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PARAMAGNETIC SUSCEPTIBILITY OF METALS IN THE THEORY OF Q-DEFORMED FERMI-DIRAC STATISTICS

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Abstract. *Contribution of the free electrons to the paramagnetic susceptibility of metals at low temperature is investigated by using the q-deformed Fermi-Dirac statistics. Besides the general Pauli term, in our analytic expression of the paramagnetic susceptibility, the contribution of the q-deformed is also taken into account. Our numerical evaluation for some typical metals Na, K, Cs, Rb and Ba shows the adequation with one measured in experimental. In the low temperature limit, we also pointed out the weakly temperature dependence of the paramagnetic susceptibility of the metals.*

I. INTRODUCTION

In metal many electrons can move freely throughout the crystal that leads the metal often to be a high electrical conductivity candidate with the electrical conductivity typically being around 10^6 to 10^8 $\Omega^{-1}m^{-1}$. For instance, if each atom in material contains only one free electron, there would be about 10^{22} conduction electrons in a cm^3. Depending on which distribution function used to consider the free-electron gas, a different theory could be established: (i) Once free electrons are considered as simplest classical gas settling on the same energy, the Drudes theory can be used to analyze issues arising on the metal; (ii) In the case of using the Maxwell-Boltzmann distribution function for the classical gas, the metal can be described in the framework of the Lorentzs theory; (iii) In the quantum feature with the Fermi-Dirac distribution function being used, the Sommerfelds theory is proposed instead. In the mean of these theories, the paramagnetic susceptibility of the free electrons in the metals had been studied in detail [2, 5]. In this article, we propose another way to apply the statistical distribution of Fermi-Dirac -q deformation to investigate the paramagnetic susceptibility of metals at low temperature. We will point out the analytical expressions of the paramagnetic susceptibility of metals as well as the q-deformed parameter. Our numerical evaluation for some typical metals Cs, Na, K, Rb and Ba will be discussed and compared with one measured in experiments [8, 9, 10, 11].

II. THEORY

According to the classical free electron theory, the paramagnetic susceptibility of the free electrons must obey the Curie's law [2, 5].

$$\chi = \frac{\mathrm{I}}{\mathrm{H}} = \frac{\mathrm{N}\mu_{\mathrm{B}}^2}{k_{\mathrm{B}}T} \tag{1}$$

where I is the magnetization, H is magnetic field, N is the total number of free electrons, μ_B is magneton Bohr, k_B is the Boltzmann constant and T is the absolute temperature. The paramagnetic susceptibility of the free electrons in equations (1) shows its inverse proportion to the temperature.
In the quantum theory, Pauli pointed out another expression for the paramagnetic susceptibility of the free electrons, which does not depend on temperature [5].

$$\chi = \frac{3}{2}\frac{\mathrm{N}\mu_{\mathrm{B}}^2}{k_{\mathrm{B}}T_F}. \tag{2}$$

Here T_F is the Fermi temperature.
Now we consider aramagnetic susceptibility of metals in the theory of q-deformed Fermi-Dirac statistiec.
In the q-deformed formalism, the Fermions oscillator operators satisfy the following commutative relations [3, 4, 6, 7].

$$\hat{b}\hat{b}^{+} + q\hat{b}^{+}\hat{b} = q^{-\hat{N}} \tag{3}$$

where

$$\hat{b}^{+}\hat{b} = \left\{\hat{N}\right\}_q \tag{4}$$

$$\hat{b}\hat{b}^{+} = \left\{\hat{N}+1\right\}_q \tag{5}$$

with the q-deformed Fermions number:

$$\{N\}_q = \frac{q^{-n} - (-1)^n q^n}{q + q^{-1}} \tag{6}$$

In statistical physics, the thermal average expression of the operator $\hat{F}$ reads:

$$\left\langle \hat{F} \right\rangle = \frac{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}.\hat{F}\right)}{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}\right)} \tag{7}$$

Where μ is the chemical, $\widehat{H}$ is the Hamiltonian operator of the system, $\beta = \frac{1}{k_B T}$.
From equation (7) one can evaluate the average number of particles with the same energy as follows:

$$\left\langle \hat{N} \right\rangle = \frac{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}\hat{\mathrm{N}}\right)}{Tr\left(\exp\left\{-\beta(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}})\right\}\right)} \tag{8}$$

The calculations give the following results:

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

$= \frac{1}{q+q^{-1}}\left[\sum\limits_{n=0}^{\infty}\left(q^{-1}.e^{-\beta(\varepsilon-\mu)}\right)^n - \sum\limits_{n=0}^{\infty}\left(-q.e^{-\beta(\varepsilon-\mu)}\right)^n\right]$
$= \frac{1}{q+q^{-1}}\left[\frac{1}{1-q^{-1}.e^{-\beta(\varepsilon-\mu)}} - \frac{1}{1+q.e^{-\beta(\varepsilon-\mu)}}\right]$

$$= \frac{e^{-\beta(\varepsilon-\mu)}}{1+(q-q^{-1})e^{-\beta(\varepsilon-\mu)} - e^{-2\beta(\varepsilon-\mu)}} \qquad (9)$$

On the other hand:
$Tr\left(\exp\left\{-\beta(\hat{H}-\mu\hat{N})\right\}\right) = \sum\limits_{n=0}^{\infty}\langle n|e^{-\beta(\varepsilon-\mu)\hat{N}}\,|n\rangle$
$= \sum\limits_{n=0}^{\infty}\langle n|e^{-\beta(\varepsilon-\mu)n}\,|n\rangle = \sum\limits_{n=0}^{\infty} e^{-\beta(\varepsilon-\mu)n}$

$$= \frac{1}{1-e^{-\beta(\varepsilon-\mu)}} \qquad (10)$$

Substituting equation (9) and equation (10) into equation (8), we obtain the q-deformed Fermi-Dirac distribution function as following:

$$\overline{n}(\varepsilon) = f_q(\varepsilon) = \frac{e^{\beta(\varepsilon-\mu)} - 1}{e^{2\beta(\varepsilon-\mu)} + (q-q^{-1})\,e^{\beta(\varepsilon-\mu)} - 1} \qquad (11)$$

In quantum mechanics, the temperature dependence of density of state on energy must read $f_q(\varepsilon, T) \times D(\varepsilon)$ [2, 5].
Therefore

$$f_q(\varepsilon, T) \times D(\varepsilon) = \frac{e^{\beta(\varepsilon-\mu)} - 1}{e^{2\beta(\varepsilon-\mu)} + (q-q^{-1})\,e^{\beta(\varepsilon-\mu)} - 1} \cdot \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \varepsilon^{\frac{1}{2}} \qquad (12)$$

In magnetic field, the free electrons would be redistributed. Part of the electrons with spin settling opposite with the magnetic field can reverse their spins and with the rest ones modify the total magnetization. That means, the magnetization changes to

$$\mathrm{I} = (\mathrm{N}_+ - \mathrm{N}_-)\,\mu_{\mathrm{B}} \qquad (13)$$

where

$$\mathrm{N}_+ = \frac{1}{2}\int\limits_{-\mu_{\mathrm{B}}\mathrm{H}}^{\varepsilon_F} d\varepsilon f_q(\varepsilon, T) D(\varepsilon + \mu_{\mathrm{B}}\mathrm{H}) = \frac{1}{2}\mathrm{I}_{1q} \qquad (14)$$

$$\mathrm{N}_- = \frac{1}{2}\int\limits_{+\mu_{\mathrm{B}}\mathrm{H}}^{\varepsilon_F} d\varepsilon f_q(\varepsilon, T) D(\varepsilon - \mu_{\mathrm{B}}\mathrm{H}) = \frac{1}{2}\mathrm{I}_{2q}. \qquad (15)$$

Substituting equation (14) and equation (15) into equation (13) one delives:

$$\mathrm{I} = \frac{1}{2}(\mathrm{I}_{1q} - \mathrm{I}_{2q})\,\mu_{\mathrm{B}} \qquad (16)$$

with

$$\begin{aligned} \mathrm{I}_{1q} &= \int\limits_{-\mu_{\mathrm{B}}\mathrm{H}}^{\varepsilon_F} d\varepsilon f_q\left(\varepsilon,T\right) D\left(\varepsilon+\mu_{\mathrm{B}}\mathrm{H}\right) \\ &= \int\limits_{-\mu_{\mathrm{B}}\mathrm{H}}^{\varepsilon_F} \frac{e^{\frac{\varepsilon-\mu}{kT}}-1}{e^{2\cdot\frac{\varepsilon-\mu}{kT}}+(q-q^{-1})e^{\frac{\varepsilon-\mu}{kT}}-1}\cdot\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}(\varepsilon+\mu_{\mathrm{B}}\mathrm{H})^{\frac{1}{2}}d\varepsilon \end{aligned} \tag{17}$$

and

$$\begin{aligned} \mathrm{I}_{2q} &= \int\limits_{+\mu_{\mathrm{B}}\mathrm{H}}^{\varepsilon_F} d\varepsilon f_q\left(\varepsilon,T\right) D\left(\varepsilon-\mu_{\mathrm{B}}\mathrm{H}\right) \\ &= \int\limits_{+\mu_{\mathrm{B}}\mathrm{H}}^{\varepsilon_F} \frac{e^{\frac{\varepsilon-\mu}{kT}}-1}{e^{2\cdot\frac{\varepsilon-\mu}{kT}}+(q-q^{-1})e^{\frac{\varepsilon-\mu}{kT}}-1}\cdot\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}(\varepsilon-\mu_{\mathrm{B}}\mathrm{H})^{\frac{1}{2}}d\varepsilon \end{aligned} \tag{18}$$

Integrals in equation (17) and equation (18) can be evaluated approximately and we obtain

$$\mathrm{I}_{1q} = \alpha\frac{2}{3}\varepsilon_F^{\frac{3}{2}}\left(1+\frac{3}{2}\frac{\mu_{\mathrm{B}}\mathrm{H}}{\varepsilon_F}\right)+\alpha\varepsilon_F^{-\frac{1}{2}}\left(1-\frac{1}{2}\frac{\mu_{\mathrm{B}}\mathrm{H}}{\varepsilon_F}\right)F\left(q\right)\left(k_BT\right)^2 \tag{19}$$

$$\mathrm{I}_{2q} = \alpha\frac{2}{3}\varepsilon_F^{\frac{3}{2}}\left(1-\frac{3}{2}\frac{\mu_{\mathrm{B}}\mathrm{H}}{\varepsilon_F}\right)+\alpha\varepsilon_F^{-\frac{1}{2}}\left(1+\frac{1}{2}\frac{\mu_{\mathrm{B}}\mathrm{H}}{\varepsilon_F}\right)F\left(q\right)\left(k_BT\right)^2 \tag{20}$$

Where $\alpha = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}$ and

$$F\left(q\right) = -\frac{1}{q^2+1}\left[q\left(q-1\right)\sum_{k=1}^{\infty}\frac{\left(q\right)^k}{k^2}+\left(1+q\right)\sum_{k=1}^{\infty}\frac{\left(-q\right)^k}{k^2}-q\sum_{k=1}^{\infty}\frac{\left(q\right)^k}{k^3}+\sum_{k=1}^{\infty}\frac{\left(-q\right)^k}{k^3}\right] \tag{21}$$

From Eqs. (16), (19) and (20) we have:

$$\mathrm{I} = \alpha\varepsilon_F^{\frac{1}{2}}\mu_B^2H-\frac{1}{2}\frac{\mu_B^2}{\varepsilon_F^{\frac{3}{2}}}\alpha\varepsilon_F^{-\frac{1}{2}}HF\left(q\right)\left(k_BT\right)^2 \tag{22}$$

Thus

$$\chi = \frac{\mathrm{I}}{\mathrm{H}} = \alpha\varepsilon_F^{\frac{1}{2}}\mu_B^2-\frac{\mu_B^2}{2\varepsilon_F^{\frac{3}{2}}}\alpha\varepsilon_F^{-\frac{1}{2}}F\left(q\right)\cdot\left(k_BT\right)^2 \tag{23}$$

with the following notations:

$$\alpha = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}, \mathrm{N} = \frac{V}{3\pi^2}\left(\frac{2m\varepsilon_F}{\hbar^2}\right)^{\frac{3}{2}}, \varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2\mathrm{N}}{V}\right)^{\frac{2}{3}} \tag{24}$$

Equation (23) can be rewritten and our paramagnetic susceptibility expression finally reads.

$$\chi = \frac{\mathrm{I}}{\mathrm{H}} = \frac{3}{2}\frac{N\mu_B^2}{\varepsilon_F}-\frac{3}{4}\frac{N\mu_B^2}{\varepsilon_F^3}F\left(q\right)\left(k_BT\right)^2 \tag{25}$$

Table 1. The experimental data for the Fermi energy and the obtained results of F(q) [5, 12].

$Metals$	Cs	K	Na	Rb	Ba
$\varepsilon_F\ (eV)$	1.58	2.12	3.23	1.85	3.65
$F(q)$	1.17585	1.02554	1.03666	1.03695	2.29199

Table 2. The experimental and theoretical valuas of the paramagnetic susceptibility of metals.

$Metals$	Cs	K	Na	Rb	Ba
$\chi_{\exp} \times 10^{-6} cm^3.mol^{-1}$	+29	+20.8	+16	+17	+20.6
$\chi_{theo} \times 10^{-6} cm^3.mol^{-1}$	+30.67	+22.86	+15	+16.21	+21.86

III. NUMERICAL RESULTS AND DISCUSSIONS

In the CGS units, the paramagnetic susceptibility in the q-deformed theory can be evaluated belonging to according (25). values.

Table 2 shows a comparison of our results with ones observed in experimental [2, 8, 9, 10, 11, 12]. At T=0K, equation (25) leads to the paramagnetic susceptibility of the free electrons evaluated according to the Pauli quantum theory [5]:

$$\chi = \frac{3}{2}\frac{\mathrm{N}\mu_{\mathrm{B}}^2}{k_{\mathrm{B}}T_F} \tag{26}$$

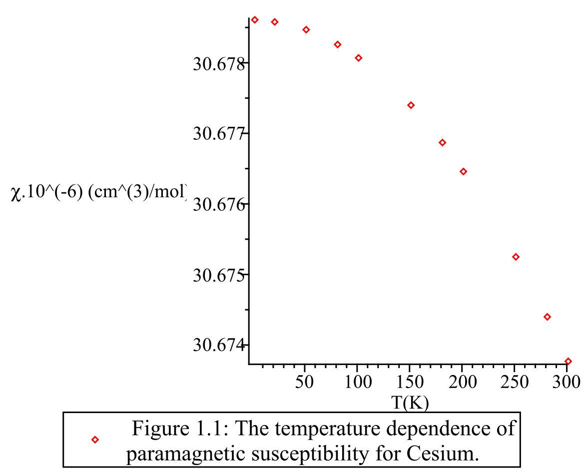

Fig. 1. The temperature dependence of paramagnetic susceptibility for cesium.

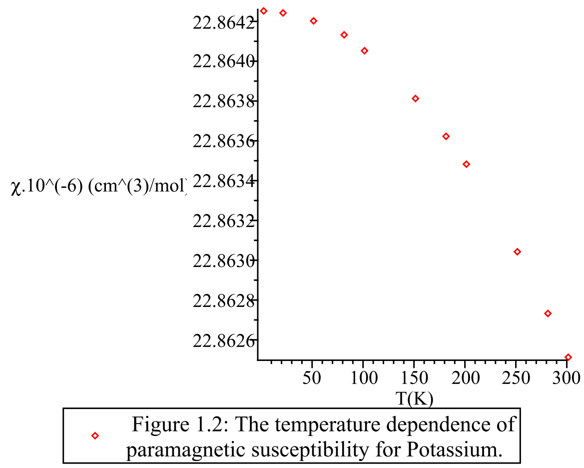

Fig. 2. The temperature dependence of paramagnetic susceptibility for potassium.

Whereas at low temperature, the adjustment quantity can be derived from the components that depend on the q-deformed. The result reads

$$-\frac{3}{4}\frac{N\mu_B^2}{\varepsilon_F^3}F\left(q\right)\left(k_BT\right)^2 \tag{27}$$

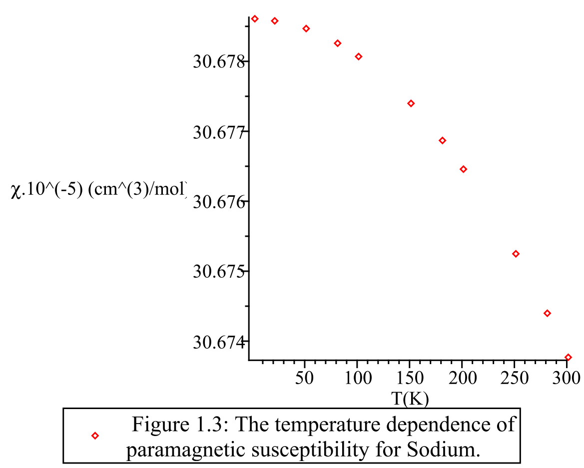

Fig. 3. The temperature dependence of paramagnetic susceptibility for sodium.

Using Maple, distortion parameter q can be obtained in corresponding to $F(q)$(Table. 1) for each metal, which was reported in the online proceeding of 36th $NCTP$. Evaluating equation (27) indicates that the adjustment quantity is quite small. That

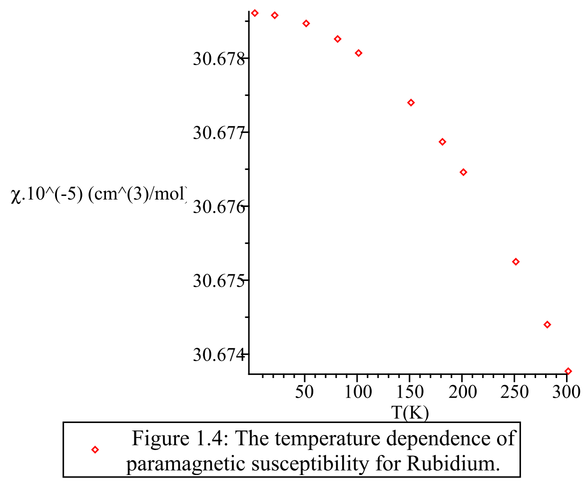

Fig. 4. The temperature dependence of paramagnetic susceptibility for rubidium .

concludes the slight temperature dependence of paramagnetic susceptibility of the free electrons in metals as observed in experiment. Molt paramagnetic susceptibility in metals versus temperature for each metal is displayed in Figs. 1.1-1.4 In addition, when taking the contribution of the deformation into account, the paramagnetic susceptibility results for some typical metals are more suitable with ones evaluated by Pauli. Our results are also looks better in comparing with the observations in the experiments [8, 9, 10, 11].

IV. CONCLUSIONS

Consulting the empirical data to the q-deformed Fermi-Dirac statistics we have considered the electron contribution to the paramagnetic susceptibility. Obtained results show an agreement with that observed in experiments [8, 9, 10, 11]. At low temperature, we point out that the paramagnetic susceptibility of the metal seems to be independent on temperature. Comparing with experiments, in the presence of the deformation, our results look better than ones evaluated from equation of Pauli. Increasing temperature leads to the decimation of the paramagnetic susceptibility. That behavior one more affirms the advantages of the q-deformation contribution in evaluating the paramagnetic susceptibility if one compares to that observed in bulk paramagnetic susceptibility. Without the q-deformation contribution, our result return to the Pauli theory to describe paramagnetic susceptibility in the metal [5].

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