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# SOLUTIONS MANUAL FOR EXERCISES IN QUANTUM MECHANICS I: THE FUNDAMENTALS

by

S. Rajasekar and R. Velusamy



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### Preface

Quantum mechanics is the study of the behaviour of matter and energy at the molecular, atomic, nuclear levels and even at sub-nuclear level. This book is intended to provide a broad introduction to fundamental and advanced topics of quantum mechanics. Volume I is devoted for basic concepts, mathematical formalism and application to physically important systems. Volume II covers most of the advanced topics of current research interest in quantum mechanics. Both the volumes are primarily developed as a text at the graduate level and also as reference books. In addition to worked-out examples, numerous collection of problems are included at the end of each chapter. Complete details of solutions of the problems are provided in the CD attached with each volume. Some of the problems serve as a mode of understanding and highlighting the significances of basic concepts while others form application of theory to various physically important systems/problems. Developments made in recent years on various mathematical treatments, theoretical methods, their applications and experimental observations are pointed out wherever necessary and possible and moreover they are quoted with references so that readers can refer them for more details.

The volume I consists of 21 chapters and 7 appendices. Chapter 1 summarizes the needs for the quantum theory and its early development (old quantum theory). Chapters 2 and 3 provide basic mathematical framework of quantum mechanics. Schrödinger wave mechanics and operator formalism are introduced in these chapters. Chapters 4 and 5 are concerned with the analytical solutions of bound states and scattering states respectively of certain physically important microscopic systems. The basics of matrix mechanics, Dirac's notation of state vectors and Hilbert space are elucidated in chapter 6. The next chapter gives the Schrödinger, Heisenberg and interaction pictures of time evolution of quantum mechanical systems. Description of time evolution of ensembles by means of density matrix is also described. Chapter 8 is concerned with Heisenberg's uncertainty principle. A brief account of wave function in momentum space and wave packet dynamics are presented in chapters 9 and 10 respectively. Theory of angular momentum is covered in chapter 11. Chapter 12 is devoted exclusively for the theory of hydrogen atom.

Chapters 13-16 are mainly concerned with approximation methods such as time-independent and time-dependent perturbation theories, WKB method and variational method. The elementary theory of elastic scattering is pre-

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sented in chapter 17. Identical particles are treated in chapter 18. The next chapter presents quantum theory of relativistic particles with specific emphasize on Klein–Gordon equation, Dirac equation and its solution for a free particle, particle in a box (Klein paradox) and hydrogen atom. Chapter 20 examines the strange consequences of role of measurement through the paradoxes of EPR and a thought experiment of Schrödinger. A brief sketch of Bell's inequality and the quantum mechanical examples violating it are given. Considering the rapid growth of numerical techniques in solving physical problems and significances of simulation studies in describing complex phenomena, the final chapter is devoted for a detailed description of numerical computation of bound state eigenvalues and eigenfunctions, transmission and reflection probabilities of scattering potentials, transition probabilities of quantum systems in the presence of external fields and electronic distribution of atoms. Some supplementary and background materials are presented in the appendices.

The pedagogic features volume I of the book, which are not usually found in text books at this level, are the presentation of bound state solutions of quantum pendulum, Pöschl—Teller potential, solutions of classical counter part of quantum mechanical systems considered, criterion for bound state, scattering from a locally periodic potential and reflectionless potential, modified Heisenberg relation, wave packet revival and and its dynamics, hydrogen atom in *D*-dimension, alternate perturbation theories, an asymptotic method for slowly varying potentials, Klein paradox, EPR paradox, Bell's theorem and numerical methods for quantum systems.

The volume II consists of 10 chapters. Chapter 1 describes the basic ideas of both classical and quantum field theories. Quantization of Klein-Gordon equation and Dirac field are given. The formulation of quantum mechanics in terms of path integrals is presented in chapter 2. Application of it to free particle and linear harmonic oscillator are considered. In chapter 3 some illustrations and interpretation of supersymmetric potentials and partners are presented. A simple general procedure to construct all the supersymmetric partners of a given quantum mechanical systems with bound states is described. The method is then applied to a few interesting systems. The next chapter is concerned with coherent and squeezed states. Construction of these state and their characteristic properties are enumerated. Chapter 5 is devoted for Berry's phase, Aharonov-Bohm and Sagnac effects. Their origin, properties, effects and experimental demonstration are presented. The features of Wigner distribution function are elucidated in chapter 6. In a few decades time, it is possible to realize a computer built in terms of real quantum systems that operate in quantum mechanical regime. There is a growing interest on quantum computing. Basic aspects of quantum computing is presented in chapter 7. Deutsch-Jozsa algorithm of finding whether a function is constant or not, Grover's search algorithm and Shor's efficient quantum algorithm for integer factorization and evaluation of discrete logarithms are described. Chapter 8 deals with quantum cryptography. Basic principles of classical cryptography and quantum cryptography and features of a few quantum cryptographic

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systems are discussed. A brief introduction to other advanced topics such as quantum gravity, quantum Zeno effect, quantum teleportation, quantum games, quantum cloning, quantum diffusion and quantum chaos is presented in chapter 9. The last chapter gives features of some of the recent technological applications of quantum mechanics. Particularly, promising applications of quantum mechanics in ghost imaging, detection of weak amplitude objects, entangled two-photon microscopy, detection of small displacements, lithography, metrology and teleportation of optical images are briefly discussed.

During the preparation of this book we have received great supports from many colleagues, students and friends. In particular, we are grateful to Prof. N. Arunachalam, Prof. K.P.N. Murthy, Prof. M. Daniel, Dr. S. Sivakumar, Mr. S. Kanmani, Dr. V. Chinnathambi, Dr. P. Philominathan, Dr. K. Murali, Dr. S.V.M. Sathyanarayana, Dr. K. Thamilmaran, Dr.T. Arivudainambi and Dr.V.S. Nagarathinam for their suggestions and encouragement. It is a great pleasure to thank Dr. V.M. Gandhimathi, Dr. V. Ravichandran, Dr. S. Jeyakumari, Dr. G. Sakthivel, Dr. M. Santhiah, Mr.R. Arun, Mr. C. Jeevarathinam, R. Jothimurugan, Ms. K. Abirami and Ms. S. Rajamani for typesetting some of the chapters. Finally, we thank our family members for their unflinching support, cooperation and encouragement during the course of preparation of this work.

Tiruchirapalli May, 2014 S. Rajasekar R. Velusamy

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### About the Authors



Shanmuganathan Rajasekar was born in Thoothukudi, Tamilnadu, India in 1962. He received his B.Sc. and M.Sc. in Physics both from the St. Joseph's College, Tiruchirapalli. In 1987, he received his M.Phil. in Physics from Bharathidasan University, Tiruchirapalli. He was awarded Ph.D. degree in Physics (Nonlinear Dynamics) from Bharathidasan University in 1992 under the supervision of Prof.M. Lakshmanan. He was a visiting scientist during 1992-93 at the Materials Science Division, Indira Gandhi Centre for Atomic Research, Kalpakkam and worked on

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Ramiah Velusamy was born in Srivilliputhur, Tamilnadu, India in the year 1952. He received his B.Sc. degree in Physics from the Ayya Nadar Janaki Ammal College, Sivakasi in 1972 and M.Sc. in Physics from the P.S.G. Arts and Science College, Coimbatore in 1974. He worked as a demonstrater in the Department of Physics in P.S.G. Arts and Science College during 1974-77. He received M.S. Degree in Electrical Engineering at Indian Institute of Technology, Chennai in the year 1981. In the same year, he joined in the Ayya Nadar Janaki Ammal College

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# Why was Quantum Mechanics Developed?

1.1 Calculate the energy of a photon of 253.6 nm light. State the energy in eV (1eV =  $1.6 \times 10^{-19}$  J).

We obtain

$$E = hc/\lambda$$

$$= \frac{6.626 \times 10^{-34} \text{Js} \times 3 \times 10^8 \text{ms}^{-1}}{253.6 \times 10^{-9} \text{m}}$$

$$= 7.83832 \times 10^{-19} \text{J}$$

$$= \frac{7.83832 \times 10^{-19}}{1.6 \times 10^{-19}} \text{ eV}$$

$$= 4.89895 \text{ eV}.$$

 $1.2\,$  Calculate the wavelength of a quantum of electromagnetic radiation with energy  $4000\,\mathrm{eV}.$ 

We have  $\lambda = hc/E$ . We have

$$hc = 6.626 \times 10^{-34} \text{Js} \times 3 \times 10^8 \text{ms}^{-1}$$

Since E is in eV we express hc in units of eV. The conversion factor is  $1J = 1/(1.6 \times 10^{-19}) \, \text{eV}$ . So

$$\begin{array}{lcl} hc & = & \frac{6.626\times 10^{-34} \mathrm{eV}\times 3\times 10^8 \mathrm{m}}{1.6\times 10^{-19}} = 1242.375\times 10^{-9} \mathrm{eVm} \\ & = & 1242.375 \mathrm{eVnm} \:. \end{array}$$

Then the wavelength of a quantum of electromagnetic radiation with energy  $4000 \mathrm{eV}$  is

$$\lambda = \frac{1242.375 eV nm}{4000 eV} = 3.106 \times 10^{-10} m = 3.106 \mathring{A}^{\circ}.$$

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- **2** Solutions to the Exercises in Quantum Mechanics I: The Fundamentals
  - 1.3 A light of wavelength 1000 nm produces photoelectrons from a metal. The threshold potential  $V_0$  is 0.5V. Calculate the work function  $\phi_0$ .

The work function  $\phi_0$  is given by

$$\phi_0 = \frac{hc}{\lambda} - |e|V_0 .$$

hc is calculated as

$$hc = 6.626 \times 10^{-34} \text{Js} \times 3 \times 10^8 \text{ms}^{-1}$$
  
=  $\frac{6.626 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19}} \text{ eVm}$   
=  $1242.375 \text{ eVnm}$ .

An electron accelerated by 1V will have 1eV of kinetic energy. Therefore, an electron accelerated by  $0.5\,\rm V$  will have the kinetic energy of  $0.5\,\rm eV.$  Then

$$\phi_0 = \frac{1242.375\,\mathrm{eVnm}}{1000\,\mathrm{nm}} - 0.5\,\mathrm{eV} = 0.742375\,\mathrm{eV} \;.$$

1.4 Consider the previous problem. Calculate the threshold wavelength  $\lambda_c$ .

We obtain

$$\lambda_{\rm c} = \frac{hc}{E} = \frac{1242.375\,{\rm eVnm}}{0.742375\,{\rm eV}} = 1674\,{\rm nm} \; .$$

1.5 Calculate the frequency of light required to produce electrons of kinetic energy  $5\,\mathrm{eV}$  from illumination of a material whose work function is  $0.5\,\mathrm{eV}$ .

According to conservation of energy

Energy of a photon = K.E. of an emitted electron + Work function .

We obtain the energy of the incident light as

$$E = \frac{1}{2}mv_{\text{max}}^2 + \phi_0 = 5\text{eV} + 0.5\text{eV} = 5.5\text{ eV}.$$

Then

$$\nu = \frac{E}{h} = \frac{5.5 \,\text{eV}}{6.626 \times 10^{-34} \,\text{Js}} \,.$$

Since  $1 \text{eV} = 1.6 \times 10^{-19} \text{J}$  we get

$$\nu = \frac{5.5 \times 1.6 \times 10^{-19} \text{J}}{6.626 \times 10^{-34} \text{Js}} = 1.3281 \times 10^{15} \text{Hz} .$$

1.6 Light of wavelength 500 nm is incident on a metal with work function  $(\phi_0)$  of 0.75 eV. What is the maximum kinetic energy  $(K_{\text{max}})$  of the ejected photoelectrons?

$$K_{\text{max}}$$
 is  $h\nu - \phi_0$ . We obtain

$$K_{\text{max}} = h\nu - \phi_0 = \frac{hc}{\lambda} - \phi_0$$
  
=  $\frac{6.626 \times 10^{-34} \text{Js} \times 3 \times 10^8 \text{ms}^{-1}}{500 \times 10^{-9} \text{m}} - 0.75 \times 1.6 \times 10^{-19} \text{J}$   
=  $2.7756 \times 10^{-19} \text{J}$ .

1.7 Suppose you are standing in front of a 40 W incandescent light bulb 5 m away. If the diameter of your pupils is about 2 mm, about how many photons, n, enter your eye every second?

Intensity at the eye is

$$I = \frac{40\pi d^2}{4\pi r^2} = \frac{10d^2}{r^2} W ,$$

where d is the diameter of the pupil and r is the distance between the eye and light source. We get

$$I = \frac{10 \times (0.002)^2}{5^2} W = 1.6 \times 10^{-6} Js^{-1}$$
.

The number of photons that enters the eye every second is obtained as

$$n = \frac{I}{h\nu} = \frac{1.6 \times 10^{-6} \text{Js}^{-1}}{6.626 \times 10^{-34} \text{Js} \times \nu} = \frac{0.2414729 \times 10^{28}}{\nu} \text{s}^{-2}.$$

If  $\nu$  is stated in Hz then

$$n = \frac{2.414729 \times 10^{27}}{\nu} \text{s}^{-1} \ .$$

1.8 Calculate the minimum voltage required for an electron to give all of its energy in a collision with a target and produce an electromagnetic radiation of wavelength 0.05nm.

When an electron is accelerated through a potential difference V, it acquires an energy |e|V. If this energy goes into producing a photon of energy E with associated wavelength  $\lambda$ , we get  $E = hc/\lambda$ . So

$$E = \frac{6.626 \times 10^{-34} \text{Js} \times 3 \times 10^8 \text{ms}^{-1}}{0.05 \times 10^{-9} \text{m}}$$

$$= \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-19} \times 0.05 \times 10^{-9}} \text{ eV}$$

$$= 24847.5 \text{ eV}.$$

**4** ■ Solutions to the Exercises in Quantum Mechanics I: The Fundamentals

Now,

$$V = \frac{E}{|e|} = \frac{24847.5 \times 1.6 \times 10^{-19} \text{J}}{1.6 \times 10^{-19} \text{C}}$$
$$= 24847.5 \text{JC}^{-1}$$
$$= 24847.5 \text{V}.$$

1.9 Assume that the resolving power of a microscope is equal to the wavelength of the light used. If electrons are used as the light source calculate the kinetic energy of electrons needed to have the resolving power as  $10^{-11}$ m.

From  $\lambda = h/p = h/mv$  we get (using  $1J = 1 \text{ kgm}^2/\text{s}^2$ )

$$v = \frac{h}{m\lambda}$$

$$= \frac{6.626 \times 10^{-34} \text{Js}}{9.11 \times 10^{-31} \text{kg} \times 10^{-11} \text{m}}$$

$$= 7.273326 \times 10^7 \text{m/s}.$$

Then the kinetic energy  $E = mv^2/2$  required is

$$E = \frac{1}{2} \times 9.11 \times 10^{-31} \text{kg} \times (7.273326 \times 10^7 \text{m/s})^2 \times \frac{1 \text{eV}}{1.6 \times 10^{-19} \text{J}}$$
  
= 15060.33 eV.

1.10 Suppose a laser provides 100 TW of power in 1ns pulses at a wavelength of  $0.26\,\mu m$ . How many photons are contained in a single pulse?

From dW/dt = P we obtain

$$dW = Pdt = 100 \times 10^{12} W \times 1 \times 10^{-9} s = 10^5 J$$
.

That is,  $nh\nu = 10^5 \text{J}$  or  $nhc/\lambda = 10^5 \text{J}$ . So

$$n = \frac{\lambda}{ch} 10^5 \text{ photons}$$
  
=  $\frac{0.26 \times 10^{-6} \text{m} \times 10^5 \text{J}}{3 \times 10^8 \text{ms}^{-1} \times 6.626 \times 10^{-34} \text{Js}} \text{ photons}$   
=  $130797 \times 10^{18} \text{ photons}.$ 

1.11 Express the change in wavelength in terms of Compton wavelength of electron when light is scattered through an angle  $\pi/4$  by a proton.

For a proton

$$\Delta \lambda = \lambda_{\rm c} \frac{m_{\rm e}}{m_{\rm p}} \left( 1 - \frac{1}{\sqrt{2}} \right) = 0.29289 \frac{m_{\rm e}}{m_{\rm p}} \lambda_{\rm c} \ .$$

1.12 A beam of X-rays of wavelength  $\lambda=0.738\text{Å}^{\circ}$  is Compton scattered by electrons through an angle  $\pi/2$ . Calculate the wavelength and the energy of the scattered radiation.

Change in wavelength for the given problem is

$$\Delta \lambda = \lambda' - \lambda = \lambda_{c} (1 - \cos \phi)$$

$$= \lambda_{c}$$

$$= \frac{h}{m_{e}c}.$$

Substituting the values of h,  $m_{\rm e}$  and c we get

$$\Delta \lambda = \frac{6.626 \times 10^{-34} \text{Js}}{9.11 \times 10^{-31} \text{kg} \times 3 \times 10^8 \text{ms}^{-1}}$$
$$= 2.42444 \times 10^{-12} \text{m}$$
$$= 0.02424 \text{Å}^{\circ}.$$

Then  $\lambda'=\lambda+\lambda_c=0.738\text{Å}^\circ+0.02424\text{Å}^\circ=0.76224\text{Å}^\circ.$  Next,

$$E = \frac{hc}{\lambda}$$

$$= \frac{6.626 \times 10^{-34} \text{Js} \times 3 \times 10^8 \text{m/s}}{0.76224 \times 10^{-10} \text{m}}$$

$$= 2.60784 \times 10^{-15} \text{J}.$$

1.13 Show that the de Broglie wavelength  $\lambda_{\rm d}$  associated with photons is equal to the electromagnetic wavelength  $\lambda$ .

The momentum p of a photon of energy  $E(=h\nu)$  is

$$p = \frac{E}{c} = \frac{h\nu}{c} \; .$$

Since c is  $\nu\lambda$  we get

$$\lambda_{\rm d} = \frac{h}{p} = \frac{h}{h\nu/c} = \frac{c}{\nu} = \frac{\nu\lambda}{\nu} = \lambda$$
.

1.14 A 5.78 MeV  $\alpha$ -particle (assume that its velocity is  $\ll c$ ) is emitted in the decay of radium. If the diameter of the radium nucleus is  $2 \times 10^{-14}$ m, how many  $\alpha$ -particle de Broglie wavelengths fit inside the nucleus?

We obtain

$$E = \frac{p^2}{2m} = 5.78 \times 10^6 \text{eV} = 9.248 \times 10^{-13} \text{J}.$$

**6** ■ Solutions to the Exercises in Quantum Mechanics I: The Fundamentals

Then 
$$p = \sqrt{2mE}$$
 gives

$$\begin{array}{lcl} p & = & \left[2 \times 6.62 \times 10^{-27} \times 9.248 \times 10^{-13}\right]^{1/2} \, \mathrm{kgm/s} \\ & = & 11.06542 \times 10^{-20} \mathrm{kgm/s} \; . \end{array}$$

Next, the de Broglie wavelength of  $\alpha$ -particle is

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}}{11.06542 \times 10^{-20}} \,\mathrm{m} = 0.5988 \times 10^{-14} \mathrm{m} \;.$$

Then

$$n = \frac{2 \times 10^{-14}}{\lambda} = \frac{2 \times 10^{-14}}{0.5988 \times 10^{-14}} = 3.34 \; .$$

1.15 A diatomic gas molecule consisting of two atoms of mass m separated by a fixed distance d is rotating about a central axis perpendicular to the line joining the two atoms. Assuming that its angular momentum is quantized as in the Bohr atom, determine the possible angular velocities  $(\omega)$  and the possible quantized rotational energies (E).

We have  $L = I\omega$  and  $L = n\hbar$ . These give  $\omega = n\hbar/I$ . Then

$$E = \frac{L^2}{2I} = \frac{n^2 \hbar^2}{2I}$$
,  $n = 1, 2, \cdots$ .