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APPLICATION OF Q-DEFORMED FERMI-DIRAC STATISTICS TO THE SPECIFIC HEAT CAPACITY OF FREE ELECTRONS OF METALS

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Abstract. *In this article, the contribution of free electrons to the specific heat capacity of metals in low temperature has been investigated by using the q-deformed fermi-dirac statistics. We have obtained the analytical expressions of the specific heat capacity of metals and the value of q-deformed parameter. Present theoretical calculations of specific heat capacity for some kinds of alkali and transition metals have been performed and compared with the experimental results showing the agreement.*

I. INTRODUCTION

Metal is a solid which contains many electrons that can move freely throughout the crystal. So it has a good electrical conductivity which is about 10^6 to 10^8 $\Omega^{-1}m^{-1}$. Each atom in material has only one electron, there would be about 10^{22} valence electrons in a cm^3. Depending on the distribution function used to consider free-electron gas we will have different theories: If free electrons are considered as simplest classical gas which have the same energy value, we use Drudes theory to analyze issues about metal. If the Maxwell-Boltzmann distribution function is used to analyze classical gas, it is applied according to Lorentzs theory. If the Fermi-Dirac distribution function is used to do this, it is applied according to Sommerfelds theory. The specific heat capacity of the free electrons in metals have been studied from these theories [1, 2, 3]. In present article, we propose other plan applying the statistical distribution of Fermi-Dirac -q deformation to study the heat capacity of free-electron gas in metals at low temperatures [4, 6]. We have obtained the analytic expressions of the specific heat capacity of metals and the value of q-deformed parameter. Present theoretical calculations of specific heat capacity for some kinds of alkali and transition metals have been performed and compared with the experimental results.

II. THEORY

At very low temperature, free electron gas in metals via the fermi-dirac statistics and the heat capacity at constant volume ratio is linear with absolute temperature [2, 3].

$$C_V^e = \gamma T \tag{1}$$

In the q-deformed Fermions oscillator operators satisfying the relation contrast commutative [4, 5, 6].

$$\hat{b}\hat{b}^{+} + q\hat{b}^{+}\hat{b} = q^{-\hat{N}} \tag{2}$$

where $\widehat{\mathrm{N}}$ is oscillator number operator and q is a deformation parameter.
with the q-deformed Fermions:

$$\{n\}_q = \frac{q^{-n} - (-1)^n q^n}{q + q^{-1}} \tag{3}$$

In statistical physics the thermal average expression of the operator $\hat{F}$ is given as:

$$\left\langle \hat{F} \right\rangle = \frac{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}.\hat{F}\right)}{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}\right)} \tag{4}$$

where μ is the chemical, $\widehat{H}$ is the Hamiltonian operator of the system, $\beta = 1/kT$, k is Boltzmann constant, T is the absolute temperature. From equations (4) the average number of particles with the same level of energy can be calculated as

$$\left\langle \hat{N} \right\rangle = \frac{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}.\hat{\mathrm{N}}\right)}{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}\right)} \tag{5}$$

The calculations give following results:

$$Tr\left(\exp\left\{-\beta(\hat{H} - \mu\hat{N})\right\}.\left\{\hat{N}\right\}_q\right) = \sum_{n=0}^{\infty} \langle n| e^{-\beta(\varepsilon-\mu)\hat{N}} \left\{\hat{N}\right\}_q |n\rangle$$
$$= \sum_{n=0}^{\infty} \langle n| e^{-\beta(\varepsilon-\mu)n} \{n\}_q |n\rangle = \sum_{n=0}^{\infty} e^{-\beta(\varepsilon-\mu)n} \{n\}_q$$
$$= \sum_{n=0}^{\infty} e^{-\beta(\varepsilon-\mu)n}.\tfrac{q^{-n}-(-1)^n q^n}{q+q^{-1}}$$
$$= \tfrac{1}{q+q^{-1}} \left[\sum_{n=0}^{\infty} \left(q^{-1}.e^{-\beta(\varepsilon-\mu)}\right)^n - \sum_{n=0}^{\infty} \left(-q.e^{-\beta(\varepsilon-\mu)}\right)^n\right]$$
$$= \tfrac{1}{q+q^{-1}} \left[\tfrac{1}{1-q^{-1}.e^{-\beta(\varepsilon-\mu)}} - \tfrac{1}{1+q.e^{-\beta(\varepsilon-\mu)}}\right]$$
$$= \frac{e^{-\beta(\varepsilon-\mu)}}{1 + (q - q^{-1})e^{-\beta(\varepsilon-\mu)} - e^{-2\beta(\varepsilon-\mu)}} \tag{6}$$

$$Tr\left(\exp\left\{-\beta(\hat{H} - \mu\hat{N})\right\}\right) = \sum_{n=0}^{\infty} \langle n| e^{-\beta(\varepsilon-\mu)\hat{N}} |n\rangle$$
$$= \sum_{n=0}^{\infty} \langle n| e^{-\beta(\varepsilon-\mu)n} |n\rangle = \sum_{n=0}^{\infty} e^{-\beta(\varepsilon-\mu)n}$$
$$= \frac{1}{1 - e^{-\beta(\varepsilon-\mu)}} \tag{7}$$

Substituting equation (6) and equation (7) into equation (5), we obtain the Fermi-Dirac distribution function q-deform Fermi Dirac as:

$$\bar{n}(\varepsilon) = \left\langle \hat{N} \right\rangle = \frac{e^{\beta(\varepsilon-\mu)} - 1}{e^{2\beta(\varepsilon-\mu)} + (q - q^{-1})e^{\beta(\varepsilon-\mu)} - 1} \tag{8}$$

Total number of free electrons and the total energy of free electron gas at temperature T are [1, 2].

$$N = \int_0^\infty \rho(\varepsilon).\bar{n}(\varepsilon)d\varepsilon \tag{9}$$

$$E = \int_0^\infty \varepsilon.\rho(\varepsilon).\bar{n}(\varepsilon)d\varepsilon \tag{10}$$

where $\rho(\varepsilon)$ is the density of states defined as:

$$\rho(\varepsilon) = \frac{g(\varepsilon).V}{4\pi^2\hbar^3}(2m)^{3/2}.\varepsilon^{1/2} \tag{11}$$

Here $\bar{n}(\varepsilon)$ is the average number of particles with energies ε and $g(\varepsilon)$ is the multiple degeneracy of each energy level ε.
From equations (8), (9), (10) and using $\alpha = \frac{V.(2m)^{3/2}}{2\pi^2\hbar^3}$ we can be rewritten as

$$N = \alpha \int_0^\infty \varepsilon^{1/2}.\frac{e^{\frac{\varepsilon-\mu}{kT}} - 1}{e^{2\frac{\varepsilon-\mu}{kT}} + (q - q^{-1})e^{\frac{\varepsilon-\mu}{kT}} - 1}d\varepsilon \tag{12}$$

$$E = \alpha \int_0^\infty \varepsilon^{3/2}.\frac{e^{\frac{\varepsilon-\mu}{kT}} - 1}{e^{2\frac{\varepsilon-\mu}{kT}} + (q - q^{-1})e^{\frac{\varepsilon-\mu}{kT}} - 1}d\varepsilon \tag{13}$$

Perform calculations and when $T \to 0K$ we obtained [2].

$$N = \frac{2}{3}\alpha.\mu_0^{3/2} \tag{14}$$

$$E_0 = \frac{2}{5}\alpha.\mu_0^{5/2} = \frac{3}{5}\mu_0 N \tag{15}$$

Where μ_0 is the chemical at $T = 0K$ given as:

$$\mu_0 = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} = \left(\frac{3N}{2\alpha}\right)^{\frac{2}{3}} \tag{16}$$

At very low temperature $T \neq 0K$, from equations (12), (13), (14), (15), (16) perform transformations and when $0 < q < 1$ we determine the total energy of free electron gas at temperature T:

$$E = E_0\left[1 + 5.\frac{F(q)(kT)^2}{\mu_0^2}\right] \tag{17}$$

From equation (15) and equation (17)we obtained.

$$E = \frac{3}{5} N\mu_0 \left[1 + 5.\frac{F(q)(kT)^2}{\mu_0^2} \right] \tag{18}$$

where

$$F(q) = \frac{-1}{q^2+1} \left[q(q-1)\sum_{k=1}^{\infty} \frac{(q)^k}{k^2} + (1+q)\sum_{k=1}^{\infty} \frac{(-q)^k}{k^2} - q\sum_{k=1}^{\infty} \frac{(q)^k}{k^3} + \sum_{k=1}^{\infty} \frac{(-q)^k}{k^3} \right] \tag{19}$$

Heat capacity at constant volume of free electrons gas in metals for the case of the deformation-q.

$$C_V^{el} = \left(\frac{\partial E}{\partial T} \right)_V = 6.\frac{NF(q)k^2T}{\mu_0} = \gamma^{bd}T \tag{20}$$

So at very low temperatures, the heat capacity of free-electron gas in metals when deformed q-ratio is linear with temperature. From equation (1) and equation (20) we inferred expressions as:

$$F\left(q\right) = \frac{\mu_0 \gamma}{6NK^2} \tag{21}$$

$$\gamma^{bd} = 6.\frac{N.k^2.F(q)}{\mu_0} \tag{22}$$

The experimental values of the Fermi energy and electron thermal constants of metals as Table 1 [7].

III. NUMERICAL RESULTS AND DISCUSSIONS

We replace the experimental values of the Fermi energy and electron thermal constants of metals (Table 1) in expression (21) and (22), find out the expression for $F(q)$ by using the software Maple estimates, and obtain the value of strain-q parameter for metals presented as table 2. Present calculation results also suggest that for alkali and earth metals with the same number of outer electrons layer, the value of the parameter q and the function $F(q)$ are larger than those of the transition metal, and contribute to the electron heat capacity is larger, while for the transition metals the outer electron layer of the layered d, f, the value of deformation parameter q and the function $F(q)$ that it is smaller than the alkali metals the electron contribution to heat smaller. Table 2 shown that the value of the parameter q are the same equaling 0.642 for the alkali metals, and the value of q are the same equaling 0.564 for the transition metals. We used these values of the parameter q for each metal and draw the graph in Fig. 1.1 to Fig. 1.5, shows the results fit well with the experiment.

Table 1. The experimental values of the Fermi energy and electron thermal constants of the metals.

$Metal$	Cs	K	Na	Ba	Sr	Ca	Li	Ag
$\mu_0(eV)$	1.58	2.12	3.23	3.65	3.95	4.68	4.72	5.48
$\gamma(mJ.mol^{-1}.K^{-2})$	3.20	2.08	1.38	2.7	3.6	2.9	1.63	0.646

$Metal$	Au	Cu	Cd	Zn	Ga	Al	Be	Mg
$\mu_0(eV)$	5.51	7.0	7.46	9.39	10.35	11.03	11.11	17.1
$\gamma(mJ.mol^{-1}.K^{-2})$	0.72	0.59	0.68	0.64	0.595	1.35	0.17	1.3

Table 2. Experimental and theoretical values of parameters γ and deformation parameters of the electrons in metals.

$Metal$	$\gamma^{TN}(mJ.mol^{-1}.K^{-2})$	$\gamma^{bd}(mJ.mol^{-1}.K^{-2})$	q	$F(q)$
Na	1.38	1.379	0.642	1.036662
K	2.08	2.079	0.627	1.025545
Rb	2.41	2.409	0.642	1.036954
Cs	3.20	3.199	0.835	1.175845
Be	0.17	0.215	0.279	0.559054
Cu	0.595	0.594	0.563	0.968659
Ag	0.646	0.645	0.442	0.823320
Au	0.729	0.728	0.531	0.934189
Cd	0.688	0.562	0.570	0.975432

IV. CONCLUSIONS

The heat capacity of free-electron gas in metals at low temperatures has been investigated by applying the statistical distribution of Fermi-Dirac -q deformation. We have obtained the analytic expressions of the specific heat capacity of metals and the value of q-deformed parameter. Present theoretical calculations of specific heat capacity for some kinds of alkali and transition metals have been performed and compared with the experimental results.

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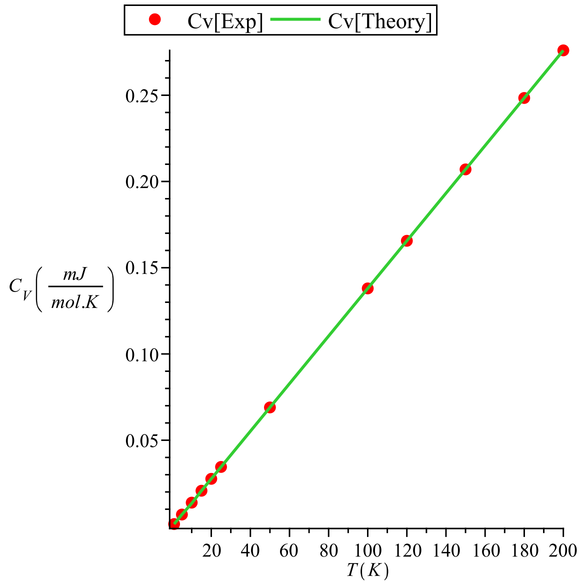

Fig. 1. Temperature dependence of the specific heat capacity of electrons for sodium.

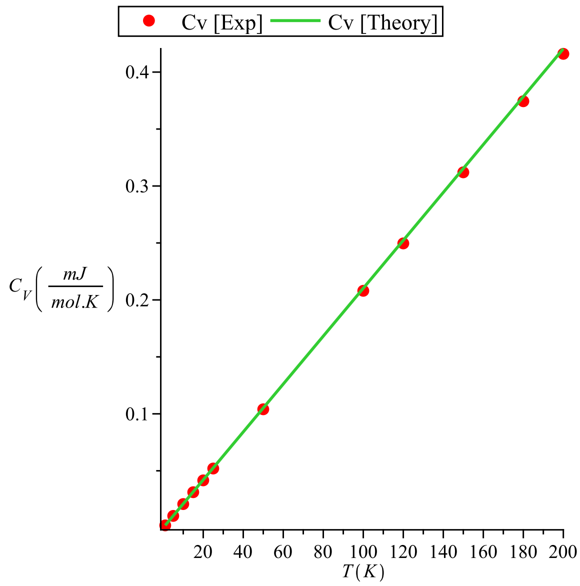

Fig. 2. Temperature dependence of the specific heat capacity of electrons for potassium.

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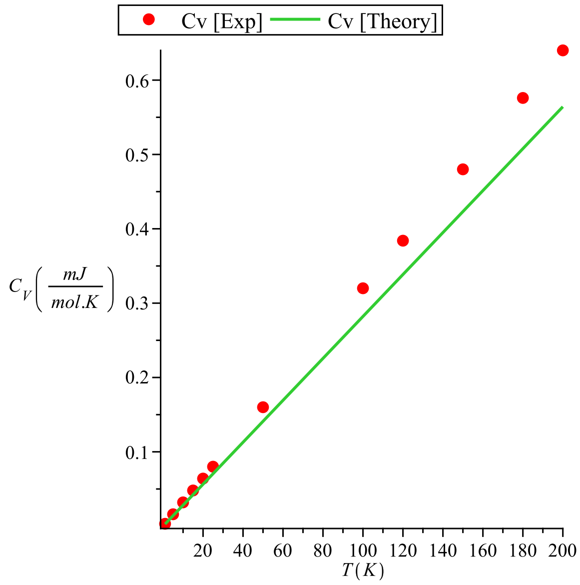

Fig. 3. Temperature dependence of the specific heat capacity of electrons for sexi.

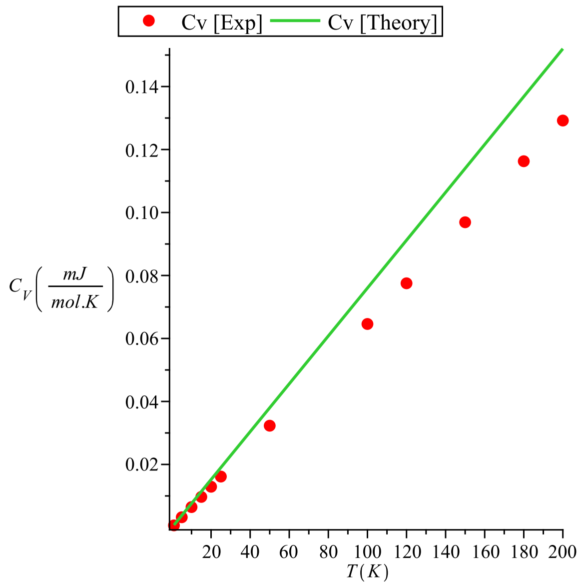

Fig. 4. Temperature dependence of the specific heat capacity of electrons for silver.

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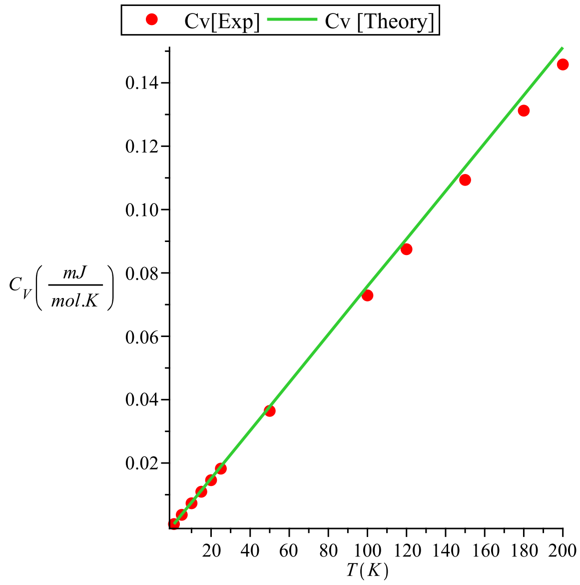

Fig. 5. Temperature dependence of the specific heat capacity of electrons for gold.

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