RESEARCH ARTICLE

Quasi-particle Contribution in Thermal Expansion and Thermal Conductivity in Metals

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Abstract: In this paper the modified Landau theory of Fermi Liquids was used to compute the thermal expansion and thermal conductivity of quasi-particles in metals. The result revealed that as temperature increases the thermal expansion of quasi-particles in metals increases in all the metals investigated. It is also observed that as the electron density parameter increases the thermal expansion of quasi-particles increases. This shows that at low density region the thermal expansion of quasi-particles is large. The result obtained for the thermal conductivity of quasi-particles in metals revealed that for all the metals computed the thermal conductivity of quasi-particles decreases as temperature increases. This seems to suggest that as temperature increases the separation between quasi-particles increases because they are not heavy particles hence, the rate of absorbing heat decreases. The computed thermal expansion and thermal conductivity of quasi-particles are in better agreement with experimental values. This suggests that the introduction of the electron density parameter is promising in predicting the contribution of quasi-particles to the bulk properties of metals. This study revealed the extent to which quasi-particles contribute to the bulk properties of metals, which assisted their potential applications in materials science and engineering development.

Keywords: Electron gas; Quasi-particles; Electron density parameter; Thermal Expansion; Thermal Conductivity

1. Introduction

The understanding of the effect of the interactions between electrons on the metallic state which is based on the Landau's Fermi-liquid theory provides the basis for understanding metals in terms of weakly interacting quasi-particles. At zero temperature a Fermi liquid has a Fermi surface, similar to the non-interacting Fermions[7]. The low lying excitations of the Fermi liquid are called quasi-particles (or Landau quasi-particles). Landau quasi-particles consist of electrons, surrounded by a cloud of spin and charge polarization. They share the same quantum numbers as free electrons but their masses can be strongly renormalized by the back flow of the surrounding fluid[1]. When materials undergo thermodynamical change, the energy received is in form of heat hence, its temperature rises and thereby changes in dimension[2]. Heat capacities, thermal expansion, thermal conductivities are few important properties often critical in the practical and engineering applications of solids. Nodar, and Levan, (2010) generalized the Landau's theory of Fermi liquids by incorporating the de Broglie waves diffraction. A newly derived kinetic equation of the Fermi particles is used to derive a general dispersion relation and the excitation of zero sound is studied. A new mode is found due to the quantum correction. It is shown that the zero sound can exist even in an ideal Fermi gas. They also disclose a new branch of frequency spectrum due to the weak interaction. Sykes and Brooker (1970) derived exact expressions for the transport properties of a degenerate Fermi liquid. The coefficients of shear viscosity, thermal conductivity, diffusion and second viscosity were evaluated giving solution for shear viscosity, and diffusion that agree within 25% with those originally quoted. However, the thermal conductivity is reduced by a factor of about 2. The coefficient of second viscosity was shown to vary with temperature like T^2. Gangadharaiah, *et al*., (2005) consider a system of 2D fermions with a short-range interaction. A straight forward perturbation theory is shown to be ill defined even for an infinitesimally weak interaction, as the perturbative series for the self-energy diverges near the mass shell. They show that the divergences result from the interaction of fermions with the zero-sound collective mode. By re-summing the most divergent diagrams, they obtain a closed form of the self-energy near the mass shell. The spectral function exhibits

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a threshold feature at the onset of the emission of the zero-sound waves. They also show that the interaction with the zero sound does not affect a non-analytic, T^2 part of the specific heat. In this work, we modified the Fermi liquid theory using the electron density parameter and the modified Fermi liquid theory is used to compute the thermal expansion and thermal conductivity of Fermi liquid in other to see the predictability of our modified Fermi liquid theory.

Quasi-particles are non-interacting quantum gases that are supposed to contribute to the bulk properties of metals. But the Landau Fermi liquid model overestimated and also underestimated the contribution of quasi-particles of most of the bulk properties of metals investigated. Hence, the modified Landau model effectively account for the over estimation and underestimation of the Landau-Fermi liquid model.

2. Theory and calculations

2.1 Thermal expansion of quasi-particles

The delocalized free-electron gas of a metal also contributes to the thermal expansion of the metal, in addition to the anharmonic atomic vibrational contribution, the pressure of the Fermi gas is given by[4],

$$\mathrm{P} = \frac{2U(T,V)}{3V} \quad (1)$$

Where, $U(T,V)$ is given as, $$U(T) = \frac{2}{5}\varepsilon_f^2 g(\varepsilon_F) + \frac{\pi^2}{6}\left(K_B T^2\right) g(\varepsilon_F) \quad (2)$$

Or, $$U(T) = \frac{3}{5}N\varepsilon_F + \frac{\pi^2}{4}NK_B\frac{T^2}{T_F} \quad (3)$$

Since the volume thermal-expansion coefficient is given by[10],

$$\beta_T = \frac{1}{B}\left(\frac{\partial p}{\partial T}\right)_V \quad (4)$$

Where B is the bulk modulus, there is a positive electronic contribution to the thermal expansion because U(T,V) is an increasing function of T. The thermal-expansion coefficient is given as, $$\beta_T = \frac{2C_v}{3BV} \quad (5)$$

Equation (5) can be written by using,

$$C_v = \frac{\pi^2}{2}NK_B\frac{T}{T_F} \quad (6)$$

and also the Bulk modulus equation given by,

$$B_{K.E} = \frac{10U_0}{9V} = \frac{2}{3}\frac{N}{V}\varepsilon_F \quad (7)$$

In atomic units the bulk modulus of metals is given by,

$$B_{K.E} = \frac{0.586}{r_s^5} \quad (8)$$

and, $$\frac{B}{B_{K.E}} = 0.2 + \frac{0.815 r_c^2}{r_s} \quad (9)$$

Hence, $$\beta_T = \frac{\pi^2}{2}\frac{K_B^2 T}{A\varepsilon_F^2} \quad (10)$$

$A = B/B_{K.E}$ a temperature independent constant, r_c (a.u) is the Ashcroft core radius and r_s is the electron density which varies between 2 and 6 for most metals. Recall that the Fermi energy of the metals at the Fermi surface is given by[3],

$$E_F = \frac{\hbar^2}{2m}\left(\frac{9\pi}{4}\right)^{\frac{2}{3}}\frac{1}{r_s^2} \quad (11)$$

Inserting equation (11) into equation (10), then, the thermal expansion of quasi-particles in terms of the electron density parameter r_s is expressed as,

$$\beta_T = \frac{2\pi^2 m^2}{\hbar^4}\frac{K_B^2 T}{A}\left(\frac{9\pi}{4}\right)^{-4/3} r_s^4 \quad (12)$$

2.2 Thermal conductivity of quasi-particles

The Boltzmann transport equation is given by[9],

$$\frac{\partial n}{\partial t} + \frac{\partial n}{\partial r}.\frac{\partial \varepsilon}{\partial p} - \frac{\partial n}{\partial p}.\frac{\partial \varepsilon}{\partial r} = \mathrm{I} \quad (13)$$

Here $n = n(p,\sigma,r)$ is the distribution function for quasi-particles. The energy $\varepsilon = \varepsilon(p,\sigma,r)$ of a given quantum level depends upon the distribution of the other particles; therefore ε can vary from place to place (even in the absence of an external field) if the liquid is inhomogeneous.

The left-hand side of the Boltzmann transport equation is expanded to

$$-\frac{1}{2}\frac{\partial n_0}{\partial \varepsilon_0} p_i \frac{\partial \varepsilon_0}{\partial p_k}\left\{\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} - \frac{2}{3}\delta_{ik} div\ u\right\} - \frac{\partial n_0}{\partial \varepsilon_0}\frac{\partial \varepsilon_0}{\partial p_k}\left\{\frac{\partial \mu}{\partial x_k} + \frac{(\varepsilon_0 - \mu)}{T}\frac{\partial T}{\partial x_k}\right\}$$

$$+\left\{\frac{\partial n_0}{\partial t} - \frac{\partial n_0}{\partial \varepsilon_0}\frac{1}{3} p_k \frac{\partial \varepsilon_0}{\partial p_k} div\ u\right\} + \frac{\partial n_0}{\partial \varepsilon_0}\frac{\partial \varepsilon_0}{\partial p_k}\frac{\partial \psi}{\partial x_k} + \frac{\partial n_0}{\partial \varepsilon_0}\frac{\partial v}{\partial t} = \mathrm{I}$$

give, (14)

The term in the left-hand side of equation (14) relevant to the thermal conductivity is given by,

$$-\frac{\partial n_0}{\partial \varepsilon_0}\frac{\partial \varepsilon_0}{\partial p}.\left\{\nabla\mu + \frac{(\varepsilon_0 - \mu)}{T}\nabla T\right\} = \mathrm{I} \quad (15)$$

Where μ is the Fermi energy. If we approximate $\frac{\partial n_0}{\partial \varepsilon_0}$ to $\frac{\partial n_0}{\partial \varepsilon}$ and change $(\varepsilon_0 - \mu)$ to kTt equation (15) becomes,

$$-\frac{\partial n_0}{\partial \varepsilon_0}\frac{\partial \varepsilon_0}{\partial p}.\nabla T(-s + kt) = \mathrm{I} \quad (16)$$

where $s = -\frac{\nabla\mu}{\nabla T}$. Here $v = \frac{\partial \varepsilon_0}{\partial p}$ is a function of energy, and is expanded as a power series in t. The direction of the polar axis is taken to be that of ∇T, which means that the left-hand side contains $\cos\Theta$ as its only spherical harmonic[6].Then we will have,

$$\frac{dT}{dz}\cos\Theta\left\{-\left[\frac{\partial \varepsilon_0}{\partial p}\right]_\mu s + \left[\frac{\partial}{\partial \varepsilon_0}\left(\frac{\partial \varepsilon_0}{\partial p}\right)\right]_\mu k^2 T t^2 + \left[\frac{\partial \varepsilon_0}{\partial p}\right]_\mu kt + ...\right\} = J(t,\Theta,\phi) \quad (17)$$

Then a solution of the form is applied and is given as,

$$\psi(t,\Theta,\phi) = \left[\frac{\partial \varepsilon_0}{\partial p}\right]_\mu \frac{dT}{dz}\cos\Theta\, q(t) \quad (18)$$

The coefficient of $q(t)$ is made a quantity that is evaluated at the Fermi surface, so that all of the variation with energy is defined to be in $q(t)$. Recall that,

$$J_s\left(t,\Theta_1,\phi_1\right)=\mathrm{B}^{-1}\sum_{n,m}p_n^{|m|}\left(\cos\Theta_1\right)e^{im\phi_1}\int dx\,k\left(t,x\right)\left\{\psi_{ns}^m\left(t\right)-\lambda_{ns}\psi_{ns}^m\left(x\right)\right\} \quad (19)$$

$$J_a\left(t,\Theta_1,\phi_1\right)=\mathrm{B}^{-1}\sum_{n,m}p_n^{|m|}\left(\cos\Theta_1\right)e^{im\phi_1}\int dx\,k\left(t,x\right)\left\{\psi_{na}^m\left(t\right)-\lambda_{na}\psi_{na}^m\left(x\right)\right\} \quad (20)$$

Then substituting equation (18) into equation (19) and equation (20), we have,

$$\int dx\,k\left(t,x\right)\left\{q_s\left(t\right)-q_s\left(x\right)\right\}=-\mathrm{B}s+\mathrm{B}'Tt^2, \quad (21) \qquad \int dx\,k\left(t,x\right)\left\{q_a\left(t\right)-\lambda_{1a}q_a\left(x\right)\right\}=At \quad (22)$$

where, $\lambda_{1s}=1$ and B' is defined as, $\mathrm{B}'=\left\{\frac{\partial^2\varepsilon_0}{\partial p^2}\left(\frac{\partial p}{\partial\varepsilon_0}\right)^2\right\}_\mu \mathrm{B}k^2$,(23)

and $A=\mathrm{B}k=\frac{8\pi^2\hbar^6}{m^{*3}kT^2}\left\{\int\frac{d\Omega}{2\pi}\frac{\omega_\eta\left(\theta,\phi\right)}{\cos\frac{1}{2}\theta}\right\}^{-1}$ (24)

Equations (21) and (22) are the integral equations that are to be solved in order to find the thermal conductivity. By considering first equation (21) it is shown that $q_s\left(t\right)$ is of the order T^{-1} , so that it is negligible beside $q_a\left(t\right)$. In addition the argument is fairly lengthy. First we have to evaluate $s=-{}^{\nabla\mu}\!/\!_{\nabla T}$. When a temperature gradient is imposed on the Fermi liquid, the physics of the liquid determines the gradient of μ , so that it must be possible to find $\nabla\mu$ from the transport equation. The required condition is provided by the conservation of momentum, given by,

$$\int d\tau\;p\mathrm{I}=0 \quad (25)$$

Using equation (14) we have,

$$0=\int dt\;p\frac{\partial\tau}{\partial p}\frac{dn_0}{dt}\left(-s+kt\right)=\left\{p\frac{\partial\tau}{\partial p}\right\}_\mu s-\left\{\frac{\partial}{\partial\varepsilon_0}\left(p\frac{\partial\tau}{\partial p}\right)\right\}_\mu\frac{\pi^2K^2T}{3}+\ldots., \quad (26)$$

S is the entropy per particle and more physically,

$$\frac{\nabla\mu}{\nabla T}=\left(\frac{\partial\mu}{\partial T}\right)_p \quad (27)$$

From equation (27) it appears that in the presence of a temperature gradient the liquid arranges itself to be at a uniform pressure [7]. Recall that,

$$\int d\tau\frac{\partial n_0}{\partial\varepsilon_0}\frac{\partial\varepsilon_0}{\partial p}\psi\left(p\right)=0 \quad (28)$$

Equation (28) can be rewritten as,

$$0=\int dt\frac{\partial\tau}{\partial p}\frac{\partial n_0}{\partial t}q\left(t\right)$$
$$=\left(\frac{\partial\tau}{\partial p}\right)_\mu\int dt\frac{dn_0}{dt}q_s\left(t\right)+KT\left\{\frac{\partial}{\partial\varepsilon_0}\left(\frac{\partial\tau}{\partial p}\right)\right\}\int dt\frac{dn_0}{dt}tq_0\left(t\right)+\ldots., \quad (29)$$

Considering equation (14), the solution consists of a particular solution and a complementary function which is zero. The thermal conductivity k is given by,

$$Q=-k\nabla T \quad (30)$$

Where Q is the flux energy, given by,

$$Q=\int d\tau\varepsilon_0 \frac{\partial\varepsilon_0}{\partial p}\frac{\partial n_0}{\partial\varepsilon}\psi(p) \quad (31)$$

Then from equation (18)

$$k=-\frac{KT}{3}\left(\frac{\partial\varepsilon_0}{\partial p}\right)_\mu \int dt\frac{\partial\tau}{\partial p}\frac{dn_0}{dt}tq(t)$$

$$=-\frac{KTv_F}{3}\left\{\left(\frac{\partial\tau}{\partial p}\right)_\mu \int dt\frac{dn_0}{dt}tq_a(t)+KT\left[\frac{\partial}{\partial\varepsilon_0}\left(\frac{\partial\tau}{\partial p}\right)\right]_\mu \int dt\frac{dn_0}{dt}t^2 q_s(t)+....\right\} \quad (32)$$

We can see that the contribution of q_s to the thermal conductivity is two factors of T smaller than that of q_a , so the even function need be considered no further . The odd function is taken into consideration, and using equation (32) and

$$-\int_{-\infty}^{\infty} dt\frac{dn_0}{dt}q(t)t=\frac{2A}{3-\lambda}H(\lambda) \quad (33)$$

Then we have,

$$k=\frac{1}{3}v_F^2\left(\frac{m^* p_F}{3\hbar^3}K^2T\right)\frac{6}{\pi^2}\frac{\mathrm{B}}{3-\lambda_{1a}}\mathrm{H}(\lambda_{1a})$$

$$=\frac{8}{3}\frac{\pi^2\hbar^3 p_F^3}{m^{*4}T}\left(\int\frac{d\Omega}{2\pi}\frac{\omega_\eta(\theta,\phi)}{\cos\frac{1}{2}\theta}\{1-\cos\theta\}\right)^{-1}\mathrm{H}(\lambda_{1a}) \quad (34)$$

where,

$$\mathrm{H}(\lambda)=\frac{3-\lambda}{4}\sum_{n=0}^{\infty}\frac{(4n+5)}{(n+1)(2n+3)\{(n+1)(2n+3)-\lambda\}}$$

$$=\frac{\lambda-3}{2\lambda}\left\{\gamma+\ln 2-1-\frac{1}{2\lambda}+\frac{1}{2}\psi\left(s_1-\frac{1}{2}\right)+\frac{1}{2}\psi\left(s_2-\frac{1}{2}\right)\right\} \quad (35)$$

and $\gamma=0.577$ while s_1 and s_2 are given as,

$$s_1=\frac{3}{4}+\frac{1}{4}\sqrt{8\lambda+1} \quad \text{and} \quad s_2=\frac{3}{4}-\frac{1}{4}\sqrt{8\lambda+1} \quad (36)$$

Recall that the Fermi momentum of the quasi-particles at the Fermi level is given as[3],

$$P_F=\hbar k_F=\hbar\left(\frac{9\pi}{4}\right)^{\frac{1}{3}}\frac{1}{r_s} \quad (37)$$

Inserting equation (37) into equation (34), then, the obtained thermal conductivity of quasi-particle in terms of the electron density parameter r_s is,

$$k=\frac{8}{3}\frac{\pi^2\hbar^6}{m^{*4}T}\left(\frac{9\pi}{4}\right)\left(\int\frac{d\Omega}{2\pi}\frac{\omega_\eta(\theta,\phi)}{\cos\frac{1}{2}\theta}\{1-\cos\theta\}\right)^{-1}\mathrm{H}(\lambda_{1a})\frac{1}{r_s^3} \quad (38)$$

3. Results and Discussion

Figure 1 and **Figure 2** show the relationship between the computed thermal expansion of quasi-particles and Landau thermal expansion of quasi-particles with temperature for some metals respectively. The results revealed that the thermal expansion of quasi-particles increases as temperature increases for all the metals investigated. Also, the computed thermal expansion of quasi-particles in metals is larger than the Landau thermal expansion of quasi-particles in metals. This may be as a result of the electron density parameter used to modify the Landau Fermi liquid theory and some approximations made. In both cases as temperature increases the thermal expansion of quasi-particles is closer to the bulk thermal expansion. But the computed thermal expansion of quasi-particles is closer to bulk thermal expansion of metals than the Landau thermal expansion of quasi-particles. This suggests that as temperature increases the amplitude of the lattice vibration of quasi-particles increases, the average interatomic distance becomes greater than the zero-temperature separation and hence thermal expansion is enhanced[4]. In all the metals investigated transition metals have lower thermal expansion than alkali and alkali earth metals. This is due to high concentration of quasi-particles in transition metals.

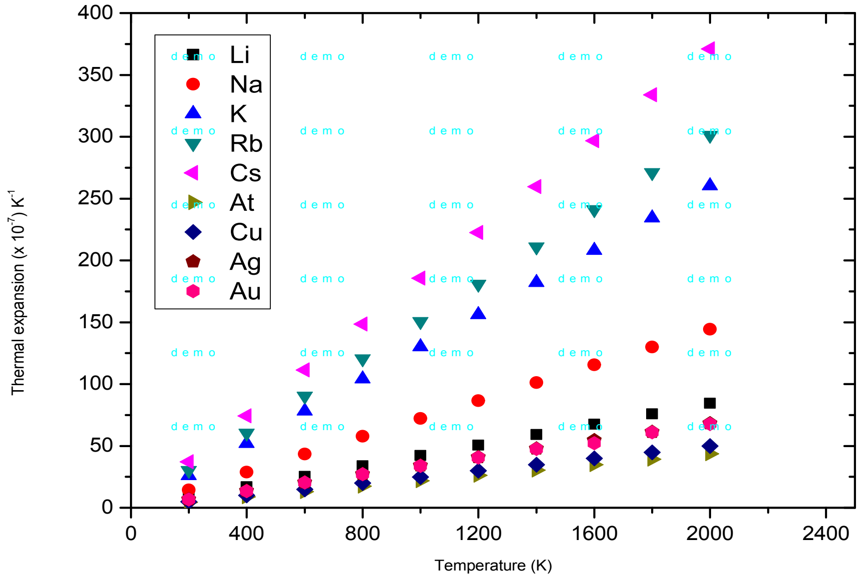

Figure 1; Variation of Calculated Thermal expansion of quasi-particles with temperature for some metals**.**

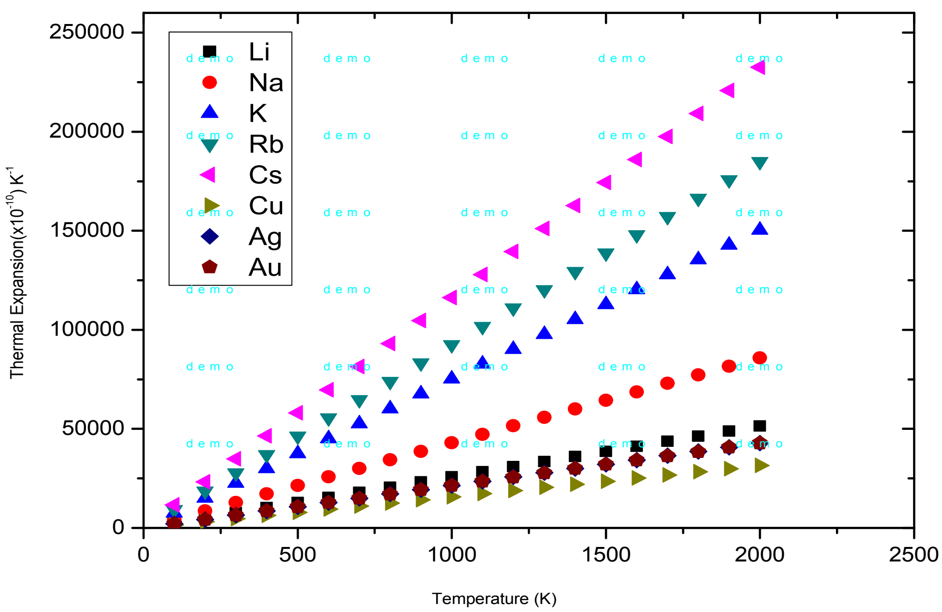

Figure 2; Variation of Landau Thermal expansion of quasi-particles with temperature for some metals [4]**.**

Figure 3 and **Figure 4** show the relationship between the computed thermal conductivity of quasi-particles and Landau thermal conductivity of quasi-particles with temperature for some metals. The result revealed that for all the metals investigated the thermal conductivity of quasi-particles decreases as temperature increases. This seems to suggest that as temperature increases the separation between quasi-particles increases because they are not heavy particles hence, the rate of absorbing heat decreases. It is also observed that the computed thermal conductivity of quasi-particles for monovalent metals is larger in transitions metals (copper (Cu), silver (Ag) and gold (Au)) than most of the alkali metals. This is due to the d-block electrons that have filled electron shell which lies high up in the conduction band in noble metals [5]. This shows that thermal conductivity of quasi-particles depends largely on the electron concentration of metals. The experimental thermal conductivity of metals is higher than the computed thermal conductivity of quasi-particles and the computed thermal conductivity of quasi-particles is higher than the Landau thermal conductivity of quasi-particles. But the value of the computed thermal conductivity of quasi-particles is closer to the value of the experimental thermal conductivity of metals. This seems to suggest that the modified Landau Fermi liquid theory can account and predict very well the contribution of quasi-particles to the thermal conductivity of metals.

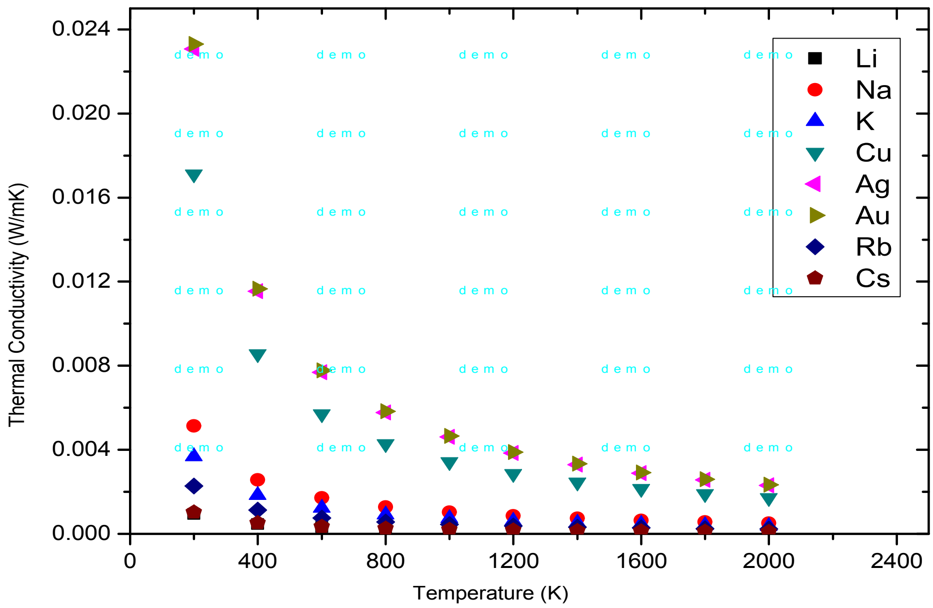

Figure 3; Variation of Calculated Thermal conductivity of quasi-particles with temperature for some metals**.**

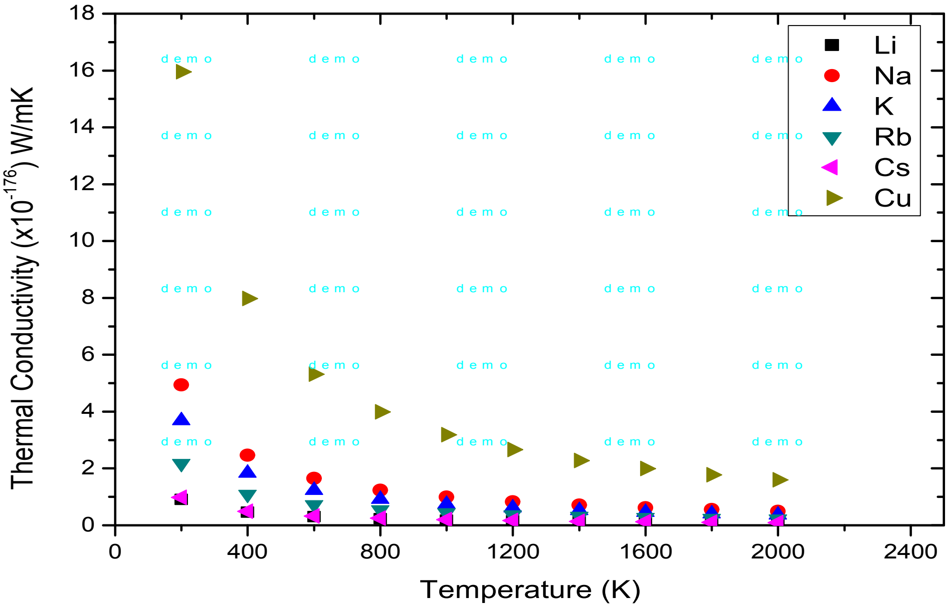

Figure 4; Variation of Landau Thermal conductivity of quasiparticles with temperature for some metals [9].

4. Conclusion

The thermal expansion of quasi-particles increases as temperature increases for all the metals investigated. In both cases as temperature increases the thermal expansion of quasi-particles is closer to the bulk thermal expansion. But the computed thermal expansion of quasi-particles is closer to bulk thermal expansion of metals than the Landau thermal expansion of quasi-particles. Also, it is observed that the experimental thermal conductivity of metals is higher than the computed thermal conductivity of quasi-particles and the computed thermal conductivity of quasi-particles is higher than the Landau thermal conductivity of quasi-particles. But the value of the computed thermal conductivity of quasi-particles is closer to the value of the experimental thermal conductivity of metals. This seems to suggest that the modified Landau Fermi liquid theory can account and predict very well the contribution of quasi-particles to the bulk thermal expansion and thermal conductivity of metals. In both properties the Landau theory of Fermi liquid under estimated the contribution of quasi-particles to bulk metals.

This study reveals the extent to which quasi-particles contribute to the bulk properties of metals, which will assist their potential applications in materials science and engineering development.

5. Application of Results

Results obtained from this work can be applied in various areas: The obtained thermodynamic properties of quasi-particles, in terms of the electron density parameter for some metals can act as a guide to experimentalists when determining the effect of temperature on the bulk properties of metals. The results obtained in this work give an insight into how the thermodynamic, transport, structural and magnetic properties of quasi-particles in metals contribute to the bulk properties of metals.

6. Recommendations for Further Studies

Having used the Landau Fermi liquid theory to develop and obtain expressions for computing some properties of quasi-particles in different metals, in terms of the electron density parameter the following recommendations are made for further studies:

This study should be extended to semiconductors and insulators to enable us have a general understanding of the contribution of quasi-particles to the bulk properties of solids.

The model should also be used to study the effect of deformation on the thermodynamics of non-interacting electron gas.

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