\vec{E} = \vec{E}_0$ is applied. Write the equation for the average electron momentum. Calculate the stationary drift (average) velocity, the DC current density \vec{J} , and the DC Drude conductivity σ_0 that relates the current density to the electric field as $\vec{J} = \sigma_0\vec{E}$.

We know that,

$$\sum \text{Forces} = m\vec{a}$$

Thus,

$$\frac{d\vec{p}}{dt} = -e\vec{E} + \vec{F}_f$$

We are in a *steady state*,

$$\frac{d\vec{p}}{dt} = 0$$

Meaning,

$$-e\vec{E} - \frac{m}{\tau}\vec{v} = 0$$

Thus,

$$\vec{v} = -\frac{\tau e}{m}\vec{E}$$

We know the current density \vec{j} ,

$$\begin{aligned}\vec{j} &= -en \times \vec{v} \\ &= (-en) \times \left(-\frac{\tau e}{m}\vec{E}_0\right) \\ &= \frac{\tau e^2 n}{m}\vec{E}\end{aligned}$$

We can re-write it,

$$\vec{j} = \sigma_0 \vec{E}$$

Thus,

$$\sigma_0 = \frac{\tau e^2 n}{m}$$

- b) An AC electric field $\vec{E} = \vec{E}_0 \exp(-i\omega t)$ is applied. Calculate the resulting oscillating velocity $\vec{v} = \vec{v}_0 \exp(-i\omega t)$, the corresponding current density, and the (complex) AC Drude conductivity $\sigma(\omega)$. Verify that the DC conductivity is recovered in the zero-frequency limit.

$$\begin{aligned} m \frac{d\vec{v}}{dt} &= -e\vec{E} - \frac{m}{\tau} \vec{v} \\ (-im\omega)\vec{v}_0 &= -e\vec{E}_0 - \frac{m}{\tau} \vec{v}_0 \\ \vec{v}_0 \left(\frac{m}{\tau} - im\omega \right) &= -e\vec{E}_0 \\ \vec{v}_0 &= -\frac{e\vec{E}_0}{\frac{m}{\tau} - im\omega} \\ \vec{v}_0 &= -\frac{e\vec{E}_0 \left(\frac{m}{\tau} + im\omega \right)}{\left(\frac{m}{\tau} \right)^2 + m^2\omega^2} \end{aligned}$$

$$\begin{aligned} \vec{j} &= (-en)\vec{v} \\ &= \frac{e^2 n \left(\frac{1}{\tau} + i\omega \right)}{m \left(\omega^2 + \frac{1}{\tau^2} \right)} \vec{E}_0 \\ &= \frac{e^2 n \tau^2}{m(\omega^2 \tau^2 + 1)} \frac{1}{\tau} (1 + i\omega\tau) \vec{E}_0 \\ &= \underbrace{\frac{e^2 n \tau}{m(1 + \omega^2 \tau^2)} (1 + i\omega\tau)}_{\sigma(\omega)} \vec{E}_0 \\ &= \sigma(\omega) \vec{E}_0 \end{aligned}$$

Thus,

$$\sigma(\omega) = \frac{e^2 n \tau}{m} \frac{(1 + i\omega\tau)}{(1 + \omega^2 \tau^2)}$$

We indeed recover what we found earlier,

$$\sigma(0) = \frac{e^2 n \tau}{m}$$

- c) Determine the real and the imaginary part of the complex AC conductivity, and explain the physical relevance of the two components.

$$\sigma(\omega) = \sigma(0) \times \frac{(1 + i\omega\tau)}{(1 + \omega^2\tau^2)}$$

$$\operatorname{Re}(\sigma(\omega)) = \frac{\sigma(0)}{1 + \omega^2\tau^2}, \quad \operatorname{Im}(\sigma(\omega)) = \frac{\sigma(0)}{1 + \omega^2\tau^2} \times \omega\tau.$$

Remark : Let $E(t)$ be any time dependent field. So we can write this field as a Fourier Transform

$$E(t) = \int d\omega \tilde{E}(\omega) e^{-i\omega t}$$

And we can do exactly the same for the velocity $v(t)$,

$$v(t) = \int d\omega \tilde{v}(\omega) e^{-i\omega t}$$

So if we plug this in the dynamic equation,

$$\frac{d}{dt} \vec{v} + \frac{1}{\tau} \vec{v} = -\frac{e}{m} \vec{E}(t)$$

Thus,

$$\int d\omega (-i\omega) \tilde{v}(\omega) e^{-i\omega t} + \frac{1}{\tau} \int d\omega \tilde{v}(\omega) e^{-i\omega t} = -\frac{e}{m} \int d\omega \tilde{E}(\omega) e^{-i\omega t}$$

All the terms have this frequency integral, so we can put all of them in the same side,

$$\int d\omega \left\{ -i\omega \tilde{v}(\omega) + \frac{1}{\tau} \tilde{v}(\omega) + \frac{e}{m} \tilde{E}(\omega) \right\} e^{-i\omega t} = 0$$

This means that

$$-i\omega \tilde{v}(\omega) + \frac{1}{\tau} \tilde{v}(\omega) + \frac{e}{m} \tilde{E}(\omega) = 0$$

and, this is the exact the same problem as we solved earlier,

$$\tilde{v}(\omega) = -\frac{e}{m} \frac{\frac{1}{\tau} + i\omega}{\frac{1}{\tau^2} + \omega^2} \tilde{E}(\omega)$$

So, solving the problem as we did on the b) allow us to generalize for any frequency.