

Mandatory assignment FYS3400 II

candidate number: 110

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Electrons I

1. Let's take a system of fermions, which follow the Fermi-Dirac distribution. This distribution gives the average number of fermions at energy ϵ , which is expressed by the following equation:

$$f_{FD}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \quad (1)$$

where μ is the chemical potential, and in general it depends on the temperature. Nevertheless, at absolute zero ($T = 0$) μ is equal to ϵ_f , where ϵ_f is the fermi energy; defined as the energy of the topmost filled orbital at absolute zero. In order to study properly a Free electron fermi gas (FEFG) we need to find out an expression for the density of states in 3D. To do this we have to solve the Schrödinger equation for a FEFG, find the allowed energies of the system and then look how many fermions there are in an interval $E+dE$. This yields to the expression of the DOS for a system of fermions:

$$DOS(\epsilon) = \frac{V}{2\pi} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \epsilon^{\frac{1}{2}} \quad (2)$$

Solving the Schrödinger equation we come across the expression for the fermi energy:

$$\epsilon_f = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{\frac{2}{3}} \quad (3)$$

To proof that at absolute zero $\mu = \epsilon_f$ we start from the Gibbs energy G . From the thermodynamics it is known that $G = N\mu$ at $T = 0$ where N is the number of particles; on the other hand G can also be expressed as a function of thermodynamics coordinates as follow:

$$G = E + pV \quad (4)$$

where E is the energy, p the pressure, and V the volume of the system. In the light of the above, the energy of the system can be calculate:

$$E = \int_0^{+\infty} DOS(\epsilon) f_{FD}(\epsilon, T, \mu) \epsilon d\epsilon \quad (5)$$

At temperature equal to 0, the Fermi-Dirac distribution has the shape of a step function $\theta(\epsilon < \epsilon_f)$, hence the integral runs from 0 to the fermi energy, because after that energy there's no fermions at $T = 0$, this yields to:

$$\begin{aligned} E &= \int_0^{\epsilon_f} DOS(\epsilon) f_{FD}(\epsilon) \epsilon d\epsilon = \int_0^{\epsilon_f} \frac{V}{2\pi} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \epsilon^{\frac{1}{2}} \epsilon d\epsilon \\ &= \int_0^{\epsilon_f} \frac{V}{2\pi} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \epsilon^{\frac{3}{2}} d\epsilon \\ &= \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \left(\frac{2}{5} \epsilon_f^{\frac{5}{2}}(V) \right) \end{aligned} \quad (6)$$

After that we have found out the value of the energy we can calculate the pressure, which is related to the energy by the following thermodynamical expression: $p = -\frac{\partial E}{\partial V}$.

$$\begin{aligned}
p &= -\frac{\partial E}{\partial V} \\
&= -\frac{2}{5} \frac{\partial}{\partial V} V \lambda^3 \epsilon_f^{\frac{5}{2}}(V) \quad \text{where } \lambda = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{1}{2}} \\
&= -\frac{2}{5} \left(\lambda^3 \epsilon_f^{\frac{5}{2}} + V \lambda^3 \left(-\frac{5}{3} \frac{\epsilon_f^{\frac{5}{2}}}{\epsilon_f} \right) \right) = \frac{4}{15} \lambda^3 \epsilon_f^{\frac{5}{2}}
\end{aligned} \tag{7}$$

Now using equation (6) and (7) in equation (4) we obtain an expression for G :

$$\begin{aligned}
N\mu = G &= E + pV \\
&= \frac{2}{5} \lambda^3 \epsilon_f^{\frac{5}{2}} + \frac{4}{15} \lambda^3 \epsilon_f^{\frac{5}{2}} \\
&= \frac{2}{3} \lambda^3 V \epsilon_f^{\frac{5}{2}} \\
&= \frac{2}{3} \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \epsilon_f^{\frac{3}{2}} \epsilon_f \\
&\quad \underbrace{\hspace{1.5cm}}_{\text{This is equal to } N} \\
&= N\epsilon_f
\end{aligned} \tag{8}$$

Yielding to the equality at $T = 0$: $\mu = \epsilon_f$. □

2. Here we assume that $\mu = \epsilon$ even if the FEFG is heated up for $T > 0$. Assuming this, we plotted the Fermi-Dirac distribution as a function of $\frac{\epsilon}{\epsilon_f}$

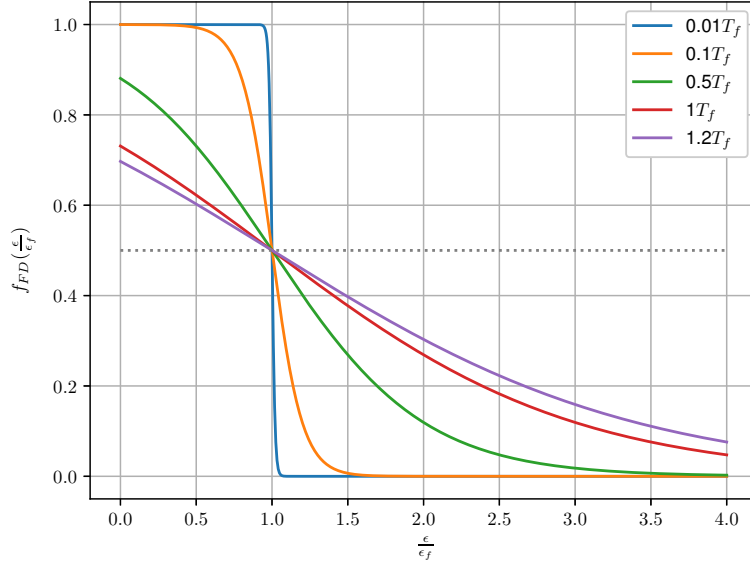


Figure 1: Caption

Looking at the figure 1. To make a proper comparison between the figure reported in Kittel on page 136 and the plotted figure, we need to plot the figure as a function of $\frac{\epsilon}{k_B T}$ or we can scale the plot in Kittel by a factor of $T_f = 5 \times 10^4$. Looking at the figures, the approximation of $\mu = \epsilon_f$ seems to hold until $T = 0.5T_f$.

3. However, μ is not constant and it changes with temperature. The approximation $\mu = \epsilon_f$ holds only in the limit of $T \rightarrow 0$. We can estimate the trend of μ as a function of temperature. As a starting point, we observe that the total number of particles in the system N , it is not changing with the

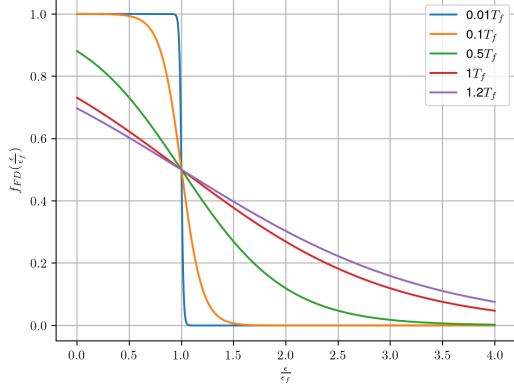


Figure 2: Fermi-Dirac distribution function (1) at the various labelled temperatures with the assumption of $\mu = \epsilon_f$. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature.

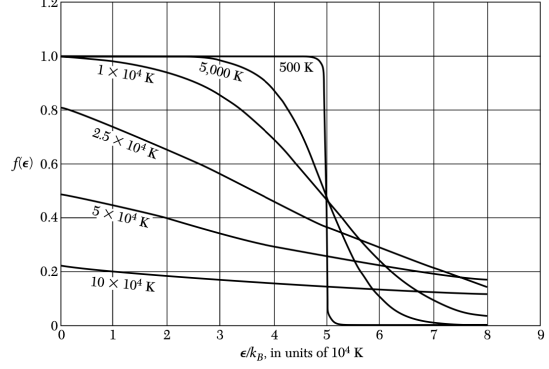


Figure 3: Fermi-Dirac distribution function (1) at the various labelled temperatures, for $T_f = \frac{\epsilon_f}{k_B} = 5 \times 10^4 K$. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature. The chemical potential μ at each temperature may be read off the graph as the energy at which $f_{FD} = 0.5$.

temperature. Hence, we will aspect that the number of particles at $T = 0$ is equal when $T > 0$. From the definition of the fermi energy (3) we can get the number of particles at $T = 0$:

$$N_0 = \frac{V}{3\pi^2} \left(\frac{2m\epsilon_f}{\hbar^2} \right)^{\frac{3}{2}} \quad (9)$$

On the other hand, when the temperature increase the number of particle can be calculated as:

$$\begin{aligned} N &= \int_0^{+\infty} DOS(\epsilon) f_{FD}(\epsilon, \mu, \beta) d\epsilon \\ &= \int_0^{+\infty} \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon-\mu)} + 1} d\epsilon \end{aligned} \quad (10)$$

The number of particles doesn't change with temperature, hence:

$$\begin{aligned} N - N_0 &= 0 \\ \int_0^{+\infty} \frac{1}{2} \frac{V}{\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon-\mu)} + 1} d\epsilon - \frac{1}{3} \frac{V}{\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \epsilon_f^{\frac{3}{2}} &= 0 \\ \int_0^{+\infty} \frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon-\mu)} + 1} d\epsilon - \frac{2}{3} \epsilon_f^{\frac{3}{2}} &= 0 \end{aligned}$$

we can normalize the expression respect ϵ_f and adjust the units in a proper way changing the variable in the integral $x = \frac{\epsilon}{\epsilon_f}$, yielding to:

$$\int_0^{+\infty} \frac{x^{\frac{1}{2}}}{e^{\frac{T_f}{T}(x-\frac{\mu}{\epsilon_f})} + 1} dx - \frac{2}{3} = 0$$

$$g(T, \mu) = 0 \quad (11)$$

To find how μ depends on T we can fix T and find for which μ the equation is satisfied. In this way for every value of chosen T we obtain the respective value of μ that solve eq:11. Since the integral is quite nasty to solve analytical, so we have chosen to solve it numerically. Then we plotted $\frac{\mu}{\epsilon_f}$ with the correspondent $\frac{T}{T_f}$ in figure 4.

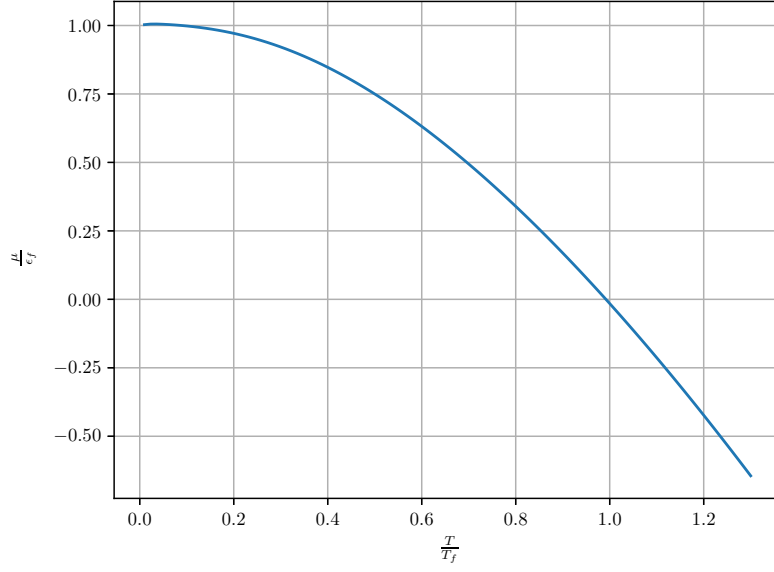


Figure 4: This plot shows the true dependence of the chemical potential μ as a function of T . From the plot we can see that the dependence on temperature of μ it goes like $\epsilon_f - aT^2$

Through a fit we see that the dependence on temperature of μ it goes like $\epsilon_f - aT^2$, where a is fit constant. This is in accordance with the literature.

4. Now we plot again the same chart of point b but with the true dependence of the chemical potential μ found in the previous point. The chart is shown in figure 5.

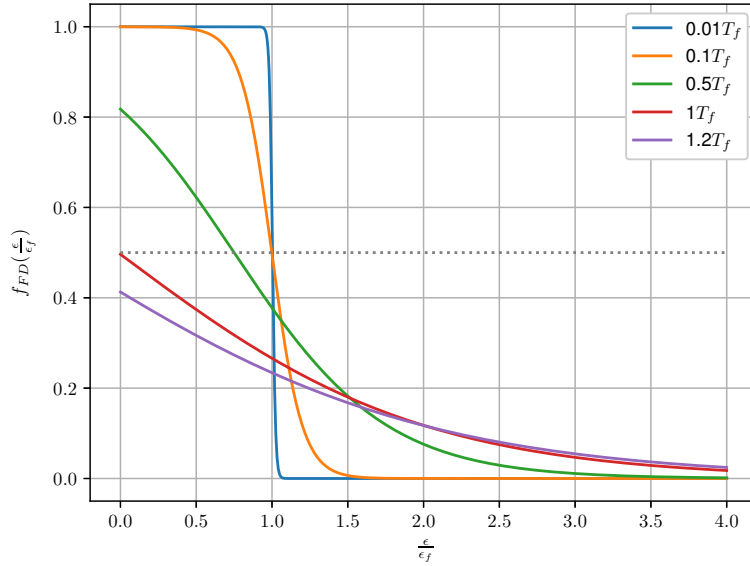


Figure 5: Fermi-Dirac distribution function (1) at the various labelled temperatures with $\mu(T)$ depending on the temperature. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature.

We can also make a comparison between f_{FD} with $\mu = \epsilon_f$ (as in the point (b)) and f_{FD} with the true dependence of the chemical potential. For the sake of illustration we overlap the 2 plot and we see that until $T = 0.1T_f$ the approximation of $\mu = \epsilon_f$ holds, but then it starts deviating.

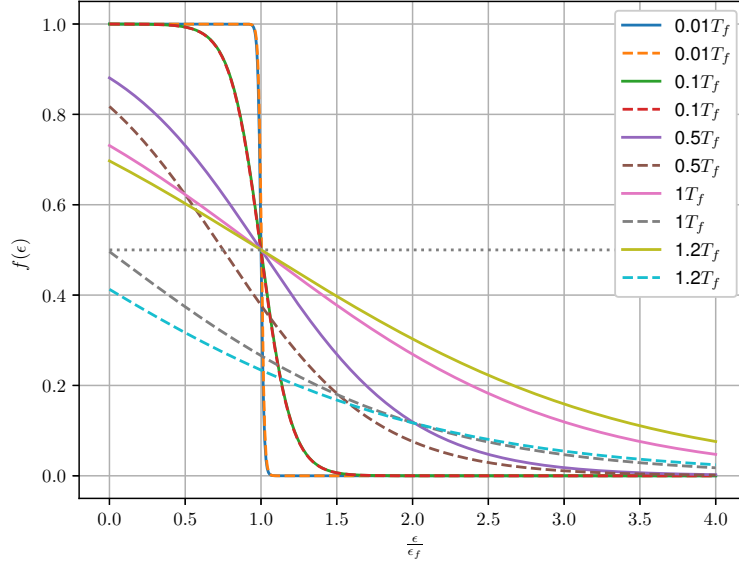


Figure 6: Comparison between the Fermi-Dirac distribution functions (1) at the various labelled temperatures with $\mu(T)$ depending on the temperature (dashed lines) and with $\mu = \epsilon_f$ (continue lines). We can see that the assumption $\mu = \epsilon_f$ holds until $T = 0.01T_f$

- When we heat the crystal from $0K$, not every electron gains an energy $\approx k_B T$ as expected classically, but only the electrons within an energy range $k_B T$ of the Fermi level ϵ_f can be excited thermally. Only those electron near the fermi energy can absorb energy as heat and jump to a new energy level above ϵ_f . The higher is T , more electron can jump and occupy new energy levels. If N is the total number of electrons, we expect that only a fraction of the order of $\frac{k_B T}{\epsilon_f}$ can be excited thermally at temperature T , only these lie within an energy range of the order of $k_B T$ around the fermi energy. Each of these $N \frac{k_B T}{\epsilon_f}$ contribute in the total kinetic thermal energy: $U \sim N \frac{k_B T}{\epsilon_f} k_B T$. The electronic heat capacity is given by: $C_{el} = \frac{\partial U}{\partial T}|_V \sim N \frac{k_B}{\epsilon_f} T$. From a qualitative analysis we see that the heat capacity of the FEFG is directly proportional to T In low temperature approximation $k_B T \ll \epsilon_f$ we can derive quantitatively the expression for the heat capacity, although a more general solution of this problem it could be given. The total energy of the system of N electrons at temperature T is given by equation 5, but for the sake of clarity we report it again here :

$$U = \int_0^{+\infty} DOS(\epsilon) f_{FD}(\epsilon, T, \mu) \epsilon d\epsilon$$

In this equation only the Fermi-Dirac distribution depends on temperature, and since we are in the low temperature we can assume $\mu \approx \epsilon_f$. The heat capacity is given by:

$$C_{el} = \frac{\partial U}{\partial T}|_V = \int_0^{+\infty} \epsilon DOS(\epsilon) \frac{\partial f_{FD}}{\partial T} d\epsilon$$

Using the fact that the number of particles doesn't change with temperature, the following equality is true:

$$0 = \epsilon_f \frac{\partial N}{\partial T} = \epsilon_f \int_0^{+\infty} DOS(\epsilon) \frac{\partial f_{FD}}{\partial T} d\epsilon$$

Putting the last two equations together we obtain:

$$C_{el} = \int_0^{+\infty} (\epsilon - \epsilon_f) DOS(\epsilon) \frac{\partial f_{FD}}{\partial T} d\epsilon$$

At low temperature $(\epsilon - \epsilon_f) \frac{\partial f_{FD}}{\partial T}$ is large only at the energies very close to the Fermi energy, thus in this regime we can ignore the variation of $DOS(\epsilon)$ under the integral. Evaluating the $DOS(\epsilon)$

at the fermi energy it is a good approximation and then we can take it outside the integral.

$$\begin{aligned}
C_{el} &\approx DOS(\epsilon_f) \int_0^{+\infty} (\epsilon - \epsilon_f) \frac{\partial f_{FD}}{\partial T} d\epsilon \\
&\approx k_B DOS(\epsilon_f) \int_0^{+\infty} (\beta^2(\epsilon - \epsilon_f)) \frac{e^{\beta(\epsilon - \epsilon_f)}}{(1 + e^{\beta(\epsilon - \epsilon_f)})^2} d\epsilon \quad \text{with } \beta = \frac{1}{k_B T} \\
&\approx \frac{k_B}{\beta} DOS(\epsilon_f) \int_{-\beta\epsilon_f}^{+\infty} x^2 \frac{e^x}{(1 + e^x)^2} dx \quad \text{with } x = \beta(\epsilon - \epsilon_f)
\end{aligned} \tag{12}$$

In low temperature limit $-\beta\epsilon_f \ll 0$, so we can extend the integration from $-\infty$ to $+\infty$.

This integral is tabulated and has a value of:

$$\int_{-\infty}^{+\infty} x^2 \frac{e^x}{(1 + e^x)^2} dx = \frac{\pi^2}{3}$$

The last thing to do is to evaluate the $DOS(\epsilon_f)$, looking at equation 2 and evaluating it in ϵ_f , we obtain:

$$DOS(\epsilon_f) = \frac{3N}{2\epsilon_f} \tag{13}$$

In conclusion the equation 12 becomes:

$$C_{el} \approx \frac{k_B}{\beta} \frac{3N}{2\epsilon_f} \frac{\pi^2}{3} = \frac{\pi^2 k_B^2 N}{2\epsilon_f} T$$

This result is in accordance with the qualitative thinking that we did before starting the calculations.

Electrons II

The Kronig-Penney model is an idealized quantum-mechanical system that describes electron motion in a period array of delta functions with magnitude V_0 : Hence, the Hamiltonian has a periodic potential

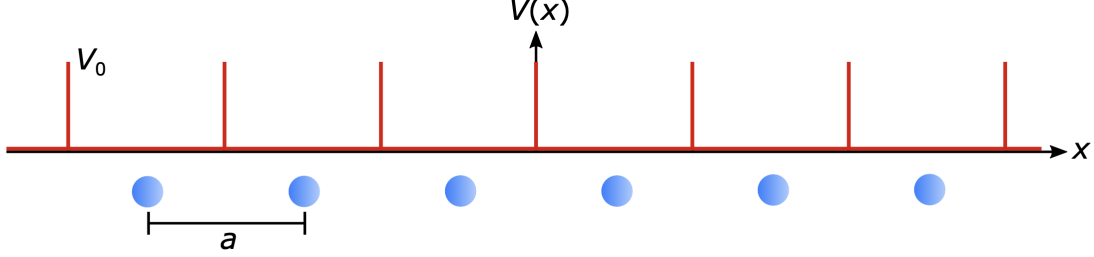


Figure 7: Kronig-Penney model with a periodic potential consisting of delta functions with magnitude V_0 with periodicity a .

with the following shape:

$$U(x) = U_0 \sum_{n=-\infty}^{+\infty} \delta(x - na)$$

where the delta is the dirac delta and a is the lattice constant. The time-independent Schrödinger equation consists:

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right) \psi(x) = E\psi(x) \quad (14)$$

Consider the function in the region $I : \forall x \in [-a, 0]$ and $II : \forall x \in [0, a]$. Since the potential energy is equal to zero inside each of the segments, the corresponding wavefunctions are the linear combinations of two plane waves. In region I the wavefunction that satisfies the Schrödinger equation 14 is:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

and in the region II the wavefunction that satisfies is:

$$\psi_{II}(x) = Ce^{ikx} + De^{-ikx} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

But according to Bloch's theorem, the wavefunction solution of the Schrödinger equation when the potential is periodic, can be written as:

$$\psi(x) = e^{iqx} u(x) \quad \text{with } q = n \frac{2\pi}{Na}$$

where $u(x)$ is a periodic function. In fact $u(x) = u(x + a)$. This yields to:

$$\begin{aligned} \psi_{II}(x) &= e^{iqa} \psi_I(x - a) \\ &= (Ae^{ik(x-a)} + Be^{-ik(x-a)}) e^{iqa} \end{aligned}$$

Now we have to impose the boundary conditions, first the continuity in 0:

$$\begin{aligned} \psi_I(0) &= \psi_{II}(0) \\ Ae^{ik \cdot 0} + Be^{-ik \cdot 0} &= (Ae^{ik(-a)} + Be^{-ik(-a)}) e^{iqa} \\ A + B &= (Ae^{-ika} + Be^{ika}) e^{iqa} \end{aligned}$$

The second boundary condition, in $x = 0$, is given by integrating the shroedinger equation, so we can integrate in a small interval around 0: from $-\epsilon$ to $+\epsilon$ with $\epsilon \rightarrow 0$:

$$\begin{aligned} -\frac{\hbar^2}{2m} \int_{-\epsilon}^{+\epsilon} \psi''(x) dx + V_0 \int_{-\epsilon}^{+\epsilon} \delta(x) \psi(x) dx &= E \int_{-\epsilon}^{+\epsilon} \psi(x) dx \\ -\frac{\hbar^2}{2m} (\psi'(+\epsilon) - \psi'(-\epsilon)) + V_0 \psi(0) &= 0 \end{aligned}$$

We can get rid of the term $E \int_{-\epsilon}^{+\epsilon} \psi(x) dx$ on the right side thanks to the continuity of the wavefunction. On the other side, however, the term $\psi'(\epsilon) - \psi'(-\epsilon)$ is not 0, in fact the derivative of the wavefunction is different if we get close from the right of the delta or from the left. Taking this into account the second boundary condition in our case is:

$$\begin{aligned}\psi'_{II}(0) - \psi'_I(0) &= \frac{2mV_0}{\hbar^2} \psi(0) \\ (Ae^{-ika} - Be^{ika})e^{iqa} - (A - B) &= \frac{2mV_0}{ik\hbar^2} (A + B)\end{aligned}$$

Putting together the boundary conditions we obtain the following system:

$$\begin{cases} A + B = (Ae^{-ika} + Be^{ika})e^{iqa} & \text{continuity} \\ (Ae^{-ika} - Be^{ika})e^{iqa} - (A - B) = \frac{2mV_0}{ik\hbar^2} (A + B) & \text{derivative} \end{cases}$$

Going a bit through the math we can write this system better:

$$\begin{cases} A(1 - e^{iqa}e^{-ika}) + B(1 - e^{iqa}e^{ika}) = 0 \\ A(e^{-ika}e^{iqa} - 1 - g) + B(-e^{ika}e^{iqa} + 1 - g) = 0 \end{cases}$$

where $g = \frac{2mV_0}{ik\hbar^2}$. For sake of notation, this system we can write this system with matrix:

$$M \times \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} (1 - e^{iqa}e^{-ika}) & (1 - e^{iqa}e^{ika}) \\ (e^{-ika}e^{iqa} - 1 - g) & (-e^{ika}e^{iqa} + 1 - g) \end{bmatrix} \times \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

This is a linear system has a solution, different from the null solution, when the matrix of coefficient (M) has determinant equal to 0. Hence:

$$\det(M) = \begin{vmatrix} (1 - e^{iqa}e^{-ika}) & (1 - e^{iqa}e^{ika}) \\ (e^{-ika}e^{iqa} - 1 - g) & (-e^{ika}e^{iqa} + 1 - g) \end{vmatrix} = 0$$

Performing the calculations

$$\begin{aligned}\det(M) &= (1 - e^{iqa}e^{-ika})(-e^{ika}e^{iqa} + 1 - g) - (1 - e^{iqa}e^{ika})(e^{-ika}e^{iqa} - 1 - g) = 0 \\ &= -e^{ika}e^{iqa} + 1 - g + e^{2iqa} - (1 - g)e^{iqa}e^{-ika} - (e^{-ika}e^{iqa} - e^{2iqa} - 1 - g + (1 + g)e^{iqa}e^{ika}) = 0 \\ &= 2e^{2iqa} + 2 - e^{iqa}e^{ika} - e^{ika}e^{iqa} + ge^{iqa}e^{ika} - ge^{iqa}e^{-ika} = 0 \\ &= 2e^{iqa}\cos(qa) - 2e^{iqa}(\cos(ka)) - 2e^{iqa}\frac{2mV_0a}{\hbar^2}\sin(ka) = 0\end{aligned}$$

This yields to a trascendental equation:

$$\cos(qa) = \frac{2mV_0a}{\hbar^2} \frac{\sin(ka)}{ka} + \cos(ka) \quad (15)$$

On the left we have a term that depend only on the lattice, on the other side of the equation we have terms that depends only on the energy, through the factor k . This equation is satisfied only for specific value of k and q . The allowed values of the energy ϵ are given by those satisfying $qa = (\frac{2m\epsilon}{\hbar^2})^{\frac{1}{2}}a$, since the number N of lattice point is big the spectrum of the possible solution is very dense for which that lie under the condition: $-1 \leq \frac{2mV_0a}{\hbar^2} \frac{\sin(ka)}{ka} + \cos(ka) \leq 1$. We can see it graphically in figure 8

For other values of the energy there are no solutions to the Schrödinger equation, so that forbidden gaps in the energy spectrum are formed. To sum up, the energy is discontinuous there are allowed and forbidden energy bands.

Now let's analyse the behaviour of the system when $V_0 \rightarrow 0$ and when $V_0 \rightarrow +\infty$.

When the module of the potential goes to zero ($V_0 \rightarrow 0$), the allowed bands get wider and forbidden bands get narrowed until we get once again the case of a Free Fermi Electron Gas with energy $E = \frac{\hbar^2 k^2}{2m}$. We also see that in the limit $V_0 \rightarrow 0$ we have $q = k$.

Instead looking at the other limit, when $V_0 \rightarrow +\infty$, the only possible value for the wavefunction is 0 in those point where there is the delta function ($x = na$), $\psi(na) = 0$. This yields to the same solution of a potential well, i.e $\sin(ka) = 0$ and the allowed energy levels are $E_n = n^2 \frac{\hbar^2 \pi^2}{2ma^2}$.

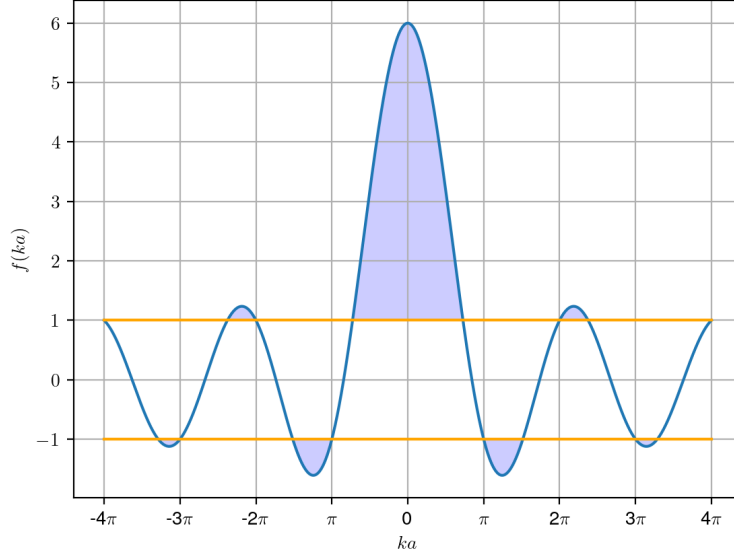


Figure 8: In this plot in blue is illustrated $P \frac{\sin(ka)}{ka} + \cos(ka)$ with $P = 5$, and in orange the boundary of $\cos(qa)$. The allowed values of the energy ϵ are given by those ranges of $qa = (\frac{2m\epsilon}{\hbar^2})^{\frac{1}{2}}a$ for which the function lies between ± 1 . Forbidden values are shaded in blue

Disordered System

In a glass there are many places where one or a group of atoms can exist in two different positions or configurations. The energies of these configurations will be very close, and the atoms can quantum tunnel between the two configurations. Hence, if we want to study the property of a glass, we can look at it as an ensemble of two level systems. The average energy for a 2 level system is given from statistical mechanics:

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1,2} E_i e^{\beta E_i}$$

where $\beta = \frac{1}{k_B T}$ and Z is the canonical partition function of the TLS, i.e the sum of all the Boltzmann weight for the allowed energies. One can set the lowest energy state as the zero of energy, so $E_1 = 0$ and as a consequence $E_2 = E$. This setting yields to an average energy for a TLS equal to:

$$\langle E \rangle = \frac{E}{1 + e^{\beta E}} \quad (16)$$

each of these TLS contributes to the heat capacity of the glass in the following way:

$$C_{TLS} = \left. \frac{\partial \langle E \rangle}{\partial T} \right|_V = k_B (\beta E)^2 \frac{e^{\beta E}}{(e^{\beta E} + 1)^2}$$

However, to calculate the total heat capacity another important ingredient is needed: the density of states of these TLS. This quantity indicates the number of TLS with energy between E and $E + dE$. In our exercise the DOS is given, and it is time-dependent:

$$DOS_{TLS}(E) = \frac{P_0}{2} \ln \left(\frac{4t_0}{\tau_{min}(E)} \right)$$

where P_0 is a constant, t_0 the time, and $\tau_{min}(E)$ is the minimum relaxation time of the TLS. In the light of the above, the total heat capacity is given by:

$$C = \int_0^{+\infty} DOS_{TLS}(E) C_{TLS} dE$$

where in our case:

$$C = \int_0^{+\infty} \frac{P_0 k_B}{2} \ln \left(\frac{4t_0}{\tau_{min}(E)} \right) (\beta E)^2 \frac{e^{\beta E}}{(e^{\beta E} + 1)^2} dE \quad (17)$$

This is a nasty integral to calculate, but we can make some useful observations. First of all, we need an expression for the relaxation time. This indicates the mean time to overcome the barrier and tunnelling on the other allowed energy of the system. One can show that the general expression for the relaxation time of our model is:

$$\frac{1}{\tau_{min}(E)} \propto E^3 \coth\left(\frac{\beta E}{2}\right)$$

. However, the integral is dominated by $(\beta E)^2 \frac{e^{\beta E}}{(e^{\beta E} + 1)^2}$, which for low temperature is a function almost 0 everywhere except for a narrow peak close to $k_B T$. If in this range the logarithm has a small variation in the narrow range of E where the dominating part of the integral is non zero, it can be considered as a constant, and it can be taken out from the integral replacing τ by $\tau_{min}(E_0)$, where E_0 is an energy of the order of $k_B T$. For the sake of simplicity, it is possible to see this from a graphical point of view as illustrated in figure 9. This yields to:

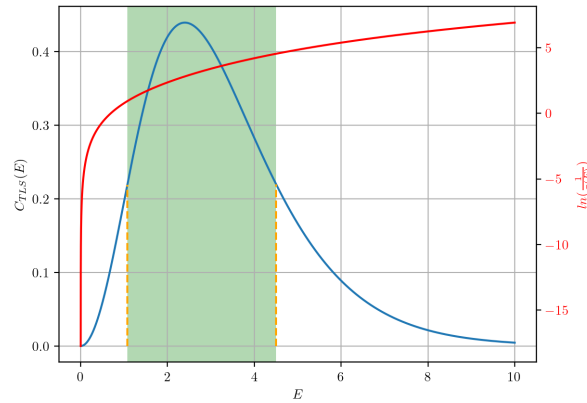


Figure 9: The figure shows the comparison at $T = 1K$ between the trend in red of the logarithmic part of the integral (see equation 17) and in blue the trend of the remaining part of the integral (C_{TLS}). In first approximation we see that the logarithm changes very slowly respect to C_{TLS} . In green is highlighted the narrow range of E where the dominating part of the integral contributes more to the value of the integral.

$$C = \frac{P_0 k_B}{2} \ln\left(\frac{4t_0}{\tau_{min}(E_0)}\right) \int_0^{+\infty} (\beta E)^2 \frac{e^{\beta E}}{(e^{\beta E} + 1)^2} dE$$

where $E_0 \sim k_B T$. Now it is left a simpler integral to evaluate:

$$\frac{1}{\beta} \int_0^{+\infty} \frac{x^2 e^x}{(e^x + 1)^2} dx \quad \text{after changing variable } x = \beta E$$

The value of this integral is known and it is equal to: $\frac{\pi^2}{6}$.

In conclusion, the solution of the problem is:

$$C = \frac{P_0 k_B^2 T}{2} \ln\left(\frac{4t_0}{\tau_{min}(E_0)}\right) \frac{\pi^2}{6} = A(T) \ln\left(\frac{4t_0}{\tau_{min}(E_0)}\right)$$

It is important to understand that the *DOS* of the *TLS* depends on the time t_0 over which we are measuring. This is because only those *TLS* with $\tau < t_0$ are active, before τ_{min} we don't have any *TLS*.

The second part of the exercise asks us to calculate the power released when the whole system has a thermal contact with a reservoir. There are at least two equivalent way to solve this exercise, one it consists in starting from the definition of energy (see eq:16), the other method consists in using the formula that we've just found.

Let's start from the first one: the released energy during the whole quasistatic process, when the glass start with temperature T and end with temperature T_{eq} when reaches the equilibrium with the reservoir.

$$q_{TLS} = E(T) - E(T_{eq})$$

This is the single mean released energy by a TLS. Using the equation (16) we obtain the mean energy of the single TLS at temperature T. To get the whole released energy from the system we have to multiply it by the $DOS(\epsilon)$ and integrate it:

$$q = \int_0^{+\infty} DOS(\epsilon) q_{TLS}(\epsilon) d\epsilon$$

The power is the derivation of q by time:

$$\dot{q} = \frac{d}{dt} \int_0^{+\infty} \frac{P}{2} \ln \left(\frac{4t_0}{\tau_{min}(E)} \right) \left[\frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_1}}} - \frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_{eq}}}} \right] d\epsilon$$

Since the process is quasistatic the time dependence it is only in the logarithmic term. The integral converges so we can differentiate under the integral sign:

$$\begin{aligned} \dot{q} &= \int_0^{+\infty} \frac{P}{2} \frac{d}{dt} \left(\ln \left(\frac{4t}{\tau_{min}(E)} \right) \right) \left[\frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_1}}} - \frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_{eq}}}} \right] d\epsilon \\ &= \frac{P}{2t} \int_0^{+\infty} \frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_1}}} - \frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_{eq}}}} d\epsilon \\ &= \frac{P}{2t} \int_0^{+\infty} \frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_1}}} d\epsilon - \int_0^{+\infty} \frac{\epsilon}{1 + e^{\frac{\epsilon}{k_B T_{eq}}}} d\epsilon \\ &= \frac{P k_B^2}{2t} (T^2 - T_{eq}^2) \int_0^{+\infty} \frac{x}{1 + e^x} dx \\ &= \frac{P k_B^2}{2t} (T^2 - T_{eq}^2) \frac{\pi^2}{12} \end{aligned}$$

This is the correct result.

The same result can be gotten integrating the heat capacity in equation :

$$\begin{aligned} E(t) &= \int_{T_{eq}}^T C(t, T) dT \\ &= \int_{T_{eq}}^T \frac{P_0 k_B^2 T}{2} \ln \left(\frac{4t_0}{\tau_{min}(E_0)} \right) \frac{\pi^2}{6} dT \\ &= \frac{P k_B^2}{2} \ln \left(\frac{4t_0}{\tau_{min}(E_0)} \right) \frac{\pi^2}{6} \left(\frac{1}{2} (T^2 - T_{eq}^2) \right) \\ &= \frac{P \pi^2 k_B^2}{24} (T^2 - T_{eq}^2) \ln \left(\frac{4t_0}{\tau_{min}(E_0)} \right) \end{aligned}$$

Note that the time dependence is only inside the logarithm. Now to get the released power we have to derive over the time:

$$\begin{aligned} \dot{q} &= \frac{d}{dt} \left(\frac{P_0 \pi^2 k_B^2}{24} (T^2 - T_{eq}^2) \ln \left(\frac{4t_0}{\tau_{min}(E_0)} \right) \right) \\ &= \frac{P \pi^2 k_B^2}{24t} (T^2 - T_{eq}^2) \end{aligned}$$

Yielding to the same result.