Direct and Quantitative Verifications of Energy Nonconservation by Urbach tail of Light Absorption in Smiconductors

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Abstract

Based on exact theory of quantum transition and precise numerical calculations, this paper demonstrates quantitatively that the Urbach tail in the diagram of light absorption coefficient of semiconductor versus photon energy are caused by energy nonconservation (ENC). This paper also points out that the light absorption is a non-example of Fermi golden rule; due to ENC the estimations on the dark energy and dark mass in our universe might be no longer to have big significance; ENC is a non-example of the first and second thermodynamic law.

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Keywords: Urbach tail; Light absorption; Quantum transition; Energy nonconservation.

1 Introduction

There are three problems, which have not yet been solved, or, are still open.

(1). Lack of a direct and quantitative verification of ENC:

Recently, more and more authors have noted the possibility of energy nonconservation (ENC) in many physical processes [1-7]. Ref. [1] argues that the Boltzmann equation in de Sitter space may violate energy conservation (EC). Ref. [2] indicates that the Goldstone model relaxation needs additional perturbation interactions providing the energy dissipation. The small ENC in the quantum transition such as photoeffect was pointed out in theory since 1930 [3,4]. Lepe et al found the sign of the amount of energy nonconservation in cosmology [5] and [6]. Based on many recent references, Cahill pointed out that in anisotropic Brownian motion and the detected in correlations between ocean temperature fluctuations and solar flare counts there might be energy nonconservation, which violate the first thermodynamics [7]. Cahill further pointed out that this energy nonconservation can explain why the earths temperature record so closely tracks solar flare counts, and fundamentally then it is implied that the Earths climate is controlled by a nonconservation of energy process.

The author of this paper also made some theoretical studies on ENC or related to ENC from 1994 to 2014 [8-12]. Ref. [8] demonstrates that ENC effect may be not small in some cases. Ref. [9] points out that the internal conversion in nuclear physics may be of strong ENC. Refs. [8,10] demonstrate that the macroscopic KWW relaxation comes from ENC of phonon absorption process, which is an indirectly verification for ENC. Refs. [11,12] gave many useful formulas on the exact transition theory of quantum mechanics, and tried to prove a quantummechanical nonconservation theorem generally.

However, until now no any body really believes ENC due to lack of direct and quantitative experimental verification. Therefore, the present biggest problem or the most pressing task is to find out even one direct and reliable experimental quantitative verification for ENC.

This paper finds that all the experimental data (since 1940) on the light absorption in semiconductors need to use the concept of ENC, and can be explained quantitatively by ENC theory.

(2). Origin of Orbach tail:

The light absorption at *photon energy* $E_{ph} <$ *gap* E_g, which is called Urbach tail and was discovered in 1940 [13]. Although Tauc pointed out in 1974 in Ref. [13] that Orbach tail cannot simply be explained by considering only the defects in semiconductors, because Orbach tail appears in both disorder and perfectly order semiconductors. However, until now all references still use the defect effect to study Orbach tail [14,15]. The ENC theory of light absorption in semiconductors in this paper can provide a unified theory of Orbach tail, appropriate to both disorder and perfectly order semiconductors.

(3). Serious departure of Tauc law at $E_{ph} = E_g$:

Until now all references such as Refs. [14,15] use Tauc law to discuss the light absorption. Tauc law said that $\alpha = (E_{ph} - E_g)^n$ [13], which means that $\alpha \equiv 0$ at $E_{ph} = E_g$. However, all experimental data tell show $\alpha >> 0$ at $E_{ph} = E_g$. Our ENC theory of light absorption can quantitatively explain $\alpha >> 0$ at $E_{ph} = E_g$.

This paper is a theoretical paper, which uses transition theory of quantum mechanics to analyze all the experimental data on the light absorption in semiconductors in the past 70 years. Section 2 introduces the now available theory of light absorption, which is an EC theory. Section 3 introduces our ENC theory. Section 4 makes conclusion and some discussions.

2 Theories Now Available

All the existing light absorption theories are established on EC. The absorption coefficient α in light absorption in semiconductors represents an attenuation of the incident light power by $1/e \approx 1/2.7 \approx 0.37$ per unit propagation length. For convenience of statement, we study the direct transition in GaAs. The formula of α is given by many textbooks [16]. For example, Eq. (11.2.12) of Ref. [16] is

$$\alpha = \frac{377(\Omega)2\hbar^2}{EphnA_\circ^2Vt}P_{cv}, \tag{1}$$

where $n = 3.6$ is the reflective index, V the unit cell volume, $A_\circ$ the amplitude of vector potential, $t(\approx \tau)$ the duration time of time-dependent perturbation (, i. e., light), τ the relaxation time, P_{cv} the transition probability from valence to conduction bands ($R = P_{cv}/t$ is the transition rate). Eq. (11.9.15) of [16] proves that Eq. (1) is equivalent to transition of reduced mass $m_r = 0.0337m_\circ$ from top of valence band to conduction band [17]. The gap $E_g = 1.42$ eV at 300 K [18]. The P_{cv} can be found in any textbooks on quantum mechanics, is $\{(10.3.7)'$ of Ref. [8]$\}$ (or see Refs. [4,3])

$$P_{cv} = \frac{1}{\hbar^2}\int_{-\infty}^{\infty}|H'_{k'k}|^2\rho(E_k)\frac{\sin^2[(E_k+E_g-E_{ph})t_\circ]/(2\hbar)}{[(E_k+E_g-E_{ph})/(2\hbar)]^2}dE_k. \tag{2}$$

The integral limit is infinite, which means, obviously, strong ENC. However, all the now available references do not really and seriously calculate this integral. On the contrary, they assume $t \to \infty$, then use the known formula $\sin^2[(E_k+E_g-E_{ph})t/(2\hbar)][(E_k+E_g-E_{ph})t/(2\hbar)]^2 = (2\pi\hbar/t)\delta(E_k+E_g-E_{ph})$. Here, the δ function is an EC factor. Of course, the integral in Eq. (2) can be finished simply in this mathematical treatment. After integration, they obtain that R is independent of t, which is called Fermi golden rule, and (Refer to (11.9.14) and (11.9.16) of Ref. [16])

$$\alpha = \begin{cases} \frac{377(\Omega)\pi e^2\hbar 2|\mathbf{a}\cdot\mathbf{p}_{cv}|^2(2m_r)^{3/2}}{n2m_\circ m_\circ E_{ph}2\pi^2\hbar^3}\sqrt{E_{ph}-E_g}, & E_{ph}\geq E_g \\ 0, & E_{ph}<E_g \end{cases}, \tag{3}$$

where the average value of $|\mathbf{a}\cdot\mathbf{p}_{cv}|^2 \approx 2\pi\hbar/b4/\pi^2$, $b = 5.86\mathring{A}$ is the lattice constant [23]. The form $\alpha \propto (E_{ph}-Eg)^q$ is called Tauc law [14,13]. The curve 1 in figure 1 is given by Eq. (3). The Tauc law cannot explain: $\alpha(E_{ph} = E_g) >> 0$ and $\alpha(E_{ph} < E_g) > 0$.

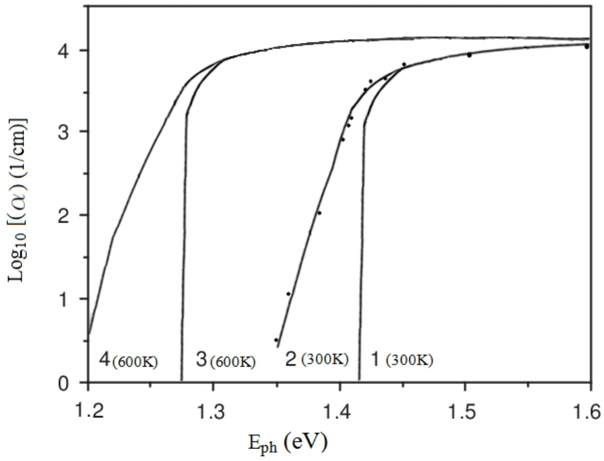

Figure 1: The data are for GaAs at 300 K [25]. The unit of α is cm^{-1}. The curves 1 and 2 come from EC (Tauc law), and ENC (this paper) for GaAs at 300 K. The curves 3 and 4 come from EC (Tauc law), and ENC (this paper) for GaAs at 600 K. $E_g(T = 600K) = 1.265$ eV [18]. The characters of curves 2 and 4 are same as the curves of $a \sim Se$ at different temperatures [13]. The curves 1 and 2 overlap at $E_{ph} \geq 1.45$ eV, and are different at $E_{ph} < 1.45$ eV. In our calculations of curve 2 and 4, we take $t = 10^{t'}$, $t' = -13.5$ for $E_{ph} > E_g$, $t' = -11.2 - (13.5 - 11.2)[(E_{ph} - (E_g - 0.07)]/0.07$ for $E_g - 0.07 < E_{ph} < E_g$, i. e., t' is a little less than -13.5.

3 Theory of This Paper

Due to that all the now available references cannot explain the experimental data, this paper tries to exactly calculate the infinite limit integral of the transition probability in Eq. (2). These exact integrations find $R \approx (t)^{-0.5}$, which violates Fermi golden rule, and the curves of α versus E_{ph} are shown as curves 2 and 4 in figure 1. The very good fitting between the data and curve 2 indicates that the region between the curve 1 and the curve 2, including the curve 2, comes completely from ENC. The region between the curve 3 and the curve 4, including the curve 4, comes completely from ENC as well.

In mathematics, the differences between our theory and the now available theory are very small. Our theory and the now available theories make exact and approximate treatment for the same Eq. (2), respectively. Although the numerical calculations in our theory are very simple, the physics behind the mathematics is very big. Our theory and the now available theories lead to ENC and EC, respectively. It is necessary to explore in detail the origin of ENC in the light absorption. For this purpose, we transform Eq. (2). For brevity, we just write the E_{ph}-dependent part in Eq. (2), which is

$$\alpha(E_{ph}) \propto \int_0^{+\infty} \sqrt{E_{ph} - E_g + E_k} \frac{\sin^2 \frac{E_k t}{2\hbar}}{(E_k)^2} dE_k + \int_0^{E_{ph}-E_g} \sqrt{E_{ph} - E_g - E_k} \frac{\sin^2 \frac{E_k t}{2\hbar}}{(E_k)^2} dE_k \equiv I + II. \quad (4)$$

The term II in Eq. (4) is equal to zero at $E_{ph} = E_g$. The factor $\sqrt{E_{ph} - E_g - E_k}$ in II tells us that if $E_{ph} < E_g$, then the processes of photon absorption in semiconductors will be prohibited. On the contrary, the term I in Eq. (4) allows the processes in case of $E_{ph} < E_g$. More clearly say, the carriers in semiconductors can still absorb a photon which's energy is less than E_g, and transit to the conduct band. For reference, we draw the figure 2. The figure 2 shows that $II < I$.

The origin of the light absorption at $E_{ph} < E_g$ is an open problem since 1940 [14,15]. For example, the four arbitrary parameter theory in 2013 thinks that the origin of Orbach tail is the existence of impurity states or structure disorder in the gap region [16]. It is obviously that the theory of Orbach tail in Ref. [14] cannot explain the existence of the same Orbach tail in perfect order semiconductors. According to our theory, the Urbach tail comes from both the light absorption of ENC. Therefore, our theory can explain at the same time the Orbach tails in both disorder and perfect order semiconductors.

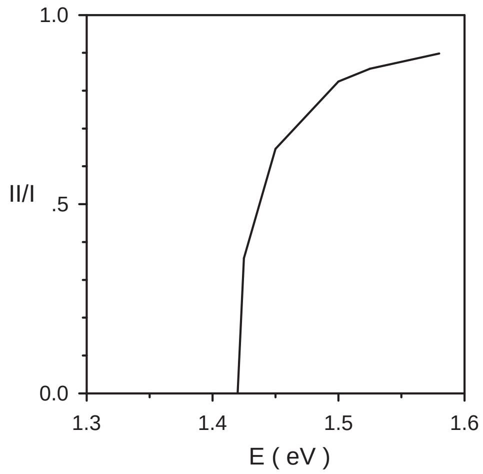

Figure 2: The I and II represent ENC and EC contributions coming from Eq. (4), respectively. $II/I < 1$ means that in light absorption of semiconductors the contribution of ENC part is always more important than the contribution of EC part.

4 Conclusion and Implications

Conclusion:

All the now available experimental data (since 1940 to 2015) of the light absorption in semiconductors have Orbach tail and $\alpha(E_{ph} = E_g) >> 0$. The now available EC theory of light absorption cannot explain these data. However, our ENC theory of light absorption, based on the exact treatment for the transition theory of quantum mechanics, can even quantitatively explain these data. Therefore, the light absorption in semiconductors provide direct and quantitative experimental verification for ENC.

In comparison of our paper with all the studies on the energy nonvconservation until now we feel that it is only that our paper can make the investigations from both the exact theory and precise measurement simultaneously.

Discussions:

(1). ENC means that the energy can be purely fictitious. For example, if $E_{ph} = Eg$, then every excited electron can obtain 0.35 eV average energy from ENC in the experiment of Fig. 1. From Einstein mass-energy relation, one can deduce further that the mass can be purely fictitious. Due to ENC the estimations on the dark energy and dark mass in our universe might be no longer to have big significance.

(2). From our exact calculations of transition probability, we can conclude that EC in transition processes such as the light absorption in semiconductors, is approximate, i. e., EC is relative, and ENC is absolute. From the equiprobability symmetry spontaneous breaking of quantum processes, proposed in Ref. [11], ENC might be understood.

(3). From 1930 people have made many conclusions by using quantum transition theory and EC. At least, 1/10 of them, such as the light absorption of semiconductors, need to be modified by considering ENC.

(4). The ENC of light absorption is a non-example of the first law of thermodynamics. If the first law thermodynamics does not hold in some cases, then the second law of thermodynamics does not hold in some cases too.

(5). The light absorption is a non-example of Fermi golden rule, because the transition rate is not a time-independent constant.

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