Quantum Mechanics

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Preface

My first visit to China took place in 1973 when the country was deep in the Cultural Revolution. In 1978, I was invited to Tsinghua University in Beijing, where I was asked to present two series of lectures. One was a general physics course on optical and thermal physics for the teaching staff, and the other was a special topic on electronic properties of semi-conductors in reduced dimensionality. The latter was open to the research staff from different universities as well as related institutes of Academia Sinica in Beijing area. I started my research collaboration with a small group of physicists pulled together just for this purpose. After that, I made almost annual visits to a large number of Chinese universities and research institutes, and developed many research collaboration projects with colleagues of various institutions around the nation.

I visited Shanxi University for the first time in 1996 upon the invitation of President Peng Kunchi. During my sabbatical in 1999, President Peng asked me to teach an intensive course on Modern Physics for one week to junior students of the Physics Base, which in effect is a center for training research and teaching physicists as designated by the Ministry of Education.

Two years after my retirement from University at Buffalo, State University of New York (SUNY), I was approached again to teach a semester course of Quantum Mechanics to the senior class of the Base. Although I had never taught undergraduate Quantum Mechanics during my thirty nine years service at SUNY-Buffalo, I did teach an intensive course for six weeks at Nankai University in 1992. Based on my visits to numerous institutions in China during the past thirty five years, my impression is that Chinese physics majors are generally better prepared than their American counterparts. Thus, I decided to take the challenge. I started my mission during the spring of 2005. The reception by students was apparently quite good, and I have been back in Taiyuan for several times since then.

The School of Physics and Electronic Engineering of Shanxi University suggests that I consider the publication of my lecture notes. In China, there have been very few, if any, books on Quantum Mechanics published in English. This is because the foreign books are in general priced prohibitively high and hardly accessible by the students. Therefore an English publication priced in line with the existing Chinese books on the same subject should be a welcome addition to the student market.

My lectures are based on notes originally prepared for the graduate level one-year course at SUNY-Buffalo, where I have taught it for many years. The textbook I assigned for the course was *Quantum Mechanics* by Kurt Gottfried. I have liberally taken materials from the textbook. However, necessary modifications in the present book have been made to suit the Chinese undergraduates. In particular, Quantum Mechanics is a semester course in Chinese universities, which means seventy-two contact hours with four per week for eighteen weeks. Although I have tried to keep the volume within a manageable size, it is nevertheless desirable to include some materials just for completeness. Sections on more advanced topics can be skipped in a semester course without any interruption of the continuity. For the convenience of instructors, I have marked those sections by the asterisk symbol.

The students are expected to have completed undergraduate courses on modern physics, classical mechanics, classical electromagnetism, as well as some background in kinetic theory and statistical physics. Since the book aims at advanced undergraduates and beginning graduates, my choice of the content emphasizes more on the understanding of physics rather than the recent developments during the last few decades. In my opinion, the latter should be more suitable for advanced courses on special topics. On the other hand, I have tried my best to relate topics as well as examples discussed in this book to practical problems in the current research whenever it is possible.

It has been a general practice in American universities that the relativistic quantum mechanics is the subject of a different course and hence it is not covered here. On the average, about ten problems of various degrees of difficulty are included at the end of each chapter. Many of them are selected from the test and examination papers of my classes over the years. Working out these problems should greatly help the students in understanding the theory, even though there have already been many problem and answer books on quantum mechanics available in China. As a textbook, I have made no effort to provide an extensive list of bibliography. However, a short list of better known titles is included for quick references. The readers may find it handy when more details or further discussion of a particular subject is needed.

I would like to thank Professors Peng Kunchi, Xie Changde, Gao Jiangrui and Zhou Fuguo of Shanxi University for their invitation, hospitality and most importantly, their continuous effort for providing everything to facilitate the publication of this book. Most of the graphic work of figures included in the Word

file was carried out by Miss Zhang Hanyin, a student of the 2005 class of Physics Base at Shanxi University. She spent all the available time out of her busy schedule for the job. Her generous help is greatly appreciated. I am very much in debt to my late parents who supported my education wholeheartedly during the most difficult time of their life in WWII, when our home and everything in the house were completely burned down by Japanese bombs. I am also grateful to late Professor Ta-You Wu from whom I took my first course on the subject. My frequent visits to China left my family behind ever since the children were babies. Without the understanding and support of my wife Sharon Lin, children Jennifer Shih-Yi and Kenneth Shih-Kang, it would be difficult to imagine how my research collaboration projects with colleagues in China could have been possible. I thank them all for letting me freely travel.

Duo-Liang Lin

December 2010 in Fremont, California

Contents

I. Brief review of historical development

1. Black body radiation

By the end of the 19th century, it was believed, even by very prominent physicists, that physics theory was almost complete. Newton's laws, Maxwell's equations plus Boltzman and Gibbs statistical mechanics would be able to explain all natural phenomena. Physics research would no longer be interesting and challenging. All experimentally observed results would eventually be understood by the existing theory, perhaps with minor modifications.

Among all the problems that appeared not understandable by the then existing theory, the black body radiation actually originated the revolutionary quantum concept. If one plots the intensity $I(\nu)$ of emission versus the radiation frequency ν, one obtains the empirical curve as shown in Fig. 1.1. The radiation intensity is of course nothing more than the energy density radiated. The problem is then to derive a theoretical formula for the energy density as a function of the frequency to account for the data.

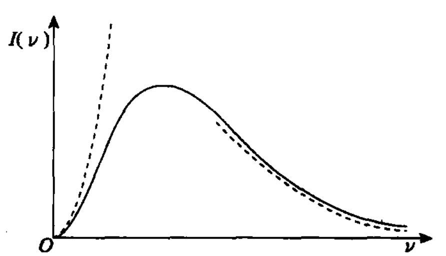

Fig. 1.1 The intensity of black-body radiation versus the frequency

Two such expressions were derived on the basis of classical physics. They are

i) Wien formula:

$$\psi_\nu = a\left(\frac{8\pi\nu^3}{c^3}\right)e^{-b\nu/T} \tag{1.1}$$

where a and b are constants, and

ii) Rayleigh and Jean formula.

$$\psi_\nu = \frac{8\pi\nu^2}{c^3}kT \qquad (1.2)$$

where k is the Boltzman constant. It is seen that Wien formula agrees qualitatively with the data in the high frequency limit while Rayleigh-Jean formula is good only in the low frequency limit. In the main region where the radiation intensity peaks, however, both theoretical curves are incorrect. The above comparison demonstrates conclusively that the classical theory fails to explain the experimental data.

Since the observed intensity distribution of the black body radiation cannot be understood by the classical physics, Planck tried without any physical basis, to reproduce the data by constructing an empirical formula. He eventually obtained the energy density distribution

$$\psi_\nu = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{h\nu/kT}-1} \qquad (1.3)$$

Attempting to understand what the formula implied, Planck was forced to introduce a revolutionary hypothesis in 1900. The atomic oscillators can radiate only discrete energies of the amount ε, 2ε, 3ε, $\cdots$, $n\varepsilon$, where the energy unit ε is directly proportional to the radiation frequency ν, or $\varepsilon = h\nu$. The proportionality constant h is now the famous Planck constant on which the whole theory of quantum mechanics is built.

2. Photoelectric effect

The observed phenomenon of photoelectric effect was never understood in classical physics. The kinetic energy of ejected electrons does not depend on the intensity of the incident light. Instead, it is directly related to the incident light frequency as shown in Fig. 1. 2.

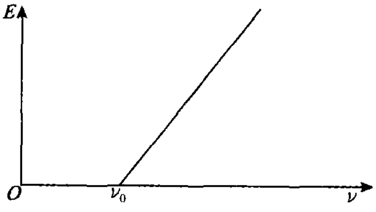

Fig. 1. 2 Kinetic energy of ejected electron from a metal surface

The observed phenomenon was explained by Einstein who introduced the quantum assumption in light waves. In 1905, Einstein proposed a theory in which the radiation energy traveling in space is not uniformly distributed over the wave front, but is concentrated into a quantum of amount $h\nu$. The quantum can be anywhere on the wave front with equal probability. When one quantum of energy $h\nu$ of light is absorbed, the atom emits an electron of energy $\frac{1}{2}mv^2$, given by

$$\frac{1}{2}mv^2 = h\nu - \phi \tag{1.4}$$

where ϕ represents the work done by the electron against the surface barrier of the substance. This formula was verified experimentally a few years later by quantitative measurements. The verification strongly supports Einstein's theory on the electromagnetic wave, that the waves only represent the probability of the quantum to be found at various points on the wave front.

3. Specific heat of solids

According to the classical theory, the specific heat of a solid is given by

$$C_V = \frac{dE}{dT} = \frac{d}{dT}(3kT) \tag{1.5a}$$

which yields the Dulong-Petit law

$$C_V = 3R = 3N_0 k \tag{1.5b}$$

Einstein replaces the classical partition energy kT, or the energy per degree of freedom by the

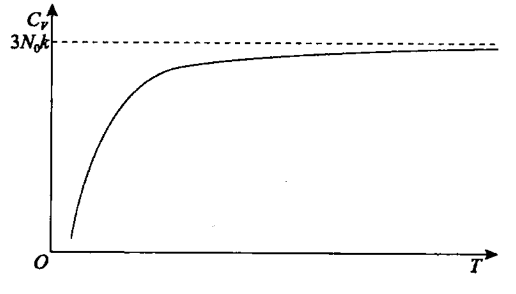

Fig. 1. 3 Specific heat of solids versus T

Planck assumption $h\nu/(e^{h\nu/kT} - 1)$. His theory gives

$$C_v = 3N_0 k \frac{x^2 e^x}{(e^x - 1)^2}, \quad x = h\nu/kT \tag{1.6}$$

As illustrated in Fig. 1. 3, Eq. (1. 6) successfully explains the decrease of the specific heat with decreasing temperature until the low temperature region. Debye introduced a critical temperature for the material under consideration, and obtained a more complicated formula that agrees with experiments all the way to nearly absolute zero. The subject is not of our concern at this stage, but it demonstrates from a different angle the success of the new quantum theory.

4. Compton effect

The experiment of light scattering from material was performed much later. In 1923, Compton observed that the wave length λ_0 of a light beam becomes longer after the scattering. The wavelength shift $\Delta\lambda$ after the scattering depends on the scattering angle θ, and is given by the relation

$$\Delta\lambda = \lambda - \lambda_0 = \frac{h}{m_0 c}(1 - \cos\theta) \tag{1.7}$$

where $\lambda_c = h/m_0 c = 0.0242$ Å is now known as the Compton wavelength of the electron. The phenomenon can easily be understood if one considers light as a particle of energy $h\nu$ and momentum $h\nu/c$, and the light quantum is scattered elastically by the atom. The conservation laws of momentum and energy then lead immediately to the above result. The calculation of scattering cross section, however, is much more complicated and is beyond the scope of the present book.

While the above experiments are all successfully accounted for by the quantum assumption, the theory of atomic spectra was also developed in parallel. We would not discuss the details but merely mention that the accumulated data of atomic spectra were not understood until the Bohr theory of hydrogen atom was proposed. Bohr model was really a product of the quantum theory of light radiation, and Rutherford experiment of the α particle scattering from gold, which established the existence of the atomic nucleus. Since the Bohr theory was so successful in predicting the frequencies of observed spectral line series such as Balmer series, it is natural to refine the theory for fine structures and so on. These topics will be treated in the future chapters.

Problems

1.1 Show that the Planck formula reduces to the Rayleigh-Jean formula in the low frequency limit and approaches the Wien formula in the high frequency limit. It is noted that the low frequency limit demonstrates the corresponding principle, that is, the quantum theory prediction approaches that of classical mechanics as $\hbar \to 0$.

1. 2 Find the maximum intensity of radiation in Planck formula and the radiation density at the peak intensity. Show that the total thermal energy radiated at a temperature T is $\psi=\pi k_B^2 T^4/15c^3\hbar^3$ which is consistent with the Stefan-Boltzmann radiation law.

1. 3 When a beam of light falls on the surface of silicon, it is found that the largest wavelength which results in the electron emission is 296 nm. Find the work function of Si. If the wavelength of incident light is 250 nm, find the kinetic energy and wavelength of the emitted electrons.

1. 4 Determine the average wavelength of electrons in thermal equilibrium at $T = 300$ K. Do the same for neutrons and α particles.

Ⅱ. Uncertainty and complementarily

We have discussed very briefly why the classical physics is not adequate and how the quantum theory is successful, at least partially, in explaining the striking atomic phenomena. The theory of quantum mechanics was formulated during 1924～1928. Perhaps it is most interesting to note that the theory started from two different groups of ideas, and developed later along different lines of thought with different mathematical formalisms. However, it was recognized later that the two distinctive approaches were mathematically equivalent. Finally, the physical foundation of the mathematical formalism was completed.

One approach begins with de Broglie, whose idea of matter wave leads Schrödinger to formulate the equation of motion. The probability amplitude interpretation of the wave function then completes the development of the wave mechanics. The other approach starts with Heisenberg, who formulates the so-called matrix mechanics with Born and Jordan. Based on the matrix approach, a more general formalism of quantum mechanics was developed by Dirac. The physical formalism was, completed by Heisenberg's uncertainty principle and Bohr's complimentarity principle. In the following, we study some of the microscopic phenomena and see how the new ideas are introduced.

It is important to remark that classical physics is not just inadequate to produce experimental results quantitatively, it is actually lack of the basic concepts to describe microscopic phenomena qualitatively. At this point, it may be useful to point out that the language we use has been developed on the basis of what we see in the macroscopic world. Thus, our daily life language is simply not sufficient to describe the microscopic phenomena.

1. Einstein relations and Bohr complimentarity principle

Let us now look more closely at the quantum theory mentioned previously. Let us first define the notation. For electromagnetic waves of frequency ν and wavelength λ, its wave number is $k=2\pi/\lambda$ and its velocity is $c=\nu\lambda$. For convenience, a different set of notation is defined, namely,

$$\omega = 2\pi\nu, \quad \lambda\!\!\!^{-} = \lambda/2\pi, \quad \hbar = h/2\pi, \quad |\boldsymbol{k}| = 2\pi/\lambda = 1/\lambda\!\!\!^{-} \qquad (2.1)$$

This set of notation is adopted in the following discussion throughout the book.

In the explanation of light scattering from electrons, Compton took the Einstein relation $E=h\nu=\hbar\omega$, and treated the light quantum as if it were a particle with the momentum $p=h\nu/c=\hbar\omega/c=\hbar/\lambda\!\!\!^{-}=\hbar k$, or $\boldsymbol{p}=\hbar\boldsymbol{k}$. The Einstein relations

$$E = \hbar\omega \tag{2.2a}$$

$$\boldsymbol{p} = \hbar\boldsymbol{k} \tag{2.2b}$$

together with the conservation laws of momentum and energy enable Compton to determine correctly the observed wavelength shift after the scattering. This is of course beyond the reach of classical physics.

We note that the light quantum or photon as called by Einstein really behaves like a particle of zero rest mass. This is clearly seen if one notes that $\omega=ck$ implies $E = pc$ which is just $E^2=p^2c^2+m_0^2c^4$ if the rest mass $m_0=0$.

It must be emphasized that the Einstein relations in (2.2) are already far beyond the classical physics because they express the *particle* properties in terms of the *wave* concepts. As you know, waves and particles in classical physics are completely independent and have nothing to do with each other at all. As a matter of fact, this wave-particle duality of light indicates already a part of Bohr's complimentarity principle, that is, *it is not possible to describe the microscopic phenomenon by any single classical concept.*

Compton's explanation of his light scattering experiment was not complete because he was not able to calculate the intensity distribution of light after the scattering. This intensity distribution or the scattering cross section is experimentally reproducible, but the cross section was not calculated until quantum mechanics was completely formulated.

Let us now come back to the property of light. We recall that historically light was regarded as a beam of particles ever since the Newton time. The particle picture was able to account for the Snell laws of reflection and refraction. But all evidences observed since then indicated conclusively that light exhibited wave properties. The Maxwell equations strengthened the wave picture tremendously because it treated all electromagnetic waves in general.

The new phenomena of photoelectric and Compton effects, on the other hand, provide definite evidences that light behaves like particles. The question is then really a particle-wave puzzle. In order to resolve this puzzle satisfactorily, we can either formulate a theory that is capable to describe both the particle and wave properties or we have to recognize that our language in classical physics is simply not sufficient for the description of microscopic phenomena. At this point,