Assignment 6

Conductivity of Metals

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Problem Statement

A classical model that describes the variation of resistivity as a function of temperature is Bloch–Grüneisen model (see the following expression). Primarily it accounts for the electron-electron scattering and electron-phonon (lattice vibration scattering) in a classical picture.

The goal is to generate a test data and least square fit the data using the procedure discussed in the class and compare it with the fitting parameters generated by LinearModelFit or FindFit.

The suggested steps are:
First, read carefully the information provided below the expression.

1. Choose a value for ρ_0 and Θ_D and generate the "test" data.(see the expression). Here x is the temperature.
2. Add suitable noise and get the "experimental data". Steps 1 and 2 can be combined if you wish so.
3. Store the data in a file on your hard disk in the .csv format.
4. Import the data and fit the data to a linear model and find the "unknown" parameters ρ_0 and α. This must be done using the procedure discussed in the class.
5. Plot the experimental data (points) and the fitted data (continuous line) together on a single plot.
6. Use the Mathematica functions LinearModelFit or FindFit to get the "unknown" parameters ρ_0 and α.
7. Compare the values of ρ_0 and α with those obtained by doing it manually.
8. Plot the experimental data and the best fit line generated using the values of ρ_0 and α obtained from Mathematica function.
9. Comment on the assignment.

If you have time left:
Find a simplified expression for the resistivity, in the limit the temperature tends to zero K and when the temperature tends to a very large value compared to Θ_D.
(You may consult "google" for help in this regard)

In[460]:=

$$(*\rho(x) = \rho_0+\alpha\left(\frac{x}{\Theta_D}\right)^5\int_0^{\Theta_D/x}\left(y^5/((1-\mathrm{Exp}[-y])\ (\mathrm{Exp}[y]-1))\right)dy;*)$$

- In the above expression ρ_0 is the residual resistivity. Θ_D is a constant called the debye temperature, α is a constant and x denotes the temperature. To generate the data, choose one value between (0.1 to 0.6) for ρ_0. The Θ_D for various metals are: Au = 175 K, Na = 202 K, Cu = 333 K, Al = 395 K, Ni = 472 K. Choose any one metal of your choice.

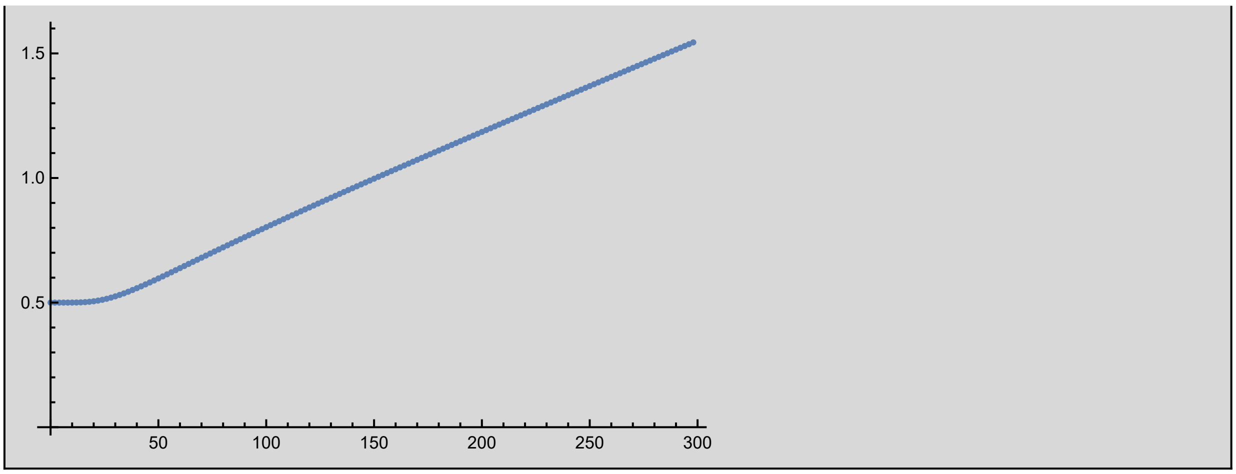
Finding the values first without and then with noise

In[461]:=

```
ρ0 = 0.5;
θD = 175; (*Au*)
α = 2.5;
ρ[x_] := ρ0 + α (x/θD)^5 NIntegrate[y^5 / ((1 - Exp[-y]) (Exp[y] - 1)), {y, 0, θD / x}]
data = Table[{x, ρ[x]}, {x, 0.01, 300, 2}];
Print["Plotting points on the graph without noise:- "]
b = ListPlot[data]
dataNoise0 = Table[{x, ρ[x] + RandomReal[{-0.05, 0.05}]}, {x, 0.01, 300, 2}];
Print["Plotting points on the graph with noise added:- "]
a = ListPlot[dataNoise]
```

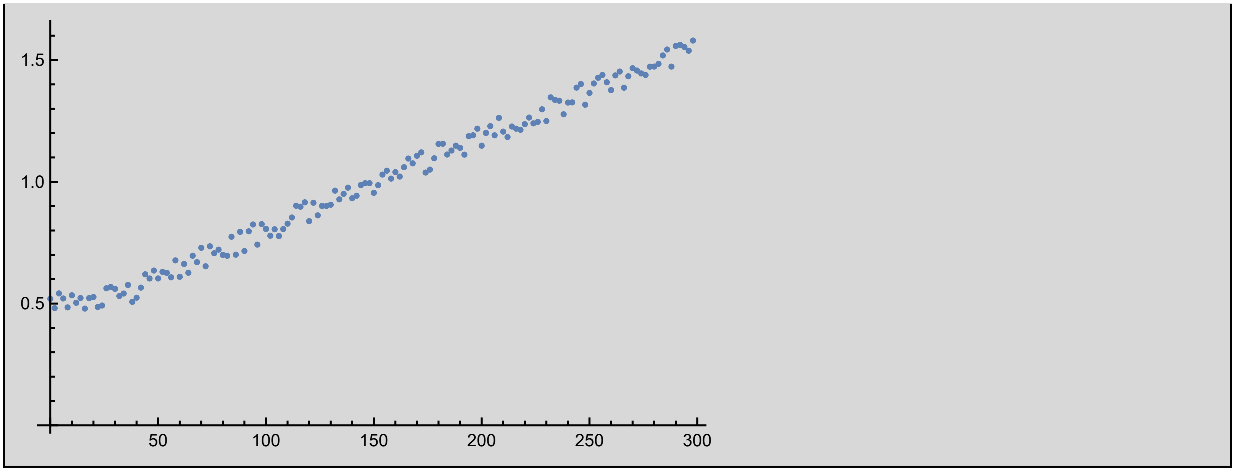
Plotting points on the graph without noise:-

Out[467]=



Plotting points on the graph with noise added:-

Out[470]=



Importing and exporting to and from the csv file

In[471]:=

```
Export["C:\\Users\\amogh\\OneDrive\\Desktop\\Assign.csv", dataNoise0];
dataNoise = Import["C:\\Users\\amogh\\OneDrive\\Desktop\\Assign.csv"];
```

Finding ρ_0 and α using Inbuilt functions

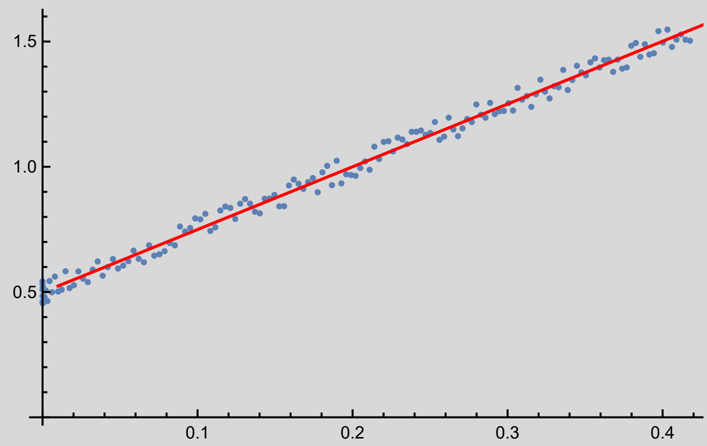
In[473]:=

```
finDat = Table[{(x/θD)^5 NIntegrate[y^5 / ((1 - Exp[-y]) (Exp[y] - 1)), {y, 0, θD / x}],
    ρ[x] + RandomReal[{-0.05, 0.05}]}, {x, 0.01, 300, 2}];
poiPlt = ListPlot[finDat];
line = Normal[LinearModelFit[finDat, x, x]]
liePlt = Plot[line, {x, 0.01, 300}, Frame → True, PlotStyle → Red];
Show[poiPlt, liePlt]
```

Out[475]=

```
0.498976 + 2.5052 x
```

Out[477]=



Finding ρ_0 and α using formulae

$$\rho(x) = \rho_0 + \alpha \left(\frac{x}{\theta_D}\right)^5 \int_0^{\theta_D/x} \frac{(y^5)}{(1-e^{-y})(e^y-1)}\, dy$$

Let $f(x) = \left(\frac{x}{\theta_D}\right)^5 \int_0^{\theta_D/x} \frac{(y^5)}{(1-e^{-y})(e^y-1)}\, dy$

Now, using the formula,

$\rho_0 + \alpha \langle f(x)\rangle = \langle y_i \rangle$

$\rho_0 \langle f(x)\rangle + \alpha \langle f^2(x)\rangle = \langle y_i\, f(x) \rangle$

where <p> is the mean of all values of p.

Solving the linear equations, we get $\alpha = \frac{\langle y\rangle\langle f\rangle - \langle y f\rangle}{\langle f\rangle^2 - \langle f^2\rangle}$ and $\rho_0 = \langle y\rangle - \alpha \langle f\rangle$

In[478]:=

```
meanf = Mean[finDat[[All, 1]]];
meany = Mean[finDat[[All, 2]]];
meanfy = Mean[finDat[[All, 1]] * finDat[[All, 2]]];
meanf2 = Mean[finDat[[All, 1]] * finDat[[All, 1]]];
alphaNet = (meany * meanf - meanfy) / (meanf^2 - meanf2)
rhoNet = meany - alphaNet * meanf
```

$$\text{alphaNet} = \frac{\text{meany} * \text{meanf} - \text{meanfy}}{\text{meanf}^2 - \text{meanf2}}$$

Out[482]=

```
2.5052
```

Out[483]=

```
0.498976
```

Comments

In[484]:=

```
Print["Note that ρ0 from inbuilt functions = y-intercept of line = ",
 rhoNet, " which is the same as calculated by the formula."]
Print["Note that α from inbuilt functions = slope of line = ",
 alphaNet, " which is the same as calculated by the formula."]
```

```
Note that ρ0 from inbuilt functions = y-intercept of line =
 0.498976 which is the same as calculated by the formula.

Note that α from inbuilt functions = slope of line =
 2.5052 which is the same as calculated by the formula.
```

Why this works:-

$$f(x) = \left(\frac{x}{\Theta_D}\right)^5 \int_0^{\Theta_D/x} \frac{(y^5)}{(1-e^{-y})\,(e^y-1))}\,dy$$

We plot a graph of $\rho_0 + \alpha\, f(x)$ vs f(x)

Assuming f(x) as X, the graph becomes $Y = \rho_0 + \alpha\, X$,

which is in the from y=mx+c where $\rho_0 = c$ and $\alpha = m$.