❖ Max-Born Interpretation of Wave Functions

In 1926, a German physicist Max Born formulated a rule which is generally called as the Born law or Born's rule of quantum mechanics, giving the probability that a measurement on a quantum system will yield a given result. In other words, it states that the probability density of finding the particle at a given point is proportional to the square of the magnitude of the particle's wavefunction at that point. The Max-Born interpretation is one of the key concepts of quantum mechanics to understand wave-particle duality.

Let us suppose that the particle under consideration is an electron whose way of existence is represented by a mathematical expression ψ which is a function of the electron's coordinates i.e. x, y, and z. Max Born actually suggested that because this mathematical expression is single-valued, continuous and finite i.e. wave-like; one can opt the same route to find it's intensity as we use in case of light or sound waves. In the case of light or sound waves, the intensity at any point can simply be obtained by squaring the amplitude i.e. ψ of the wave at the same point. Therefore, in the case of the electron, the square of the amplitude of electron wave (ψ^2) at a particular point also gives the intensity of the electron wave at the same point. In other words, the density of electron wave (probability density) at a point for a quantum mechanical state is simply obtained by the square of the magnitude of the corresponding wavefunction at the same point. Mathematically, we can show this as:

$$Probability\ density = |\psi|^2 = \psi\psi^* \tag{29}$$

Where ψ^* designates a complex conjugate of the wave function ψ. The reason for using ψ^* lies in the fact that the wave function representing a quantum mechanical state is not always real but be imaginary as well. However, as the probability density should always be real, $\psi\psi^*$ is more appropriate than simple ψ^2. In other words, if the wave function defining the quantum mechanical state is real, we can use ψ^2 as the probability density; nevertheless, if the wave function does contain the imaginary part (like $\psi = a + ib$), $\psi\psi^*$ must be used to yield real values. This can be explained by taking an imaginary expression ψ and then multiplying it by its complex conjugate ψ^* to yield real value.

$$\psi = a + ib; \qquad \psi^* = a - ib \tag{30}$$

or

$$\psi\psi^* = (a + ib) \times (a - ib) \tag{31}$$

or

$$\psi\psi^* = a^2 + b^2 \tag{32}$$

Moreover, if ψ is real, $\psi = \psi^*$, $\psi\psi^*$ becomes ψ^2, the value we have already discussed.

Now though the probability density in space is not a constant parameter (ψ is not constant), in a very small segment it can be considered constant. Now let us discuss the Max-Born interpretation for one, two and three dimensional systems.

Copyright © Mandeep Dalal

➢ ***One Dimensional Systems***

The probability of finding the particle in any one-dimensional system in the region from x to $x+dx$ must be obtained by integrating ψ^2 from x to $x+dx$ i.e. by finding the area under the curve from x to $x+dx$.

Now although the ψ^2 or $\psi\psi^*$ (because ψ is continuous) varies continuously with x, the decrease or increase in ψ^2 can be neglected and it can be assumed that it remains constant as we move from x to $x+dx$.

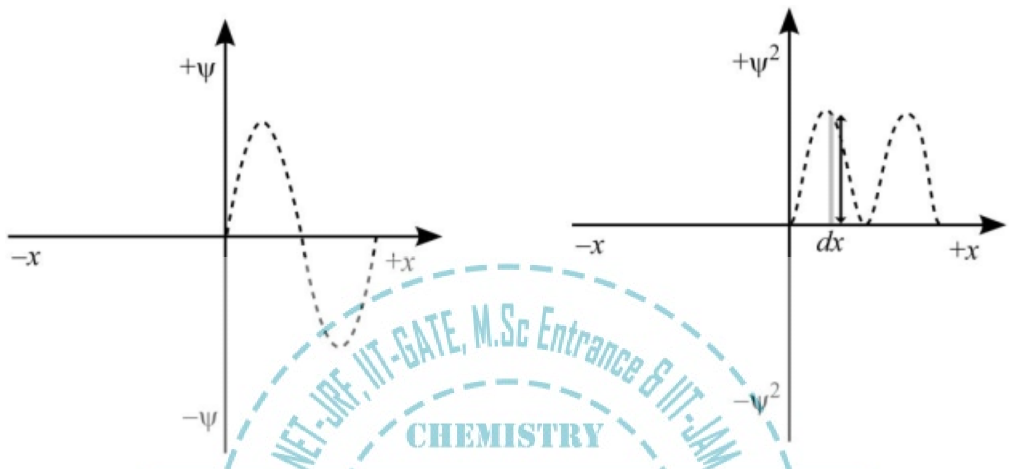

Figure 3. Born interpretation of wave function and probability density in a one-dimensional system.

NET-JRF, IIT-GATE, M.Sc Entrance & IIT-JAM
CHEMISTRY
DALAL INSTITUTE
(info@dalalinstitute.com, +91-9802825820)
www.dalalinstitute.com
SINCE 2012
Main Market, Sector-14, Rohtak, Haryana

Therefore, the area of the shaded region and hence the probability of finding the particle can be obtained just by multiplying the length (or height i.e. ψ^2) with the width (dx) of the narrow rectangle. Thus we can say that

$$Probability = |\psi|^2 \times (dx) = \psi\psi^* dx = \psi^2 dx \tag{33}$$

Since the chances of finding the particle over whole length (whole configurational space) must be unity, we get the following

$$\oint |\psi|^2 \times (dx) = \oint \psi\psi^* dx = \oint \psi^2 dx \tag{34}$$

➢ ***Two Dimensional Systems***

The probability of finding the particle in an area element $dx\, dy$ (dA), situated at a distance r distance from the center, would be $\psi\ (x, y) \times \psi^*\ (x, y) \times dx \times dy$; or in short can be written as $\psi\psi^* dA$. Hence, it must be obtained by integrating ψ^2 from (x, y) to $(x+dx, y+dy)$ i.e. by finding the area under the curve dA. Now although the ψ^2 or $\psi\psi^*$ (because ψ is continuous) varies continuously with coordinates ($x\ y$), the decrease or increase in ψ^2 can be neglected and it can be assumed that it remains constant as we move from (x, y) to $(x+dx, y+dy)$.

Therefore, the area of the shaded region and hence the probability of finding the particle can be obtained just by multiplying the magnitude of the wave function (ψ^2) with the area (dA) of the area element. Thus we can say that

Buy the complete book with TOC navigation, high resolution images and no watermark.
Copyright © Mandeep Dalal
DALAL INSTITUTE

$$Probability = |\psi|^2 \times (dA) = \psi\psi^* dA = \psi^2 dA \tag{35}$$

Since the chances of finding the particle over the whole area (whole configurational space) must be unity, we get the following

$$\oint |\psi|^2 \times (dA) = \oint \psi\psi^* dA = \oint \psi^2 dA \tag{36}$$

The pictorial representation of the area element is given below.

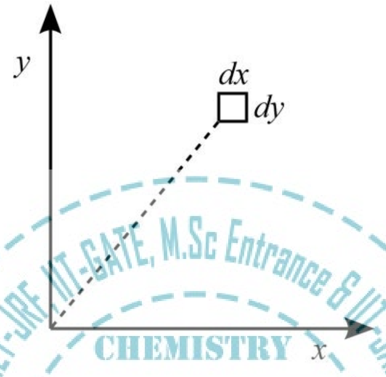

Figure 2. Born interpretation of wave function and probability density in two dimensional systems.

NET-JRF, IIT-GATE, M.Sc Entrance & IIT-JAM
CHEMISTRY
DALAL INSTITUTE
(info@dalalinstitute.com, +91-9802825820)
www.dalalinstitute.com
SINCE 2012
Main Market, Sector 14, Rohtak, Haryana

➤ ***Three Dimensional System***

The probability of finding the particle in a volume element *dx dy dz* (*dV*), situated at a distance *r* distance from the center, would be ψ (*x, y, z*) × ψ^* (*x, y, z*) × *dx* × *dy*× *dz*; or in short can be written as $\psi\psi^* dV$. must be obtained by integrating ψ^2 from (*x, y, z*) to (*x+dx, y+dy, z+dz*) i.e. by finding the area under the curve from (*x, y, z*) to (*x+dx, y+dy, z+dz*). Now although the ψ^2 or $\psi\psi^*$ (because ψ is continuous) varies continuously with coordinates (*x, y, z*), the decrease or increase in ψ^2 can neglected and it can be assumed that it remains constant as we move from (*x, y, z*) to (*x+dx, y+dy, z+dz*).

Therefore, the probability of finding the particle can be obtained just by multiplying the magnitude of the wave function (ψ^2) with the volume (*dV*) of the area element. Thus we can say that

$$Probability = |\psi|^2 \times (dV) = \psi\psi^* dV = \psi^2 dV \tag{35}$$

Since the chances of finding the particle over the whole area (whole configurational space) must be unity, we get the following

$$\oint |\psi|^2 \times (dV) = \oint \psi\psi^* dV = \oint \psi^2 dV \tag{36}$$

The pictorial representation of the area element is given below.

Copyright © Mandeep Dalal

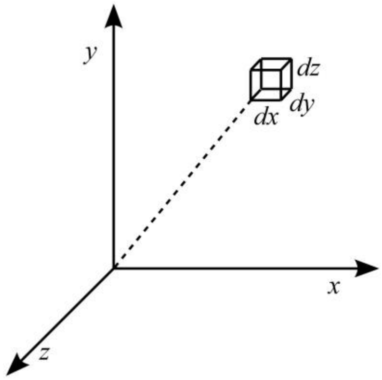

Figure 3. Born interpretation of wave function and probability density in three dimensional systems.

LEGAL NOTICE

This document is an excerpt from the book entitled "A Textbook of Physical Chemistry – Volume 1 by Mandeep Dalal", and is the intellectual property of the Author/Publisher. The content of this document is protected by international copyright law and is valid only for the personal preview of the user who has originally downloaded it from the publisher's website (www.dalalinstitute.com). Any act of copying (including plagiarizing its language) or sharing this document will result in severe civil and criminal prosecution to the maximum extent possible under law.

NET-JRF, IIT-GATE, M.Sc Entrance & IIT-JAM
CHEMISTRY
DALAL INSTITUTE
(info@dalalinstitute.com, +91-9802825820)
www.dalalinstitute.com
SINCE 2012
Main Market, Sector 14, Rohtak, Haryana

This is a low resolution version only for preview purpose. If you want to read the full book, please consider buying.

Buy the complete book with TOC navigation, high resolution images and no watermark.

DALAL INSTITUTE

Home Classes Books Videos Location Contact Us About Us Follow us:

Home

CLASSES

NET-JRF, IIT-GATE, M.Sc Entrance & IIT-JAM

Want to study chemistry for CSIR UGC – NET JRF, IIT-GATE, M.Sc Entrance, IIT-JAM, UPSC, ISRO, IISc, TIFR, DRDO, BARC, JEST, GRE, Ph.D Entrance or any other competitive examination where chemistry is a paper ?

READ MORE

BOOKS

Publications

Are you interested in books (Print and Ebook) published by Dalal Institute ?

READ MORE

VIDEOS

Video Lectures

Want video lectures in chemistry for CSIR UGC – NET JRF, IIT-GATE, M.Sc Entrance, IIT-JAM, UPSC, ISRO, IISc, TIFR, DRDO, BARC, JEST, GRE, Ph.D Entrance or any other competitive examination where chemistry is a paper ?

READ MORE

Home: https://www.dalalinstitute.com/
Classes: https://www.dalalinstitute.com/classes/
Books: https://www.dalalinstitute.com/books/
Videos: https://www.dalalinstitute.com/videos/
Location: https://www.dalalinstitute.com/location/
Contact Us: https://www.dalalinstitute.com/contact-us/
About Us: https://www.dalalinstitute.com/about-us/

Postgraduate Level Classes (NET-JRF & IIT-GATE)

Admission

Regular Program Distance Learning

Test Series Result

Undergraduate Level Classes (M.Sc Entrance & IIT-JAM)

Admission

Regular Program Distance Learning

Test Series Result

A Textbook of Physical Chemistry – Volume 1

"A Textbook of Physical Chemistry – Volume 1 by Mandeep Dalal" is now available globally; including India, America and most of the European continent. Please ask at your local bookshop or get it online here.

READ MORE

Join the revolution by becoming a part of our community and get all of the member benefits like downloading any PDF document for your personal preview.

Sign Up

International
Edition

A TEXTBOOK OF PHYSICAL CHEMISTRY

Volume I

MANDEEP DALAL

First Edition

DALAL INSTITUTE

Table of Contents

CHAPTER 1 .... **11**

Quantum Mechanics – I 11

- Postulates of Quantum Mechanics 11
- Derivation of Schrodinger Wave Equation 16
- Max-Born Interpretation of Wave Functions 21
- The Heisenberg's Uncertainty Principle 24
- Quantum Mechanical Operators and Their Commutation Relations 29
- Hermitian Operators – Elementary Ideas, Quantum Mechanical Operator for Linear Momentum, Angular Momentum and Energy as Hermitian Operator 52
- The Average Value of the Square of Hermitian Operators 62
- Commuting Operators and Uncertainty Principle (x & p; E & t) 63
- Schrodinger Wave Equation for a Particle in One Dimensional Box 65
- Evaluation of Average Position, Average Momentum and Determination of Uncertainty in Position and Momentum and Hence Heisenberg's Uncertainty Principle 70
- Pictorial Representation of the Wave Equation of a Particle in One Dimensional Box and Its Influence on the Kinetic Energy of the Particle in Each Successive Quantum Level 75
- Lowest Energy of the Particle 80
- Problems 82
- Bibliography 83

CHAPTER 2 .... **84**

Thermodynamics – I 84

- Brief Resume of First and Second Law of Thermodynamics 84
- Entropy Changes in Reversible and Irreversible Processes 87
- Variation of Entropy with Temperature, Pressure and Volume 92
- Entropy Concept as a Measure of Unavailable Energy and Criteria for the Spontaneity of Reaction 94
- Free Energy, Enthalpy Functions and Their Significance, Criteria for Spontaneity of a Process ... 98
- Partial Molar Quantities (Free Energy, Volume, Heat Concept) 104
- Gibb's-Duhem Equation 108
- Problems 111
- Bibliography 112

CHAPTER 3 .... **113**

Chemical Dynamics – I 113

- Effect of Temperature on Reaction Rates 113
- Rate Law for Opposing Reactions of Ist Order and IInd Order 119
- Rate Law for Consecutive & Parallel Reactions of Ist Order Reactions 127
- Collision Theory of Reaction Rates and Its Limitations 135
- Steric Factor 141
- Activated Complex Theory 143
- Ionic Reactions: Single and Double Sphere Models 147
- Influence of Solvent and Ionic Strength 152
- The Comparison of Collision and Activated Complex Theory 157
- Problems 158
- Bibliography 159

CHAPTER 4 .... **160**

Electrochemistry – I: Ion-Ion Interactions 160

- The Debye-Huckel Theory of Ion-Ion Interactions 160
- Potential and Excess Charge Density as a Function of Distance from the Central Ion 168
- Debye-Huckel Reciprocal Length 173
- Ionic Cloud and Its Contribution to the Total Potential 176
- Debye-Huckel Limiting Law of Activity Coefficients and Its Limitations 178
- Ion-Size Effect on Potential 185
- Ion-Size Parameter and the Theoretical Mean - Activity Coefficient in the Case of Ionic Clouds with Finite-Sized Ions 187
- Debye-Huckel-Onsager Treatment for Aqueous Solutions and Its Limitations 190
- Debye-Huckel-Onsager Theory for Non-Aqueous Solutions 195
- The Solvent Effect on the Mobility at Infinite Dilution 196
- Equivalent Conductivity (Λ) vs Concentration $C^{1/2}$ as a Function of the Solvent 198
- Effect of Ion Association Upon Conductivity (Debye-Huckel-Bjerrum Equation) 200
- Problems 209
- Bibliography 210

CHAPTER 5 .... **211**

Quantum Mechanics – II 211

- Schrodinger Wave Equation for a Particle in a Three Dimensional Box 211

- The Concept of Degeneracy Among Energy Levels for a Particle in Three Dimensional Box 215
- Schrodinger Wave Equation for a Linear Harmonic Oscillator & Its Solution by Polynomial Method 217
- Zero Point Energy of a Particle Possessing Harmonic Motion and Its Consequence 229
- Schrodinger Wave Equation for Three Dimensional Rigid Rotator 231
- Energy of Rigid Rotator 241
- Space Quantization 243
- Schrodinger Wave Equation for Hydrogen Atom: Separation of Variable in Polar Spherical Coordinates and Its Solution 247
- Principal, Azimuthal and Magnetic Quantum Numbers and the Magnitude of Their Values....... 268
- Probability Distribution Function 276
- Radial Distribution Function 278
- Shape of Atomic Orbitals (*s*, *p* & *d*) 281
- Problems 287
- Bibliography 288

CHAPTER 6 289

Thermodynamics – II 289

- Clausius-Clapeyron Equation 289
- Law of Mass Action and Its Thermodynamic Derivation 293
- Third Law of Thermodynamics (Nernst Heat Theorem, Determination of Absolute Entropy, Unattainability of Absolute Zero) And Its Limitation 296
- Phase Diagram for Two Completely Miscible Components Systems 304
- Eutectic Systems (Calculation of Eutectic Point) 311
- Systems Forming Solid Compounds A_xB_y with Congruent and Incongruent Melting Points 321
- Phase Diagram and Thermodynamic Treatment of Solid Solutions.................. 332
- Problems 342
- Bibliography 343

CHAPTER 7 344

Chemical Dynamics – II 344

- Chain Reactions: Hydrogen-Bromine Reaction, Pyrolysis of Acetaldehyde, Decomposition of Ethane 344
- Photochemical Reactions (Hydrogen-Bromine & Hydrogen-Chlorine Reactions).................. 352
- General Treatment of Chain Reactions (Ortho-Para Hydrogen Conversion and Hydrogen-Bromine Reactions) 358

- ❖ Apparent Activation Energy of Chain Reactions 362
- ❖ Chain Length 364
- ❖ Rice-Herzfeld Mechanism of Organic Molecules Decomposition (Acetaldehyde) 366
- ❖ Branching Chain Reactions and Explosions (H_2-O_2 Reaction) 368
- ❖ Kinetics of (One Intermediate) Enzymatic Reaction: Michaelis-Menten Treatment 371
- ❖ Evaluation of Michaelis's Constant for Enzyme-Substrate Binding by Lineweaver-Burk Plot and Eadie-Hofstee Methods 375
- ❖ Competitive and Non-Competitive Inhibition 378
- ❖ Problems 388
- ❖ Bibliography 389

CHAPTER 8 390

Electrochemistry – II: Ion Transport in Solutions 390

- ❖ Ionic Movement Under the Influence of an Electric Field 390
- ❖ Mobility of Ions 393
- ❖ Ionic Drift Velocity and Its Relation with Current Density 394
- ❖ Einstein Relation Between the Absolute Mobility and Diffusion Coefficient 398
- ❖ The Stokes-Einstein Relation 401
- ❖ The Nernst-Einstein Equation 403
- ❖ Walden’s Rule 404
- ❖ The Rate-Process Approach to Ionic Migration 406
- ❖ The Rate-Process Equation for Equivalent Conductivity 410
- ❖ Total Driving Force for Ionic Transport: Nernst-Planck Flux Equation 412
- ❖ Ionic Drift and Diffusion Potential 416
- ❖ The Onsager Phenomenological Equations 418
- ❖ The Basic Equation for the Diffusion 419
- ❖ Planck-Henderson Equation for the Diffusion Potential 422
- ❖ Problems 425
- ❖ Bibliography 426

INDEX 427

Mandeep Dalal
(M.Sc, Ph.D, CSIR UGC - NET JRF, IIT - GATE)
Founder & Director, Dalal Institute
Contact No: +91-9802825820
Homepage: www.mandeepdalal.com
E-Mail: dr.mandeep.dalal@gmail.com

Mandeep Dalal is an Indian research scholar who is primarily working in the field of Science and Philosophy. He received his Ph.D in Chemistry from Maharshi Dayanand University, Rohtak, in 2018. He is also the Founder and Director of "Dalal Institute", an India-based educational organization which is trying to revolutionize the mode of higher education in Chemistry across the globe. He has published more than 40 research papers in various international scientific journals, including mostly from Elsevier (USA), IOP (UK) and Springer (Netherlands) .

Other Books by the Author

A TEXTBOOK OF INORGANIC CHEMISTRY - VOLUME I, II, III, IV

A TEXTBOOK OF PHYSICAL CHEMISTRY - VOLUME I, II, III, IV

A TEXTBOOK OF ORGANIC CHEMISTRY - VOLUME I, II, III, IV

ISBN: 978-81-938720-1-7
9 788193 872017 >
MRP: Rs 800.00

DALAL INSTITUTE
Main Market, Sector-14, Rohtak, Haryana-124001
(+91-9802825820, info@dalalinstitute.com)
www.dalalinstitute.com