On the q-Deformed Thermodynamics and 
q-Deformed Fermi Level in Intrinsic Semiconductor

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Abstract

In this paper the q-deformed thermodynamic laws are investigated and q-deformed Fermi level in intrinsic semiconductor is discussed.

Keywords: q-deformed thermodynamics; q-deformed Fermi level; intrinsic semiconductor

1 Introduction

Statistical mechanics is the theoretical apparatus with which one studies the properties of macroscopic systems. systems made up of many atoms or molecules. and relates those properties to the system’s microscopic constitution. There is a growing interest in generalizing the Boltzman-Gibbs statistical mechanics. Because the entropy plays a fundamental role in the statistical physics, the entropy should be deformed so as to construct a new (deformed) theory. The first attempt has been accomplished by Tsallis \cite{1, 2}. Based on the fact that Boltzman-Gibbs theory is not adequate for various complex, natural, artificial and social system, he introduced the non-extensive entropy is given by

\[ S_q = k(\Sigma_i W_i p_i^{1-q} - 1)/q, \quad (q > 0) \]  

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where we replaced $q \rightarrow 1 - q$ in the original expression given in the Refs [1,2]. The non-extensive Boltzmann-Gibbs entropy has attracted much interest among physicists, chemists and mathematicians who study thermodynamics of complex system [3-4]. When the deformation parameter $q$ goes to 0, the non-extensive entropy reduces to the ordinary one. Tsallis entropy can be written as

$$S_q = -k \sum_{i=1}^{W} p_i^{1-q} \ln_q p_i = k \sum_{i=1}^{W} p_i \ln_q \frac{1}{p_i},$$

(2)

where $q$-logarithmic function is defined as

$$\ln_q x = \begin{cases} x^{\frac{q-1}{q}}, & (x > 0, q \neq 0) \\ \ln x & (q = 0) \end{cases}$$

(3)

and its inverse is given by

$$e_q(x) = \begin{cases} (1 + qx)^{1/q}, & (x, q \in R, q \neq 0) \\ e^x & (q = 0) \end{cases}$$

(4)

This entropy gives the MaxEnt probability distribution (MPD)

$$p_i = \frac{1}{Z_q} e_q(-\beta E_i),$$

(5)

when we impose the following constraints

$$\sum_{i=1}^{W} p_i = 1, \quad U_q = \sum_{i=1}^{W} E_i p_i^{1-q} = \text{const},$$

(6)

where

$$Z_q = \sum_{i} e_q(-\beta E_i)$$

(7)

Recently, Chung [7] proposed another type of deformed Boltzmann factor:

$$p_i = \frac{1}{Z_q} [e_q(E_i)]^{-\beta}$$

(8)

This is different from the eq.(5). In this paper from the q-deformed thermodynamic laws, we derive the eq.(8) and use it to discuss the q-deformed Fermi level in intrinsic semiconductor. This paper is organized as follows: In section 2, we discuss the q-deformed thermodynamics. In section 3, we construct the q-deformed grand partition function and q-deformed Fermi-Dirac distribution. In section IV we discuss the modification of the Fermi level for an intrinsic semiconductor.
2 The q-deformed thermodynamic laws

The q-operations that emerges from non-extensive statistical mechanics seems to provide a natural background for its mathematical formulation. The definitions of q-sum and q-difference [5, 6] is given by

\[ x \oplus y = x + y + qxy \]
\[ x \ominus y = \frac{x - y}{1 + qy} \]  

(9)

It can be easily checked that the operation \( \oplus \) satisfies commutativity and associativity. For the operator \( \oplus \), the identity additive is 0. The q-exponential and q-logarithm have the following properties:

\[
\ln_q(xy) = \ln_q x \oplus \ln_q y \quad e_q(x)e_q(y) = e_q(x \oplus y)
\]
\[
\ln_q(x/y) = \ln_q x \ominus \ln_q y \quad e_q(x)/e_q(y) = e_q(x \ominus y)
\]  

(10)

In a canonical ensemble, a system is in thermal contact with a reservoir. While energy is free to flow between the system and the reservoir, the reservoir is thought to have infinitely large heat capacity as to maintain constant temperature, \( T \), for the combined system.

If our system is in state \( s_1 \), then there would be a corresponding number of microstates available to the reservoir. Denote this number by \( \Omega_R(s_1) \). Because the combined system is isolated, all microstates are equally probable. Let \( P(s_i) \) be the probability that our system is in state \( s_i \). Then, we have

\[
\frac{P(s_1)}{P(s_2)} = \frac{\Omega_R(s_1)}{\Omega_R(s_2)}.
\]

(11)

Here, more generally, the entropy of the reservoir can be assumed to be expressed in terms of the q-logarithm:

\[
S_R = \ln_q(\Omega_R)
\]

(12)

From the eq.(11) and the eq.(12), we have

\[
\frac{P(s_1)}{P(s_2)} = e_q(S_R(s_1)) e_q(S_R(s_2)) = e_q(S_R(s_1) \ominus S_R(s_2))
\]

(13)

In the q-deformed thermodynamics, we assume that the q-deformed entropy is not additivity but q-additivity, which implies that for two subsystem A, B, we have the following total entropy

\[
S = S_A \oplus S_B
\]

(14)

If we define

\[
(x)_q = \frac{1}{q} \ln(1 + qx)
\]

(15)
we can rewrite the eq.(14) as

\[(S)_q = (S_A)_q + (S_B)_q\] (16)

Consider two systems in thermal contact, A and B. Here we assume that the q-deformed total energy is not additive but q-additive:

\[U = U_A \oplus U_B\] (17)

or

\[(U)_q = (U_A)_q + (U_B)_q\] (18)

Two systems will exchange the q-deformed energy (with \(U\) not changing) until the q-deformed entropy of the combined system is as big as possible, at which point we have equilibrium. This means that the derivative of \((S)_q\) with respect to either \((U_A)_q\) or \((U_B)_q\) must vanish at equilibrium. We have

\[d(S)_q = \frac{\partial (S_A)_q}{\partial (U_A)_q} d(U_A)_q + \frac{\partial (S_B)_q}{\partial (U_B)_q} d(U_B)_q = 0\] (19)

Using the fact that \((U)_q = (U_A)_q + (U_B)_q\) remain invariant, we have

\[d(U)_q = d(U_A)_q + d(U_B)_q = 0,\] (20)

we have

\[d(U_B)_q = -d(U_A)_q\] (21)

Inserting the eq.(21) into the eq.(19), we get

\[\frac{\partial (S_A)_q}{\partial (U_A)_q} = \frac{\partial (S_B)_q}{\partial (U_B)_q} = \beta = \frac{1}{kT}\] (22)

In a canonical ensemble (more precisely, generalized canonical ensemble), the deformed first law of thermodynamics is deformed into

\[(S_R(s_1))_q - (S_R(s_2))_q = \beta[(U_R(s_1))_q - (U_R(s_2))_q]\] (23)

where \(U_R(s_i)\) and \(E(s_i)\) denote the energies of the reservoir and the system at \(s_i\), respectively. Using the q-deformed conservation of energy \(U_R(s_i) \oplus E(s_i) = 0\), we have

\[(S_R(s_1))_q - (S_R(s_2))_q = \beta[(U_R(s_1))_q - (U_R(s_2))_q] = \beta[(E(s_2))_q - (E(s_1))_q]\] (24)
Substituting the eq.(24) into the eq.(13), we have

\[
\frac{P(s_1)}{P(s_2)} = e_q (S_R(s_1) \ominus S_R(s_2)) \\
= \exp \left( (S_R(s_1))_q - (S_R(s_2))_q \right) \\
= \exp \left[ \beta ((E(s_2))_q - (E(s_1))_q) \right] \\
= (\exp \left[ ((E(s_2))_q - (E(s_1))_q) \beta \right])^\beta \\
= \frac{[e_q(E(s_2))]^\beta}{[e_q(E(s_1))]^\beta} \\
= \frac{[e_q(E(s_1))]^{-\beta}}{[e_q(E(s_2))]^{-\beta}} 
\]

which implies, for any state s of the system

\[
P(s) = \frac{1}{Z} [e_q(E(s))]^{-\beta}, 
\]

where Z is given by

\[
Z = \sum_s [e_q(E(s))]^{-\beta}, 
\]

and the index s runs through all microstates of the system.

### 3 Grand partition function

The grand canonical ensemble is a generalization of the canonical ensemble where the restriction to a definite number of particles is removed. This is a more realistic representation of physical systems than the canonical ensemble since one can rarely fix the total number of particles in a macroscopic system.

In a grand canonical ensemble (more precisely, generalized grand canonical ensemble), we assume that the q-deformed total particle number is not additive but q-additive:

\[
N = N_A \oplus N_B 
\]

and q-deformed total energy is also q-additive:

\[
U = U_A \oplus U_B 
\]

We consider the case that the q-deformed total particle number and q-deformed total energy remain fixed. Two systems will exchange energy and particle (with \(U\) and \(N\) not changing) until the q-deformed entropy of the combined system is as big as possible, at which point we have equilibrium. This means that the
derivative of \((S)_q\) with respect to \((U)_q\), \((N)_q\) and \((N)_q\) must vanish at equilibrium. We have

\[
d(S)_q = \frac{\partial(S)_q}{\partial(U)_q} d(U)_q + \frac{\partial(S)_q}{\partial(U)_q} d(U)_q + \frac{\partial(S)_q}{\partial(N)_q} d(N)_q + \frac{\partial(S)_q}{\partial(N)_q} d(N)_q = 0
\]  
(30)

Using the fact that \((U)_q = (U)_A + (U)_B\) remain invariant, we have

\[
d(U)_q = d(U)_A + d(U)_B = 0,
\]  
(31)

we have

\[
d(U)_B = -d(U)_A
\]  
(32)

Inserting the eq.(32) into the eq.(30), we get

\[
\frac{\partial(S)_A}{\partial(U)_A} = \frac{\partial(S)_B}{\partial(U)_B} = \beta = \frac{1}{kT}
\]  
(33)

Using the fact that \((N)_q = (N)_A + (N)_B\) remain invariant, we have

\[
d(N)_q = d(N)_A + d(N)_B = 0,
\]  
(34)

we have

\[
d(N)_B = -d(N)_A
\]  
(35)

Inserting the eq.(35) into the eq.(33), we get

\[
\frac{\partial(S)_A}{\partial(N)_A} = \frac{\partial(S)_B}{\partial(N)_B} = \mu\beta = \frac{\mu}{kT}
\]  
(36)

where \(\mu\) is a chemical potential. In a grand canonical ensemble (more precisely, generalized grand canonical ensemble), the deformed first law of thermodynamics is

\[
(S_R(s_1))_q - (S_R(s_2))_q = -\beta((E(s_1))_q - (E(s_2))_q) + \beta\mu((N(s_1))_q - (N(s_2))_q)
\]  
(37)

From the eq.(37), we have

\[
\frac{P(s_1)}{P(s_2)} = \frac{[e_q(E(s_1))]^{-\beta}[e_q(N(s_1))]^{\mu\beta}}{[e_q(E(s_2))]^{-\beta}[e_q(N(s_2))]^{\mu\beta}}
\]  
(38)

which implies, for any state \(s\) of the system

\[
P(s) = \frac{1}{Z}[e_q(E(s))]^{-\beta}[e_q(N(s))]^{\mu\beta}
\]  
(39)

where \(Z\) is given by

\[
Z = \sum_s [e_q(E(s))]^{-\beta}[e_q(N(s))]^{\mu\beta}
\]  
(40)

and the index \(s\) runs through all microstates of the system.
4 q-Deformed Fermi-Dirac statistics and Fermi level

Now let us consider two-level system whose ground energy is zero and excited energy is $E$. In this case the q-deformed partition function is

$$Z = 1 + [e_q(E)]^{-\beta} [e_q(N)]^{\mu\beta}$$  \hspace{1cm} (41)

The internal energy is given by

$$U = Ef_q(E),$$  \hspace{1cm} (42)

where the q-deformed Fermi-Dirac distribution function is

$$f_q(E) = \frac{1}{1 + [e_q(E)]^{\beta} [e_q(N)]^{-\mu\beta}}$$  \hspace{1cm} (43)

We will examine how many allowed states are near an energy of interest, and the probability that those states will actually be filled with electrons. Density of states and particle statistics concepts are indispensable in study of bulk materials. The electrons at the bottom of a conduction band (and holes at the top of the valence band) behave approximately like free particles (with an effective mass $m^*$) trapped in a box.

The conduction and valence band densities of states near the band edges in real materials, the mass $m$ of the particle is replaced by the appropriate carrier effective mass. The density of states for conduction band and valence band are given by

$$N_c(E) = \frac{m^* \sqrt{2m^*(E - E_c)}}{\pi^2 h^3} \quad (E \geq E_c)$$  \hspace{1cm} (44)

$$N_v(E) = \frac{m^*_p \sqrt{2m^*_p(E_v - E)}}{\pi^2 h^3} \quad (E \leq E_v)$$  \hspace{1cm} (45)

Now let us assume that electrons and holes in each bands obey the q-deformed Fermi-Dirac distribution. In this case the q-deformed Fermi-Dirac distribution function is

$$f(E) = \frac{1}{1 + (1 + qE)^{\beta/q} (1 + qE_F)^{-\beta/q}}$$  \hspace{1cm} (46)

Then, the concentration of electrons in the conduction band at equilibrium is

$$n_0 = \int_{E_c}^{\infty} f(E) N_c(E) dE = \frac{m^*_n \sqrt{2m^*_n}}{\pi^2 h^3} \int_{E_c}^{\infty} dE \frac{\sqrt{E - E_c}}{1 + (1 + qE)^{\beta/q} (1 + qE_F)^{-\beta/q}}$$  \hspace{1cm} (47)
Because $E_c - E_F \gg kT$, we have

\[
n_0 \approx \frac{m^* \sqrt{2m^*_n}}{\pi^2 \hbar^3} \int_{E_c}^\infty dE \sqrt{E - E_c} (1 + qE)^{-\beta/q} (1 + qE_F)^{\beta/q}
\]  

(48)

If we replace

\[
u = \frac{E - E_c}{E - E_F}
\]

(49)

in the eq.(48), we get

\[
n_0 = \frac{m^* \sqrt{2m^*_n}}{\pi^2 \hbar^3} (1 + qE_F)^{\beta/q} (1 + qE_c)^{-\beta/q} (E_c - E_F)^{3/2}
\times \int_0^1 du \left[ 1 - \frac{1 + qE_F}{1 + qE_c} u \right]^{-\beta/q} u^{1/2} (1 - u)^{\beta/q - 5/2}

= \frac{2}{3} \frac{m^* \sqrt{2m^*_n}}{\pi^2 \hbar^3} (1 + qE_F)^{\beta/q} (1 + qE_c)^{-\beta/q} (E_c - E_F)^{3/2} F_1 \left( \frac{3}{2}, \frac{5}{2}, \beta, \frac{5}{2}; 1, \frac{1 + qE_F}{1 + qE_c} \right)

(50)

where Appell’s hypergeometric functions of two variables [11] is defined by

\[
F_1(a, b, b', c; x, y) = \sum_{m=0}^\infty \sum_{n=0}^\infty \frac{(a)_m (b)_n (b')_n (c)_m}{(c)_{m+n}} x^m y^n
\]

(51)

and the Pochhammer symbol is

\[
(a)_n = a(a+1)(a+2)\cdots(a+n-1), \quad (n \geq 1), \quad (a)_0 = 1
\]

(52)

The concentration of holes in the valence band at equilibrium is

\[
p_0 = \int_{-\infty}^{E_v} (1 - f(E)) N_v(E) dE
\]

\[
= \frac{m^* \sqrt{2m^*_p}}{\pi^2 \hbar^3} \int_{-\infty}^{E_v} dE \sqrt{E_v - E} \left( 1 - \frac{1}{1 + (1 + qE)^{\beta/q} (1 + qE_F)^{-\beta/q}} \right)
\]

(53)

Because $E_F - E_v \gg kT$, we have

\[
p_0 \approx \frac{m^* \sqrt{2m^*_p}}{\pi^2 \hbar^3} \int_{-\infty}^{E_v} dE \sqrt{E_v - E} (1 + qE)^{\beta/q} (1 + qE_F)^{-\beta/q}
\]

(54)

If we replace

\[
u = \frac{E_v - E}{E_F - E}
\]

(55)

in the eq.(54), we get

\[
p_0 = \frac{m^* \sqrt{2m^*_p}}{\pi^2 \hbar^3}
\]
\( \times (1+qE_v)^{\beta/q}(1+qE_F)^{-\beta/q}(E_F-E_v)^{3/2} \int_0^1 \frac{1}{u} \left[ 1 - \frac{1 + qE_F}{1 + qE_v}u \right]^{\beta/q} u^{1/2} (1-u)^{-\beta/q-5/2} \)

\[
= \frac{2 m_p^* \sqrt{2 m_p}}{3 \pi^2 h^3} (1+qE_v)^{\beta/q}(1+qE_F)^{-\beta/q}(E_F-E_v)^{3/2} F_1 \left( \frac{3}{2}, \frac{5}{2}; \frac{\beta}{q}; \frac{\beta}{q}; 1, \frac{1 + qE_F}{1 + qE_v} \right)
\]

(56)

Although we can express \( n_0 \) and \( p_0 \) in a closed form with the help of the Appell's hypergeometric functions of two variables, we will consider the case of sufficiently small \( q \) for the theory of intrinsic semiconductor where the concentration of electrons and concentration of holes are same. For small \( q \), up to a first order in \( q \), we have the following approximation:

\[
[e_q(E)]^\beta = (1 + qE)^{-\beta/q} \approx e^{\beta E} \left( 1 - \frac{1}{2} \beta^2 E^2 \right)
\]

(57)

The electron and hole concentrations in equilibrium described by derived formulas are valid whether the material is intrinsic or doped, which are approximately given by

\[
n_0 = N_c e^{E_{F} - E_c} / kT, \quad p_0 = N_v e^{E_v - E_F} / kT
\]

(58)

where

\[
N_c = 2 \left( \frac{2 \pi m_n^* kT}{h^2} \right)^{3/2} \left[ 1 + q \left( \frac{15}{8} kT + \frac{3}{2} E_c + \frac{E_c^2 - E_F^2}{2kT} \right) \right]
\]

(59)

and

\[
N_v = 2 \left( \frac{2 \pi m_p^* kT}{h^2} \right)^{3/2} \left[ 1 + q \left( -\frac{15}{8} kT + \frac{3}{2} E_v + \frac{E_F^2 - E_v^2}{2kT} \right) \right]
\]

(60)

For intrinsic material, Fermi level \( E_F \) lies at some intrinsic level \( E_i \) near the middle of the band gap. The intrinsic electron and hole concentrations are:

\[
n_i = \tilde{N}_c e^{E_i - E_c} / kT, \quad p_i = \tilde{N}_v e^{E_v - E_i} / kT
\]

(61)

where

\[
\tilde{N}_c = 2 \left( \frac{2 \pi m_n^* kT}{h^2} \right)^{3/2} \left[ 1 + q \left( \frac{15}{8} kT + \frac{3}{2} E_c + \frac{E_c^2 - E_i^2}{2kT} \right) \right]
\]

(62)

and

\[
\tilde{N}_v = 2 \left( \frac{2 \pi m_p^* kT}{h^2} \right)^{3/2} \left[ 1 + q \left( -\frac{15}{8} kT + \frac{3}{2} E_v + \frac{E_F^2 - E_v^2}{2kT} \right) \right]
\]

(63)

For intrinsic (undoped) semiconductor, the electron concentration \( n_i \) and hole concentration \( p_i \) are same:

\[
n_i = p_i = \sqrt{\tilde{N}_c \tilde{N}_v e^{-E_g/kT}}
\]

(64)
The Fermi level for an intrinsic semiconductor is obtained by equating $n_i = p_i$:

$$E_i = E_F = \frac{E_c + E_v}{2} + \frac{3}{4} \left( \frac{m_p^*}{m_n^*} \right) kT$$

$$+ q \left[ -\frac{1}{4} (E_c^2 + E_v^2) - \frac{1}{8} (E_c + E_v) + \frac{15}{8} (kT)^2 - \frac{3}{4} E_g kT - \frac{3}{16} \left( \frac{m_p^*}{m_n^*} \right) kT \right]$$

(65)

At room temperature $kT$ is very small, so the above relation is approximated as

$$E_i = E_F = \left( \frac{E_c + E_v}{2} + \frac{3}{4} \left( \frac{m_p^*}{m_n^*} \right) kT \right) \left( 1 - \frac{q}{4} \right) - \frac{q}{4} (E_c^2 + E_v^2)$$

(66)

Thus, the Fermi level for an intrinsic semiconductor in the q-deformed theory increases (or decreases) when $q$ is negative (or positive).

## 5 Conclusion

In this paper we formulated the q-deformed thermodynamics where the Boltzmann factor is given by $p_i = \frac{1}{Z_q} [e_q(E_i)]^{-\beta}$. We replaced the ordinary logarithm with the q-logarithm in defining the entropy. We deformed the thermodynamic law by using q-addition and q-difference, hence we obtained the above-mentioned q-deformed Boltzmann factor. We constructed the q-deformed grand partition function and q-deformed Fermi-Dirac distribution. We applied them to the semiconductor physics to obtain the modification of the Fermi level for an intrinsic semiconductor. We found that the Fermi level for an intrinsic semiconductor in the q-deformed theory increases (or decreases) when $q$ is negative (or positive).

**Acknowledgements.** This work was supported by the National Research Foundation of Korea Grant funded by the Korean Government (NRF-2015R1D1A1A01057792) and by the Gyeongsang National University Fund for Professors on Sabbatical Leave, 2016.

**References**


https://doi.org/10.1126/science.300.5617.249

https://doi.org/10.1016/s0034-4877(03)80040-x


**Received: December 4, 2016; Published: February 25, 2017**