Radiation and Bioinformation

辐射与生物信息

〔德〕 Qiao Gu (顾樵)

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内 容 简 介

生物系统能够产生光子辐射。它携带着生物系统的微观信息，对系统内部的变化和外界环境的影响有高度的敏感性。本书利用分子生物学和现代物理学方法，系统地描述生物光子辐射的量子统计性质，并介绍生物光子检测技术在医疗诊断、制药技术、农业科学、水质分析和环境监测、食品和饮料工业等领域的应用。

图书在版编目（CIP）数据

辐射与生物信息=Radiation and Bioinformation/顾樵著. —北京：科学出版社，2003. 10

ISBN 7-03-012208-9

I. 光… II. 顾… III. 生物光子学—研究—英文 IV. Q63

中国版本图书馆 CIP 数据核字（2003）第 086359 号

责任编辑：马学海/责任印制：刘士平 / 封面设计：王 浩

Published by Science Press
16 Donghuangchenggen North Street
Beijing 100717, P.R.China

科学出版社 出版
北京东黄城根北街16号
邮政编码:100717
http://www.sciencep.com
新蕾印刷厂 印刷
科学出版社总发行 各地新华书店经销
*
2003年10月第 一 版 开本：B5 (720×1000)
2003年10月第一次印刷 印张：25 3/4
印数：1—1 500 字数：504 000

定价：70.00元

（如有印装质量问题，我社负责调换〈新欣〉）

Professor Dr. Qiao Gu（顾樵）

Preface

How to obtain bioinformation by means of physical technology has been investigating with the development of life science. Appearance of optical microscope causes a revelation of information on cell, which drives thus the ancient biology to the horizontal of a cellar understanding. Application of X-ray technology to biological systems demonstrates bioinformation in the molecular level, which provides the basis for establishment of molecular biology. Since a half century a large number of the modern physical technologies has been used to expose bioinformation. Recently developed one of them concerns "biophoton". It is based on detection of a biological radiation to gain bioinformation in the quantum domain.

In connection with biological radiation, luminescence of firefly is a well-known phenomenon, which is regarded "bioluminescence". It displays such a relatively high intensity that one can see it by eye. There actually is a universal phenomenon of radiation in the biological kingdom, termed "biophoton emission". It concerns a ultraweak emission of the electromagnetic radiation, and its intensity is typically only 100 photons/s$\cdot$cm^2. This means that a typical biophoton flux is in the order 10^{-17} W/cm^2, which is much lower than the bioluminescence. The biophoton emission was first registered by the use of a photomultiplier tube in 1955, with cereals as the measured samples. With the improvement of detecting technology, this phenomenon has been already observed in various biological samples, involving animals and their organs, tissues, cells, and even molecules in living state; plants and their roots, stems, leaves, flowers, fruits; and the various kinds of microbes. The biophoton spectrum is found to be almost continuous within the range 200-800 nm, which corresponds to the spectral response of a normally used detector. Biophotons are believed to originate from a transition of molecules from their excited states to the downer energy states. In fact, the excited states in a biological system are occupied with quite a high molecular population, because it is essentially an open system and uninterruptedly absorbs energy from the external environment. Biophoton emission, therefore, is able to carry information on the microscopic properties of a biological system. The biophoton emission has been known to correlate closely to the various biological activities, such as DNA conformation, cell division and differentiation, stress, disease, and the death of an organism. On the other hand, it responds sensitively to the external influences, such as the change of environmental temperature, the addition of agents, exposure to the external electromagnetic fields, etc.

Biophoton emission is a complicated life phenomenon, a comprehensive description for it requires hence the multilateral disciplines, involving molecular biology, microbiology, biochemistry, thermodynamics, quantum optics, nonequilibrium statistical physics, information theory, modern photoelectric detection theory, etc. Professor Popp accomplished the earliest theoretical research in this field at the begging of the 1970's. With the help of fresh knowledge, a series of the theoretical works have been performed for the further description of biophoton emission. All of these investigations have formed recently an emergent branch of learning, so-called "biophotonics". It is of, in addition to an academic significance, great applicable values. The obtained conclusions can provide for various observations of biophoton emission with a principle understanding, a qualitative explanation, or even a quantitative analysis. They have offered a great deal of suggestions for the experimental works, for instance, the most reasonable design and arrangement of the devices located in the detecting system, choice of the optimum conditions of observing the biophoton phenomena, the most powerful way to evaluate observed data, etc. Fortunately, some of the theoretical investigations have predicted the new methods of detection, which lead to the inventions of the more advanced detectors.

With the development of biophotonics, "biophoton technology" as a new analytical tool has been appropriately worked out. Unlike the traditional analytical methods, the biophoton technology grants the holistic information of a measured sample, which serves as a summary factor characterizing the sample. The biophoton analytical method has already opened up many applications, e.g.,

1. Examination and control of food quality, including measurement of food freshness,
2. Analysis of water quality and water pollution, examination of the efficacy of water-treatment tools and technologies,
3. Research of the properties of soft and hard drinks, characteristic identification of the particular spirits,
4. Rapid measurement of concentration of bacteria in a solution, monitoring of contamination on assembly line of producing drinks,
5. Research of the biophysical properties of plants, for example, choice of the optimum conditions for growing of the plants,
6. Research of seed quality, such as germination capacity, water content, genetic treatment, etc.,
7. Research of the efficacy of medicines, in particular, choice of the optimum medicine of anti-tumor for a particular patient,

8. Application in bio-pharmacy procedure, exploration of new drugs by using living samples and/or the standard bio-indicators as measured samples, and
9. The diagnostic and therapeutic treatment of different kinds of illness, such as immune diseases and cancer.

The present monograph aims mainly at a systemic presentation of the quantum statistical theories of biophoton emission and their applications. For this purpose, we first give out the quantum statistical description of the radiation field in terms of quantum entropy, through Chapter 1 and Chapter 2. In Chapter 3 and Chapter 4, we handle in detail two typical radiation systems: the Jaynes-Cummings model and the Dicker model, the former concerns interaction of a single two-level atom with a single-mode radiation field while the later cooperative emission of a many-atomic system. Above four chapters supply the background knowledge concerning the quantum statistical properties of a general radiation field, which provides the basis for understanding the biophoton natures. The main features of biophoton emission and the fundamental conceptions of biophotonics as well as the technical notes of biophoton detection are introduced basically in Chapter 5; and the more detailed substances are referenced with the various original publications. The Popp's coherence theory on biophoton emission is narrated in Chapter 6, which lays a foundation of all the theoretical descriptions in terms of coherence concept. Based on such a concept we further present the quantum theory of biophoton emission in Chapter 7, where the steady-state behavior of biophoton emission and its dynamic aspects are systematically investigated. The applications of this theory are then exposited essentially for the various practical bio-samples. As a generalization of the quantum theory of biophoton emission, we enter into demonstration of the nonequilibrium statistical properties of a biological system by the biophoton patterns, mentioned in Chapter 8 and Chapter 9. The obtained results elucidate the macroscopic order growth dynamics in the seed germinating process and the nonequilibrium phase transition phenomena in the special biophoton actions, involving bifurcation and hysteresis. The semiclassical theory of interaction of radiation with matter is reviewed in Chapter 10, and one of the consequences is used to describe quantitatively the interference effect in the biophotons from a swarming of the animals. The quantum interference between coherent states is formulated generally in Chapter 11 and Chapter 12. The related consequence predicts a method, by which the high-degree coherence of biophoton emission has been demonstrated experimentally. In Chapter 13, we consider a sonoluminescence, which may be understood as a product of interaction between photon and phonon models, and present the quantum theory for describing the photon and phonon dynamics. The obtained results have been used not only to characterize the synchronous picosecond sonoluminescence from the gaseous system but also to explain the temperature effect of the biophoton emission with the special kinetic course. In the last two chapters we turn to investigate especially luminescence of an electrochemical system in solution, in particular, the complicated system containing microbes. A phenomenological theory has been developed for description of the total dynamics of the system, including excitation and relaxation processes, and its consequences have exhibited widespread applications in the measurements of the liquid properties, in particular, the rapid measurement of the bacterial contamination in the solution.

The author of this monograph would like to thank Professor Dr. Fritz A. Popp for the wonderful discussions in this field and for the scientific cooperation for many years in International Institute of Biophysics, in Germany.

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October 2003

Contents

Chapter 1

Entropy of Radiation Fields

Abstract. Based on the elucidation for definition of entropy, we present a general method for calculating entropy of a quantum system in mixed state and use it to the radiation fields in the typically mixed states. The results demonstrate that the quantum entropy is correlated to the fluctuation of the radiation fields, it may therefore describe the coherence properties of the radiation fields. As an example, the evolution of entropy of a dissipative system is investigated then.
Key words. Entropy, uncertainty in stochastic variable, information content, radiation field in mixed state, fluctuation of radiation field, and dynamics of quantum entropy.

1.1 Definition of Entropy

Entropy is an important concept used in many fields such as physics, statistics, information theory, etc. The well-known definition of entropy is given by Boltzmann as $S = k \ln W$, where k is the Boltzmann constant and W is the number of microscopic states in an event under consideration. For a particular event, W can be determined exactly. When we toss a coin, for example, we have two possible outcomes, so $W = 2$. Or when we throw a die we have six possible outcomes, then $W = 6$. The entropy increases as the number of states increases.

In classically statistical mechanics, entropy of an ensemble of system is defined by the relation ($k = 1$)

$$S = -\sum_i p_i \ln p_i \,, \tag{1.1.1}$$

where p_i is the probability of finding the system in state i , subject to the normalization condition

$$\sum_i p_i = 1 \,. \tag{1.1.2}$$

If the system is found in all its possible states with the equal probability, that is

$p_i = 1/W$, the statistical entropy (1.1.1) reduces then to the Boltzmann's entropy $\ln W$. Thus the Boltzmann's entropy may be understood as a special case of the statistical entropy (1.1.1) for constant probability p_i. On the other hand, the statistical entropy (1.1.1) could be written as an average of the Boltzmann's entropy $\ln(1/p_i)$ in the ensemble, as $S = \langle \ln(1/p_i) \rangle$.

Shannon and Weaver establish the relation of entropy to information theory [1.1]. Entropy may be visualized physically as a measure of the lack of knowledge of the system. If we know that the system is in a definite state *j*, then $p_i = \delta_{ij}$, we see by (1.1.1) that the entropy is zero. In this case we have complete knowledge about the system. On the other hand, if we know nothing about the system, it is equally likely to find the system in any of its possible states *i*, and the entropy reaches its maximum value $\ln W$.

Let us give a simple example to show what the fundamental feature of entropy is. Provided that the stochastic trial for shooters A, B, and C to hit and miss target is described by the probabilities shown in Table1.1, with the corresponding values of entropy. Looking at the results concerning A'shootting, we have no knowledge (it is complete uncertainty to say hitting or missing), and the entropy has value $\ln 2$, being the maximum entropy of a two-state system. In contrast, we have some knowledge about B'shootting (the uncertainty is much smaller), and the entropy reduces. For shooter C we have almost complete knowledge (the uncertainty is very small), and the entropy almost vanishes. This example demonstrates that entropy is a measure of uncertainty in measurement for a stochastic variable. In other words, it is a measure of information content obtained by observation of the stochastic variable. The uncertainty decreases (the information content increases) as the entropy decreases.

Table 1.1 The probabilities for three shooters to hit and miss target and the corresponding values of the statistical entropy (1.1.1).

shooter	hit	miss	entropy
A	0.5	0.5	0.693
B	0.9	0.1	0.325
C	0.99	0.01	0.056

We now show theoretically that maximization of the entropy leads to a constant probability p_i. We therefore maximize *S* by the method of Lagrange multipliers. If we vary the p_i s, the variation in *S* is

$$\delta S = -\sum_i (1+\ln p_i)\delta p_i = 0 , \tag{1.1.3}$$

where we set $\delta S = 0$ to find its maximum. At the same time, the variation in the constraint (1.1.2) is

$$\sum_i \delta p_i = 0 . \tag{1.1.4}$$

To apply the method of Lagrange multipliers, we multiply (1.1.4) by an undetermined parameter λ and add to (1.1.3). Then we have

$$\sum_i (1+\ln p_i + \lambda)\delta p_i = 0 . \tag{1.1.5}$$

Each δp_i is now independent, and this equation will be satisfied if and only if each term is zero:

$$1+\ln p_i + \lambda = 0 . \tag{1.1.6}$$

From this we conclude that each p_i must be a constant independent of *i*, the state of the system; that is, the probability of finding the system in any of its states is equally likely. We then have no information about the state of the system. Entropy is therefore a measure of the lack of information about the states of the elements of the ensemble, as we stated. This is the starting point of Shannon's theory of communication [1.1]. Jaynes [1.2] has proposed that entropy is used as a fundamental postulate of statistical mechanics.

It should be pointed that the statistical entropy is a very general concept: as long as one has a distribution p_i of a variable *i*, the corresponding entropy can be calculated according to (1.1.1). Consider for example a language such as English. We may label its letters *a*, *b*, *c*, ... *x*, *y*, z by the numbers $i = 1, 2, 3, \ldots 24, 25, 26$. Then we may count the frequencies of appearance of each letter in a particular paper. We define the relative frequency of a letter labeled by i as $p_i = n_i / n$, where n_i is the frequency of this letter and *n* is the total number of letters counted, $n = \sum n_i$. Then we can calculate the entropy of the system of letters contained in this paper by the use of (1.1.1). Fig. 1.1(a) plots two particular distributions, corresponding to two particular papers, which mention the completely different topics. One can see that the two distributions are very near to each other, at quite a high correlation $r = 0.99$. In contrast, Fig. 1.1(b) concerns an article in English and its German translation; the two distributions show the less correlation $r = 0.89$. Note that the total number of counted letters in the article in English is clearly less than that in its German translation, as it is generally known. However, the calculation shows that German letters seems in the lower entropy than English letters. Actually, one can see from these four distributions that the German translation has the most total number n of the letters in the four papers (the more number of states corresponds to the larger entropy), it even has the smallest value of entropy. It is believed that for every symbolic language a standard letter distribution (with an exact entropy value) can be obtained if the letters are counted in many different kinds of books or in a library perhaps.

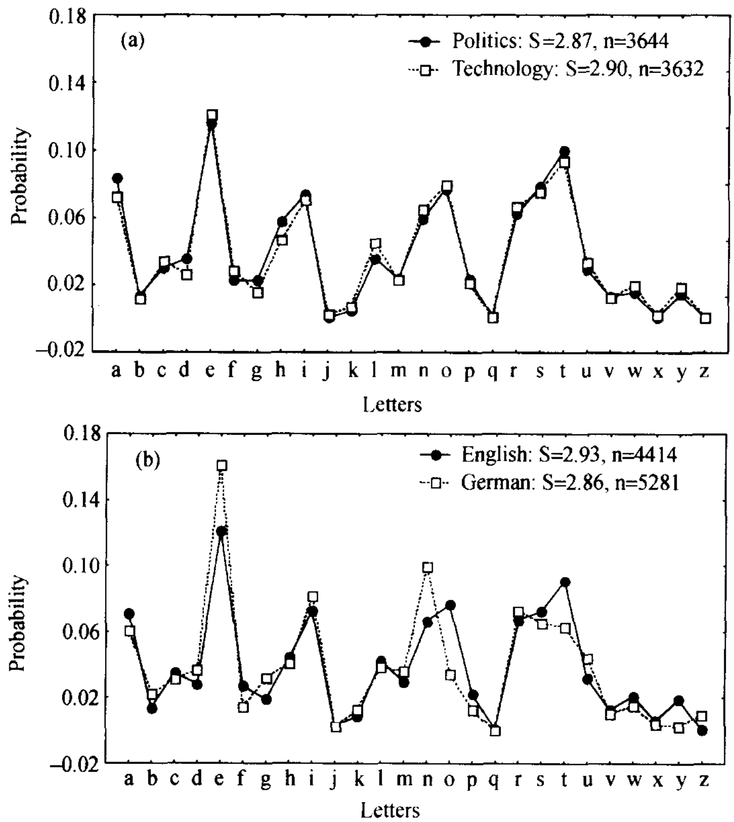

Fig.1.1 Probabilities of appearance of the 26 symbolic letters in the articles: (a) an article on politics from a newspaper and a technical notation on internet from a website, where the total numbers n of counted letters are comparable with each other. The relative deviation of entropy is 0.010%; (b) an article in English and its German translation. The entropy of the German letters is 0.024% relatively lower than that of English letters.

In many applications that we have in mind, the stochastic variables are not discrete but continuous. It corresponds to many continuously changed states. According to Jaynes's method, for a distribution function $p(x)$ with x as continuously changeable variable, the statistical entropy can also be written as integral [1.3]

$$S = -\int p(x) \ln \frac{p(x)}{m(x)} dx , \tag{1.1.7}$$

it is a generalization for (1.1.1) under continuously changed variable, where $m(x)$ is a function related to the accuracy, with which the measurement is done, and proportional to the limiting density of discrete points. Such a definition of entropy will be used to describe the evolution of organizational order of biological systems in Chapter 8.

If $m(x)$ may be treated as a constant m independent of x, one may drop it and uninteresting term $\ln m$ from (1.1.7), resulting in the well-known form

$$S = -\int p(x) \ln p(x) dx . \tag{1.1.8}$$

Following (1.1.8) one may calculate the entropy for a given distribution function. For example, for a Gaussian distribution

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-a)^2}{2\sigma^2} \right], \tag{1.1.9}$$

with σ and a being the standard deviation defined and the average value, the entropy is given by

$$S = \ln \sqrt{2\pi e}\sigma . \tag{1.1.10}$$

It is the maximum value of entropy in all the distribution functions with the same standard deviation. Eq. (1.1.10) shows that the entropy is related to only the deviation, independent of the average value.

In quantum statistical mechanics entropy is defined by von Neumann in terms of the density operator as [1.4]

$$S = -\mathrm{Tr}\, \rho \ln \rho , \tag{1.1.11}$$

subject to the constraint

$$\mathrm{Tr}\rho = 1 . \tag{1.1.12}$$

The density operator is given by

$$\rho = |\psi\rangle\langle\psi| \tag{1.1.13}$$

for a pure state and by

$$\rho = \sum_i P_i |\psi_i\rangle\langle\psi_i| \tag{1.1.14}$$

for a mixed state, where P_i is the probability of finding the system in state $|\psi_i\rangle$. The quantum entropy is zero for any pure state and positive for a mixed state. Obviously,