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校內分機：2792

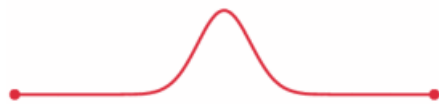
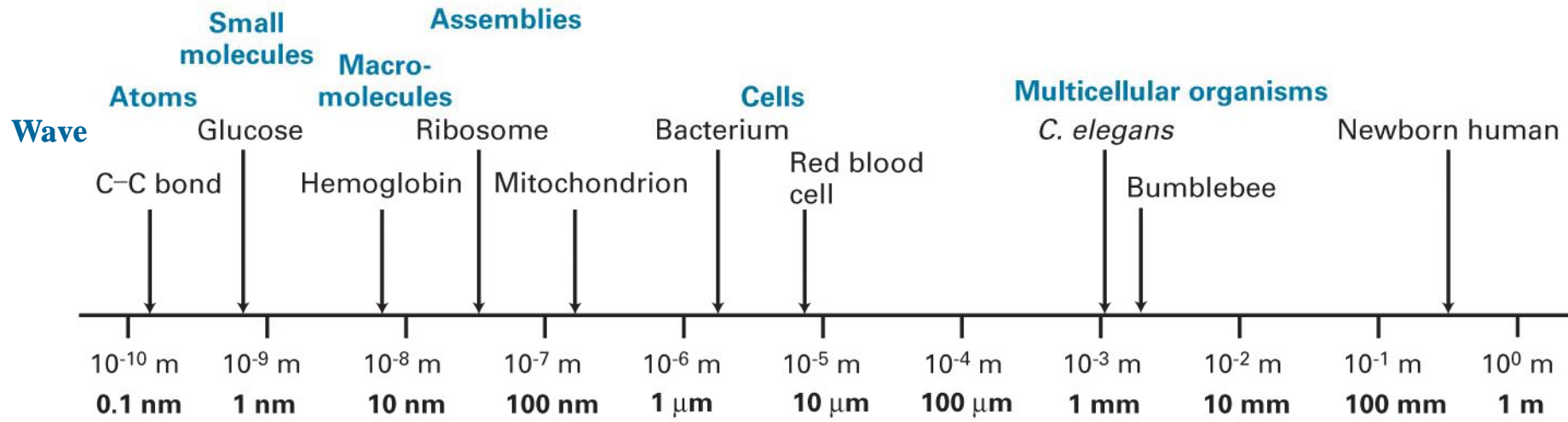
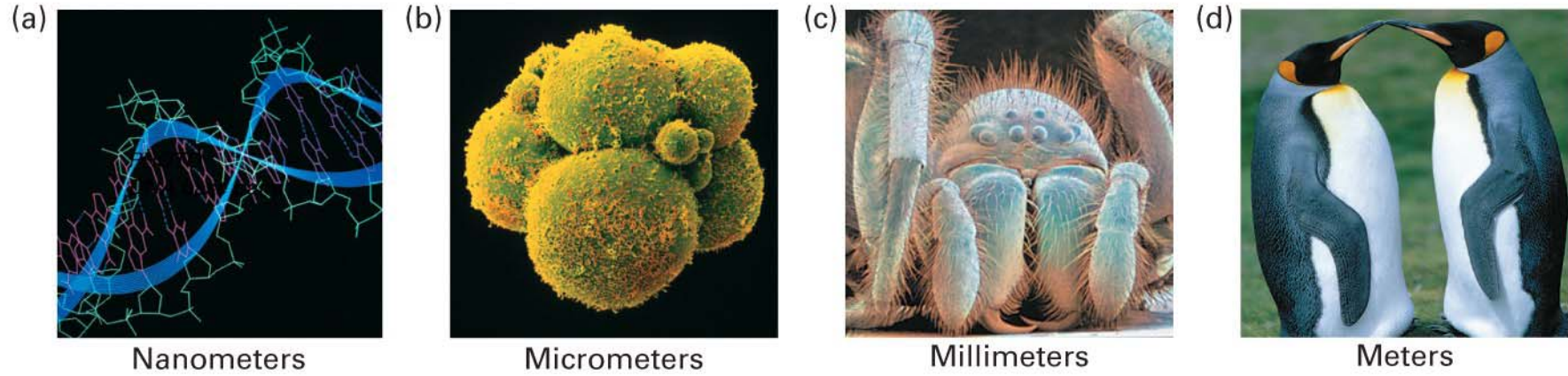
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Y. T. Lin's Presentation

Reference Books

- Physical Chemistry for the Life Sciences
(Engel, Drobny and Reid)
- Biophysical Chemistry
(James P. Allen)

Y. J. Lin's Presentation



Y. J. Lin's Presentation

生物
化學
物理



空間尺度越來越小



物質

力

表面上是粒子，
實際上是波動。

表面上是粒子。

波

能量描述

目的：反推回去
瞭解生物現象



物質

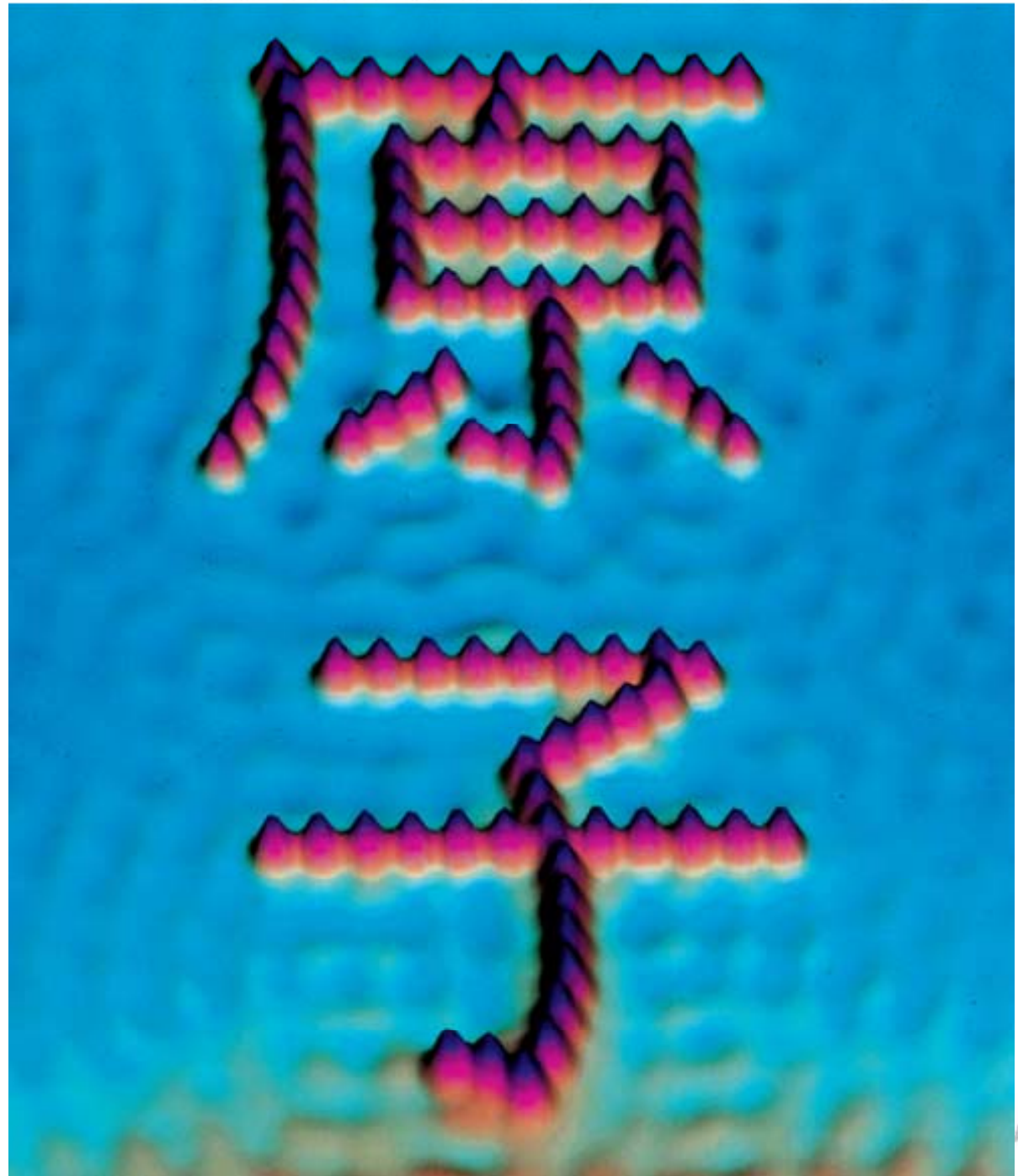
把物質切到最小，我們知道：
它表面上是粒子，實際上是波動。

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Lecture

Quantum Chemistry (I)

表面上是粒子

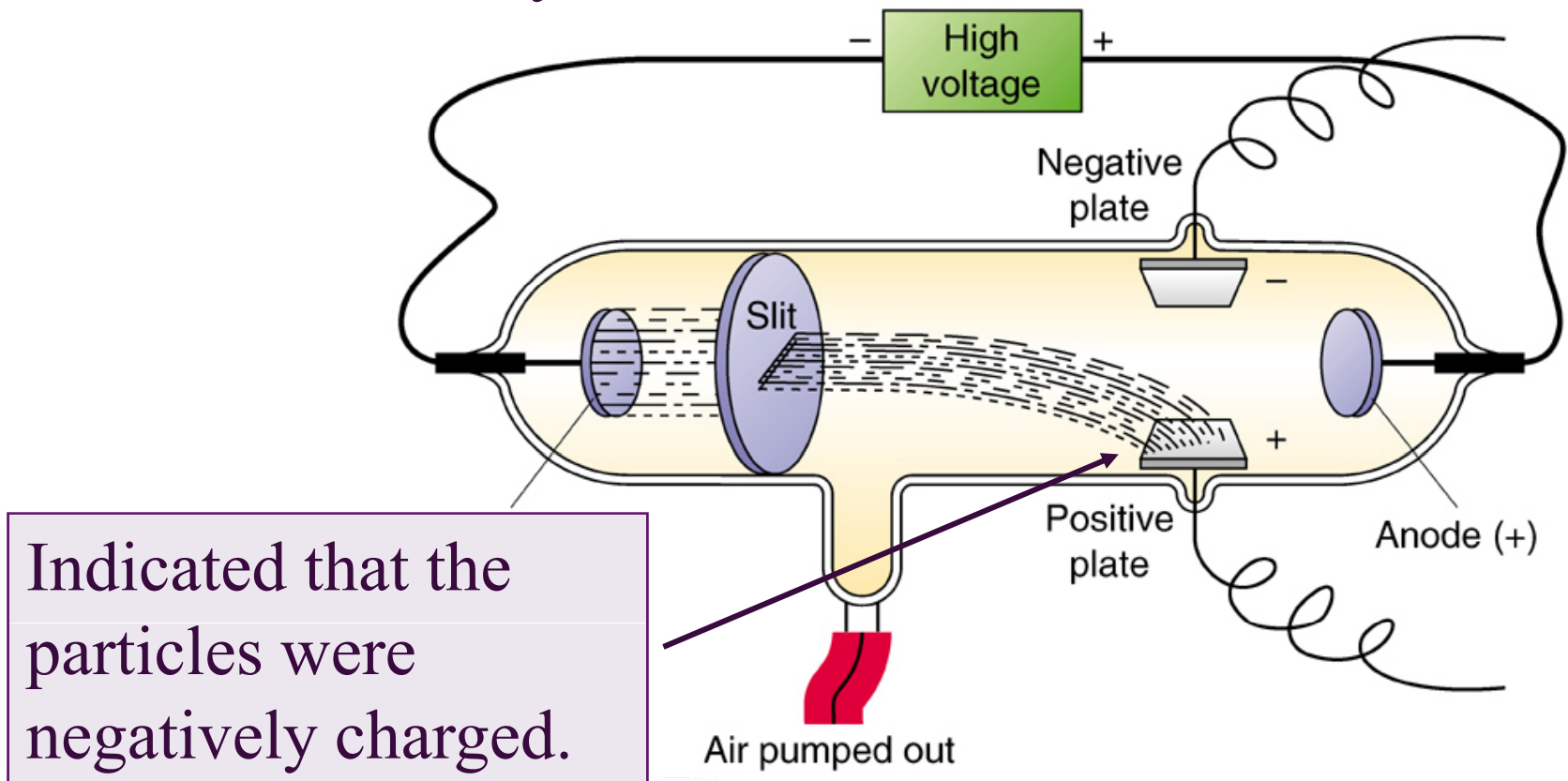


表面上是粒子

Subatomic Particles: Electrons, Protons, and Neutrons

- Electrons were the first subatomic particles to be discovered using the cathode ray tube.

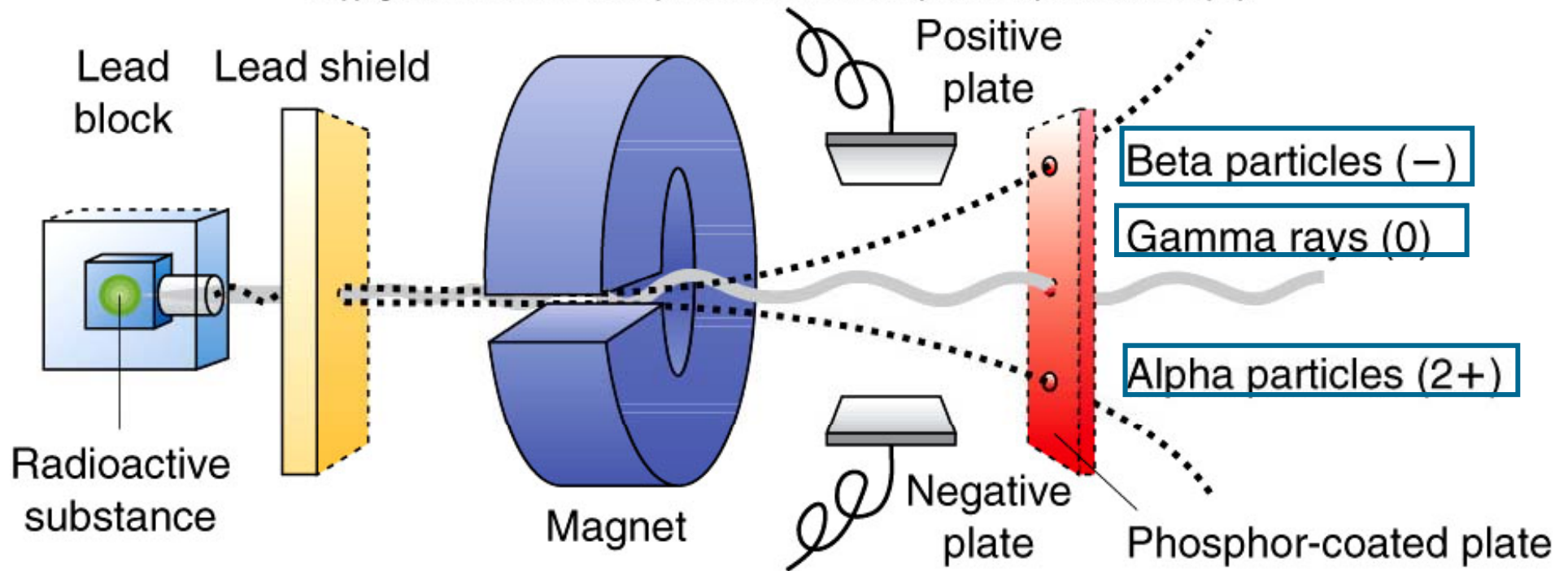
4



表面上是粒子

Radioactive Emissions

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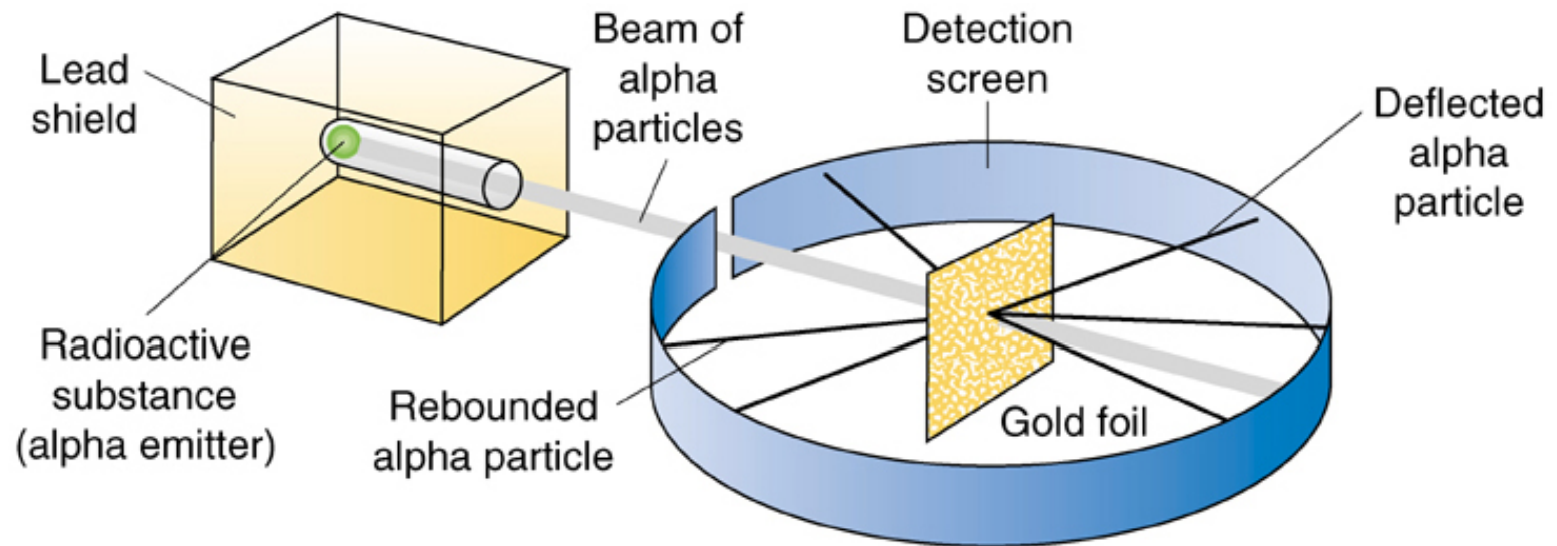


The direction taken by the radioactive emissions indicates the presence of 3 types of emissions

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表面上是粒子

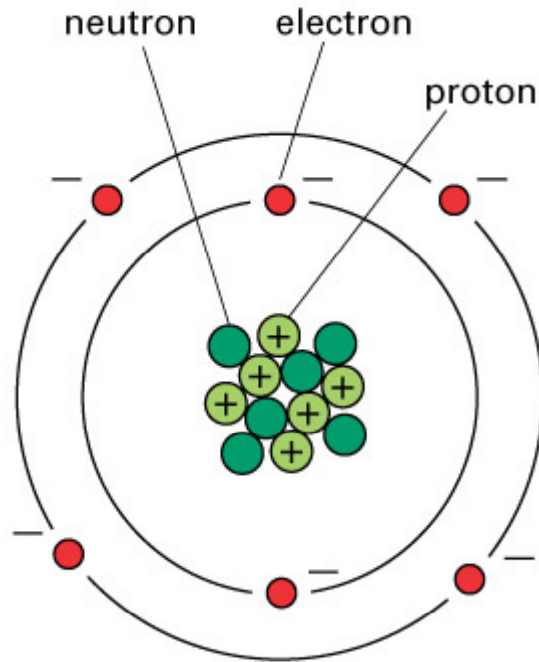
Rutherford's Gold Foil Experiment



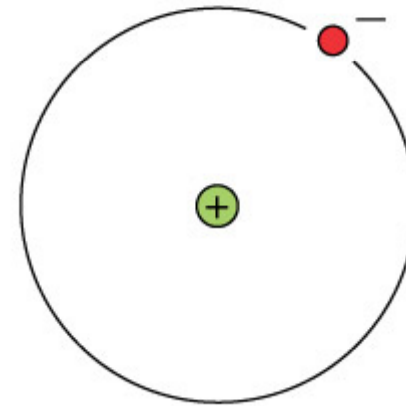
- Most of the atom is empty space
- The majority of the mass is located in a small, dense region

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表面上是粒子



carbon atom
atomic number = 6



hydrogen atom
atomic number = 1

Figure 2-2 Essential Cell Biology, 2/e. (© 2004 Garland Science)

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TABLE 2.1

Selected Properties of the Three Basic Subatomic Particles

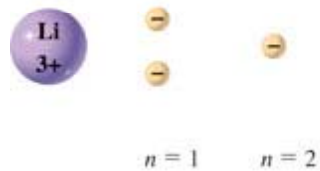
Name	Charge	Mass (amu)	Mass (grams)
Electron (e)	-1	5.4×10^{-4}	9.1095×10^{-28}
Proton (p)	+1	1.00	1.6725×10^{-24}
Neutron (n)	0	1.00	1.6750×10^{-24}

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Electron Arrangement by Energy Level

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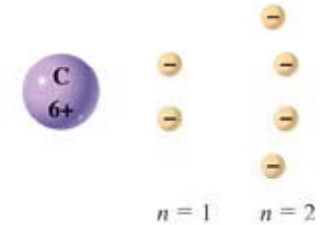
Lithium: Three-electron atom, one valence electron



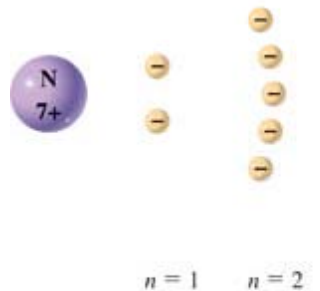
Beryllium: Four-electron atom, two valence electrons



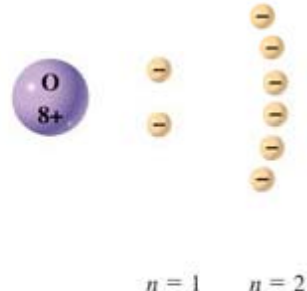
Boron: Five-electron atom, three valence electrons



Carbon: Six-electron atom, four valence electrons



Nitrogen: Seven-electron atom, five valence electrons

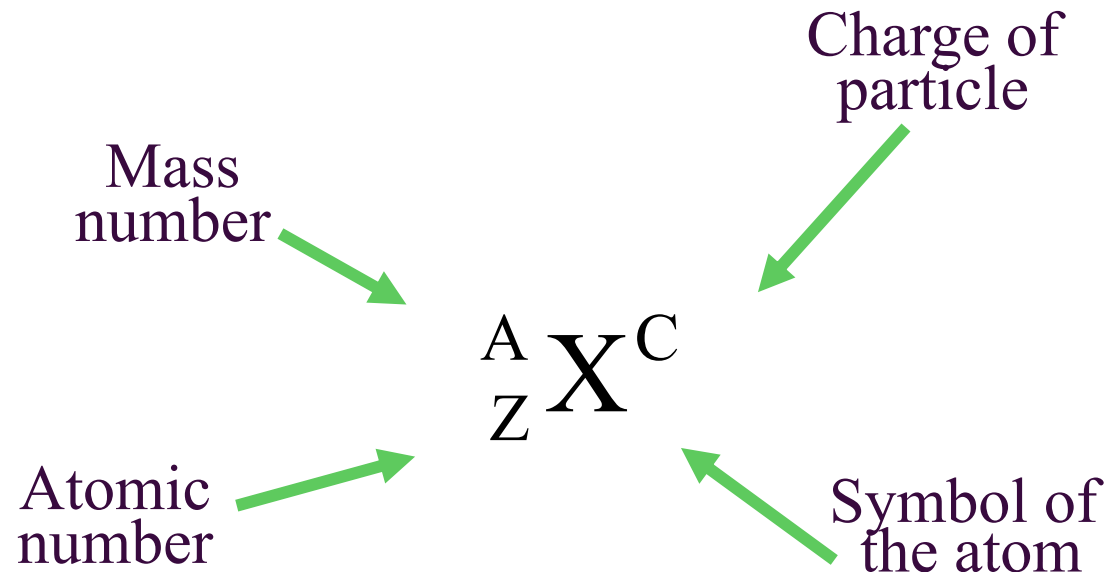


Oxygen: Eight-electron atom, six valence electrons

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Symbolic Representation of an Element

表面上是粒子的組合



- **Atomic number** (Z) - the number of protons in the atom
- **Mass number** (A) - sum of the number of protons and neutrons

表面上是粒子的組合

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REPRESENTATIVE ELEMENTS		TRANSITION ELEMENTS										REPRESENTATIVE ELEMENTS						
1A (1)												3A (13) 4A (14) 5A (15) 6A (16) 7A (17)					8A (18)	
1	1 H 1.008											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18	
2	3 Li 6.941	4 Be 9.012											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
3	11 Na 22.99	12 Mg 24.31	3B (3)	4B (4)	5B (5)	6B (6)	7B (7)	8B (8) (9) (10)			1B (11)	2B (12)	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	57 La 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.9	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (263)	105 Db (262)	106 Sg (266)	107 Bh (267)	108 Hs (277)	109 Mt (268)	110 Ds (281)	111 Rg (272)	112 Cn (285)		114 Fl (289)		116 Lv (292)		

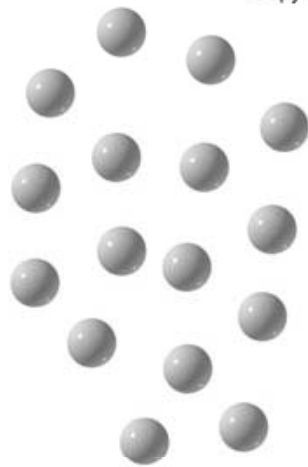
INNER TRANSITION ELEMENTS															
6	Lanthanides	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
7	Actinides	90 Th 232.0	91 Pa (231)	92 U 238.0	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

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表面上是粒子的組合

- **Dalton's Atomic Theory** - the first experimentally based theory of atomic structure of the atom

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Atoms of element X



Atoms of element Y



Compound formed from elements X and Y

(a)

(b)

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Important Biological Elements

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TABLE 2.3 Summary of the Most Important Elements in Biological Systems

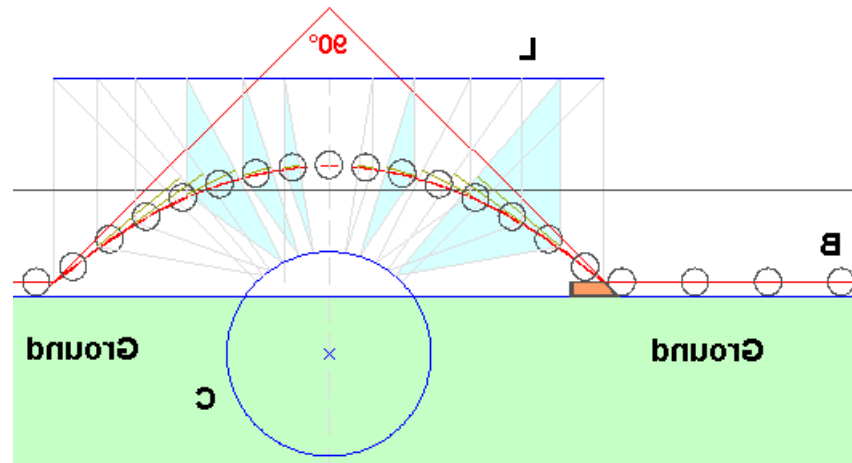
Element	Symbol	Significance
Hydrogen	H	Components of major biological molecules
Carbon	C	
Oxygen	O	
Nitrogen	N	
Phosphorus	P	
Sulfur	S	
Potassium	K	Produce electrolytes responsible for fluid balance and nerve transmission
Sodium	Na	
Chlorine	Cl	
Calcium	Ca	Bones, nerve function
Magnesium	Mg	
Zinc	Zn	Essential trace metals in human metabolism
Strontium	Sr	
Iron	Fe	
Copper	Cu	
Cobalt	Co	
Manganese	Mn	
Cadmium	Cd	"Heavy metals" toxic to living systems
Mercury	Hg	
Lead	Pb	

表面上是粒子的組合

tion

如何描述粒子？

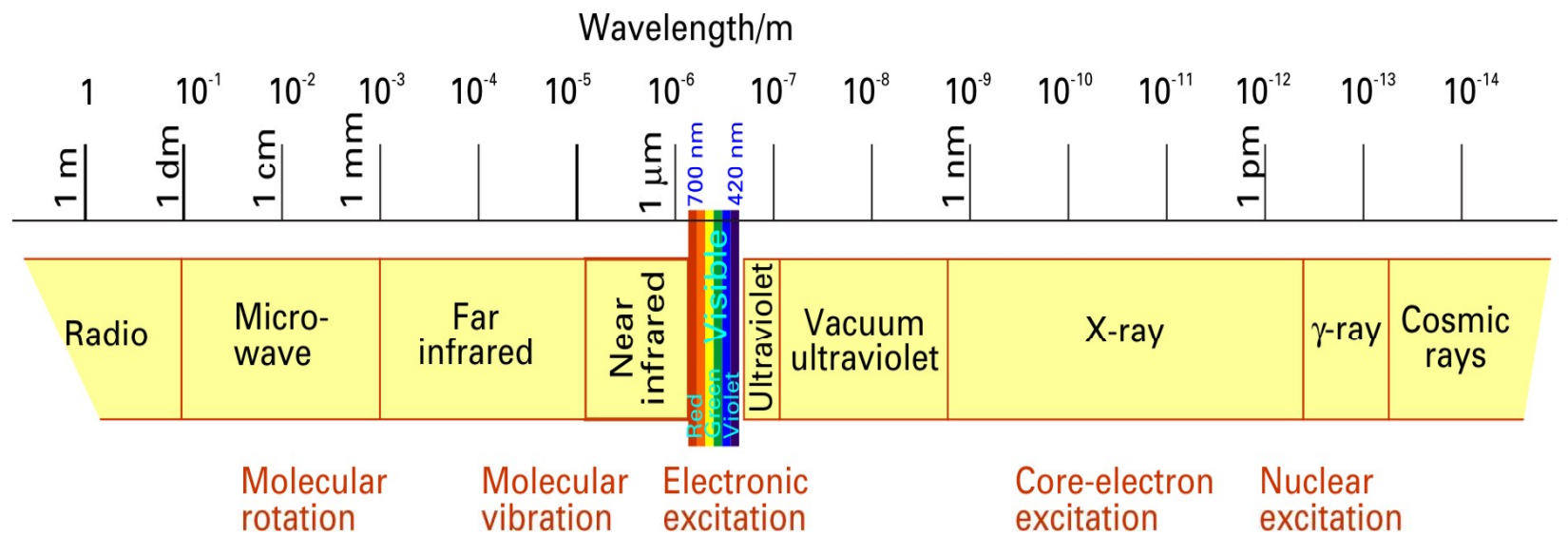
描述其動能及位能



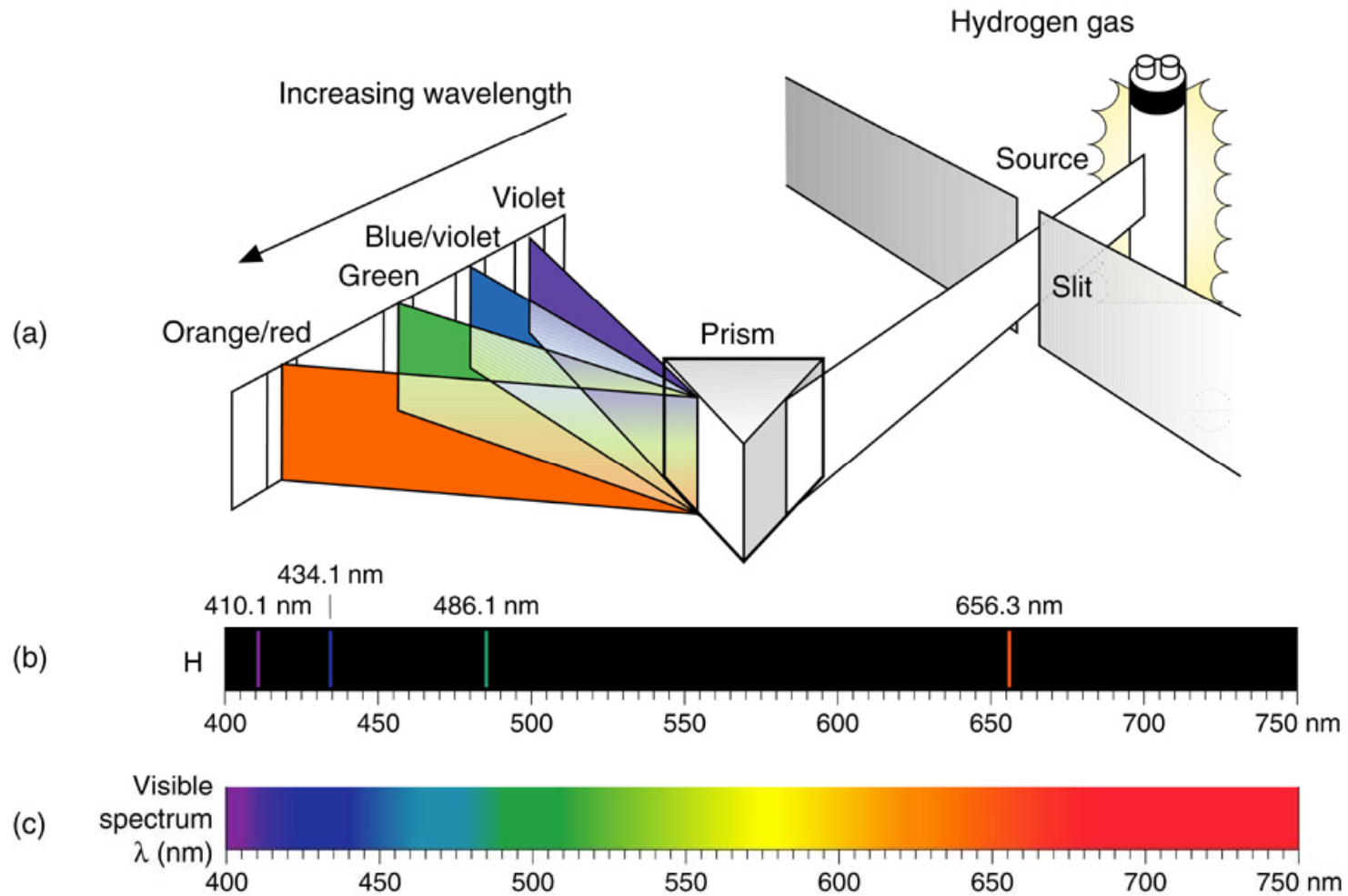
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光也是粒子

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The emission spectrum of hydrogen lead to the modern understanding of the electronic structure of the atom

重要區分

光的頻率 vs 光的亮度

光的頻率 = 單一光子的能量
光的亮度 = 所有光子的數量

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Electromagnetic Spectrum

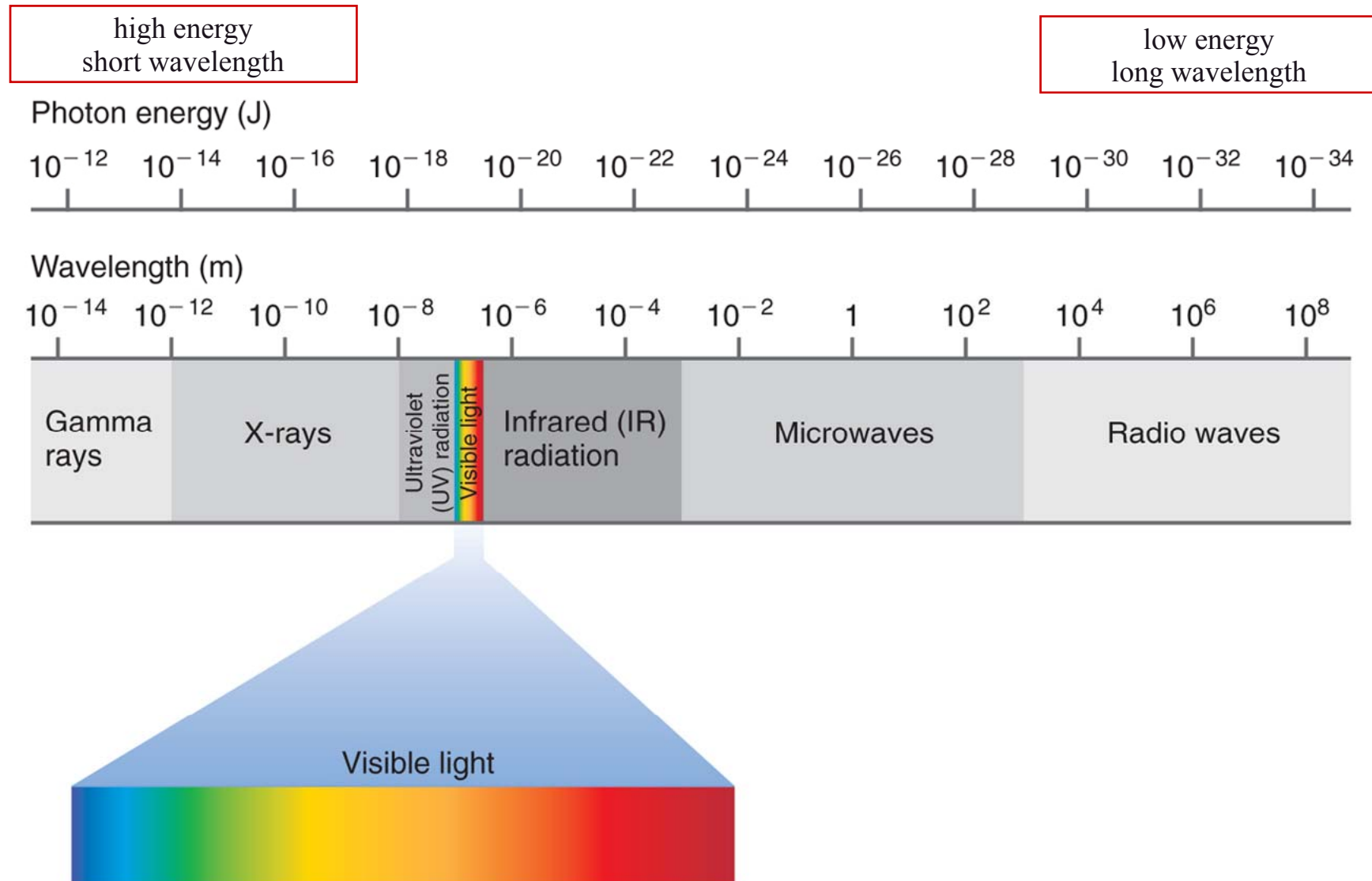
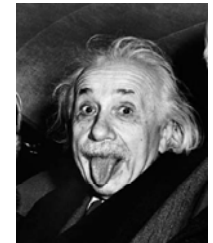
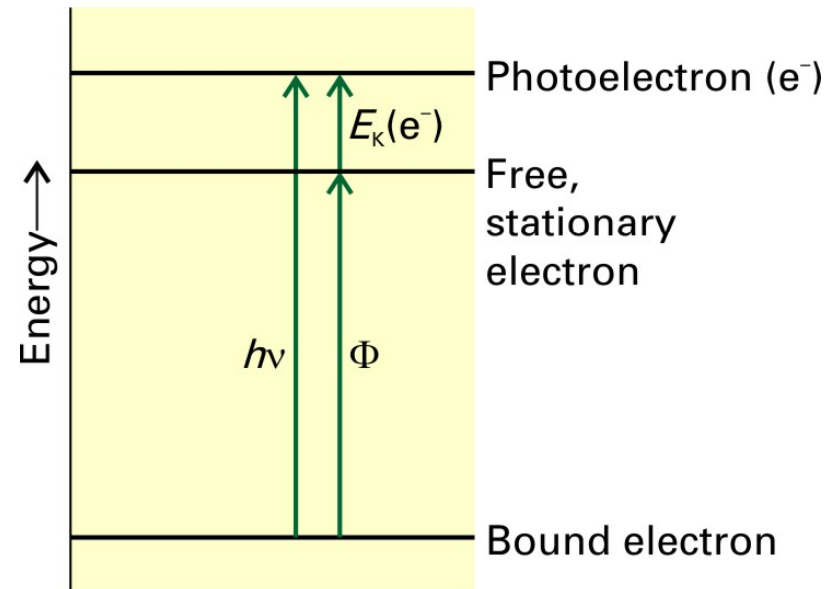
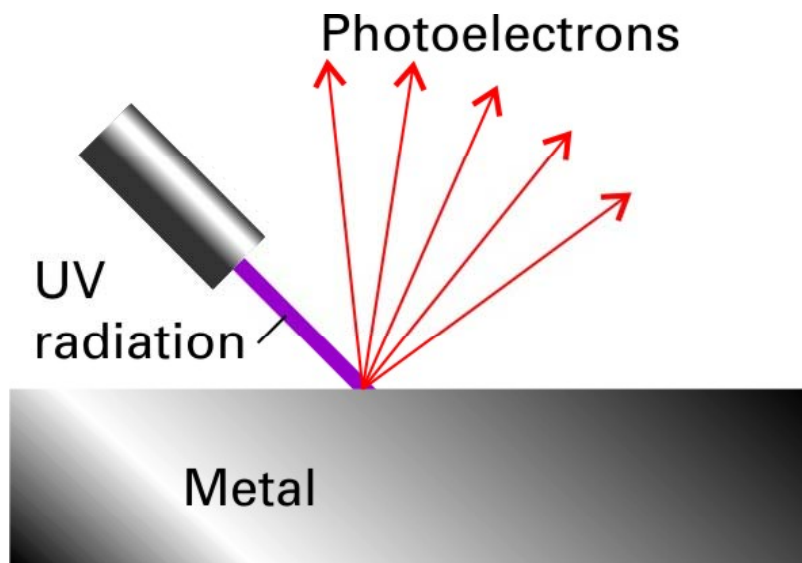


Figure: 18-01

One photon

$E = h\nu$ 光是光子。

h : plank's constant



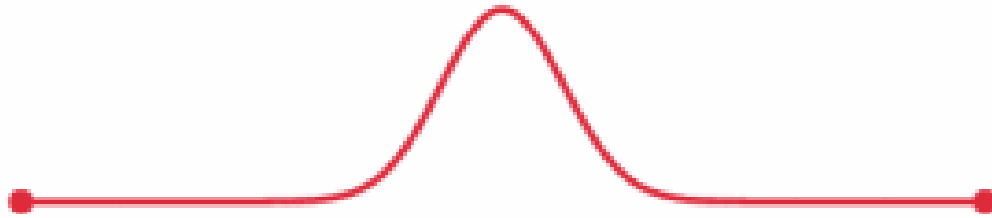
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把物質切到最小，我們知道：

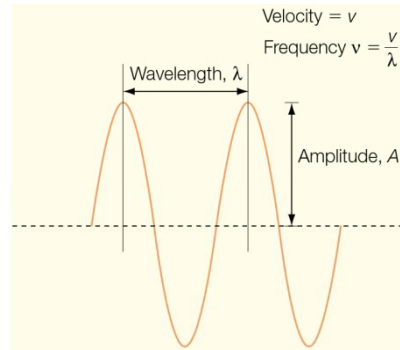
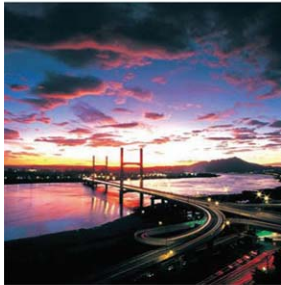
它表面上是粒子，實際上是？

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Wave



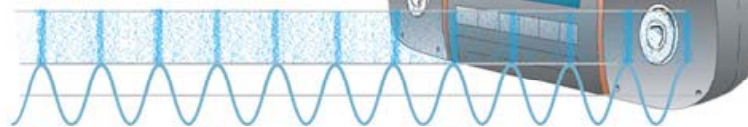
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波的特性



密部
 壓力



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波

有建設性干涉及破壞性干涉

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波 可以共振

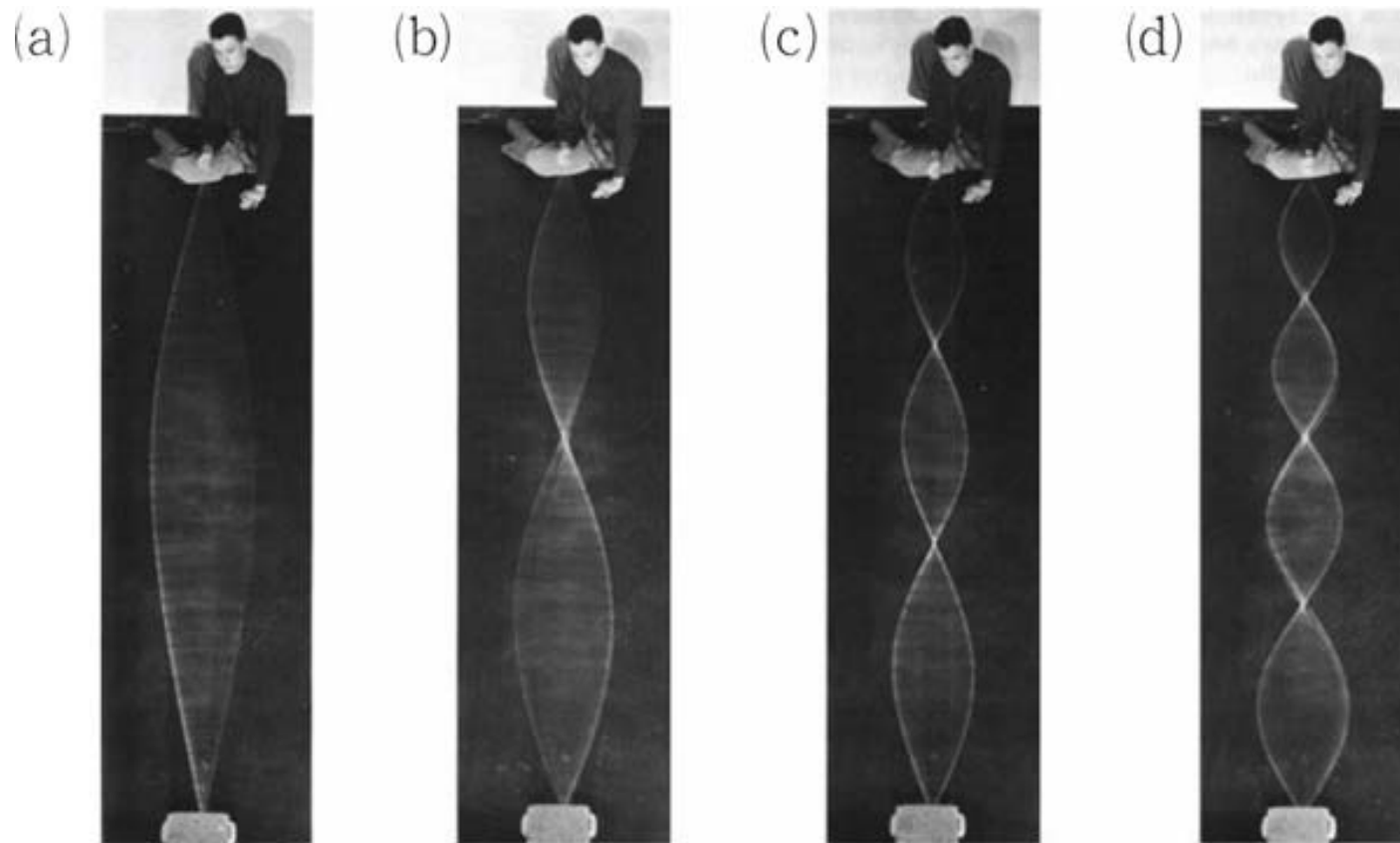
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波 可以相加減

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特定條件下，
波
形成駐波

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波 有波動方程式

描述波如何波動。

To describe how wave is waving.

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Wave equation

- Wind wave
- Airy wave theory
- Wave equation
- Acoustic wave equation
- Vibrations of a circular drum
- Standing wave
- Electromagnetic wave equation
- Schrödinger equation

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光子(Photon)也是波

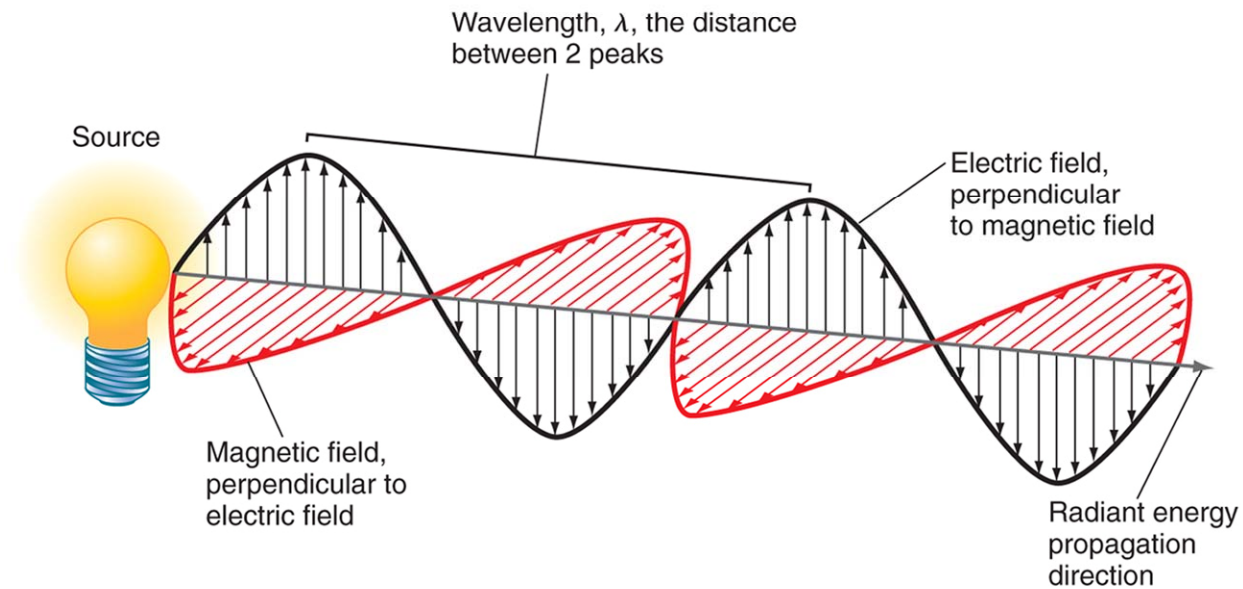


Figure: 18-02

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Tiny Particle Wave equation

- Wind wave
- Airy wave theory
- Wave equation
- Acoustic wave equation
- Vibrations of a circular drum
- Standing wave
- Electromagnetic wave equation
- **Schrödinger equation**

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Schrödinger equation



CORBIS-Bettmann

Figure 10.4 Erwin Schrödinger (1887–1961). Schrödinger proposed an expression of quantum mechanics that was different from but equivalent to Heisenberg's. His expression is useful because it expresses the behavior of electrons in terms of something we understand—waves. The Schrödinger equation is the central equation of quantum mechanics.

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The wave nature of the electrons

電子是波。

$$E = h\nu = mc^2$$

$$\lambda = c / \nu = h / mc = h / p$$

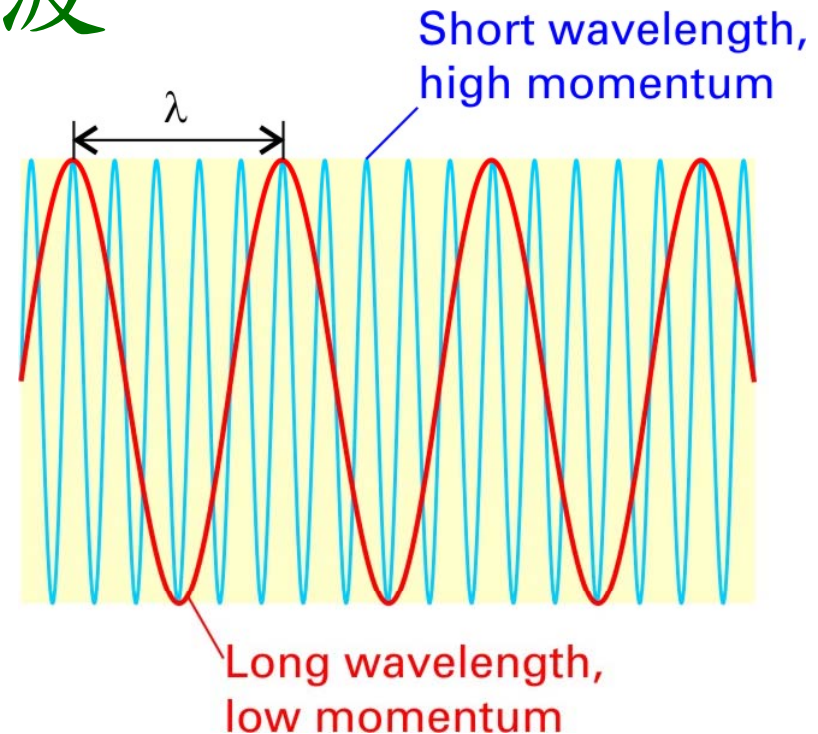
(de Broglie relation)

p : momentum

$$p = mv$$

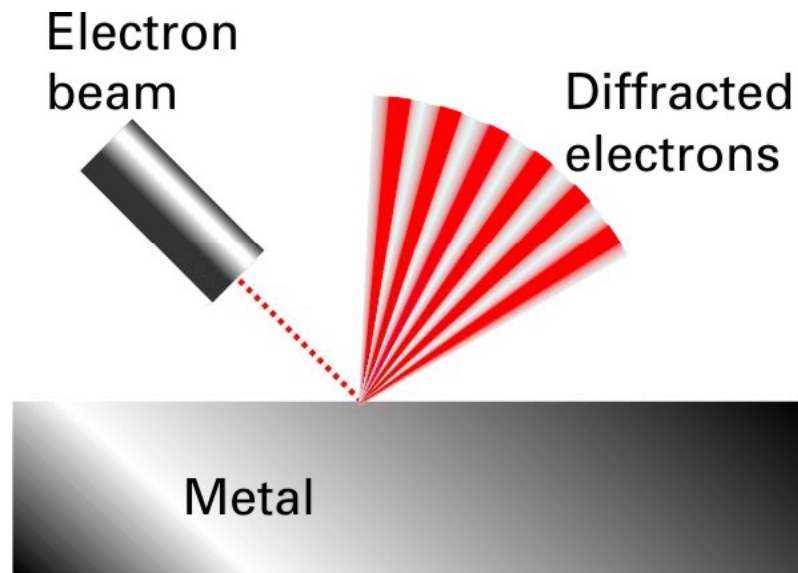
m : mass

v : velocity



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Davisson and Germer



電子是波。

$$\lambda = h / p$$

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Schrödinger equation

$$\underbrace{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}}_{\text{Kinetic energy}} + \underbrace{V\psi}_{\text{Potential energy}} = \underbrace{E\psi}_{\text{Total energy}}$$

$$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34} \text{ Js}$$

Quantum Chemistry 的七個法則

→ 用來形成 Schrödinger equation

(也就是可用來描述電子的波動方程式)

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Quantum Mechanics 的七個法則

Table 10.2 The postulates of quantum mechanics

Postulate I. The state of a system of particles is given by a wavefunction Ψ , which is a function of the coordinates of the particles and the time. Ψ contains all information that can be determined about the state of the system. Ψ must be single-valued, continuous, and bounded, and $|\Psi|^2$ must be integrable. (Discussed in section 10.2)

Postulate II. For every physical observable or variable O , there exists a corresponding Hermitian operator \hat{O} . Operators are constructed by writing their classical expressions in terms of position and (linear) momentum, then replacing “ x times” (that is, $x \cdot$) for each x variable and $-i\hbar(\partial/\partial x)$ for each p_x variable in the expression. Similar substitutions must be made for y and z coordinates and momenta. (Section 10.3)

Postulate III. The only values of observables that can be obtained in a single measurement are the eigenvalues of the eigenvalue equation constructed from the corresponding operator and the wavefunction Ψ :

$$\hat{O}\Psi = K \cdot \Psi$$

where K is a constant. (Section 10.3)

Postulate IV. Wavefunctions must satisfy the time-dependent Schrödinger equation:

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

(Section 10.14) (If it is assumed that Ψ is separable into functions of time and position, we find that this expression can be rewritten to get the time-independent Schrödinger equation, $\hat{H}\Psi = E\Psi$.) (section 10.7)

Postulate V. The average value of an observable, $\langle O \rangle$, is given by the expression

$$\langle O \rangle = \int_{\text{all space}} \Psi^* \hat{O} \Psi \, d\tau$$

for normalized wavefunctions. (Section 10.9)

Postulate VI. The set of eigenfunctions for any quantum mechanical operator is a complete mathematical set of functions.

Postulate VII. If, for a given system, the wavefunction Ψ is a linear combination of nondegenerate wavefunctions Ψ_n which have eigenvalues a_n :

$$\Psi = \sum_n c_n \Psi_n \quad \text{and} \quad \hat{A}\Psi_n = a_n \Psi_n$$

then the probability that a_n will be the value of the corresponding measurement is $|c_n|^2$. The construction of Ψ as the combination of all possible Ψ_n 's is called the *superposition principle*.

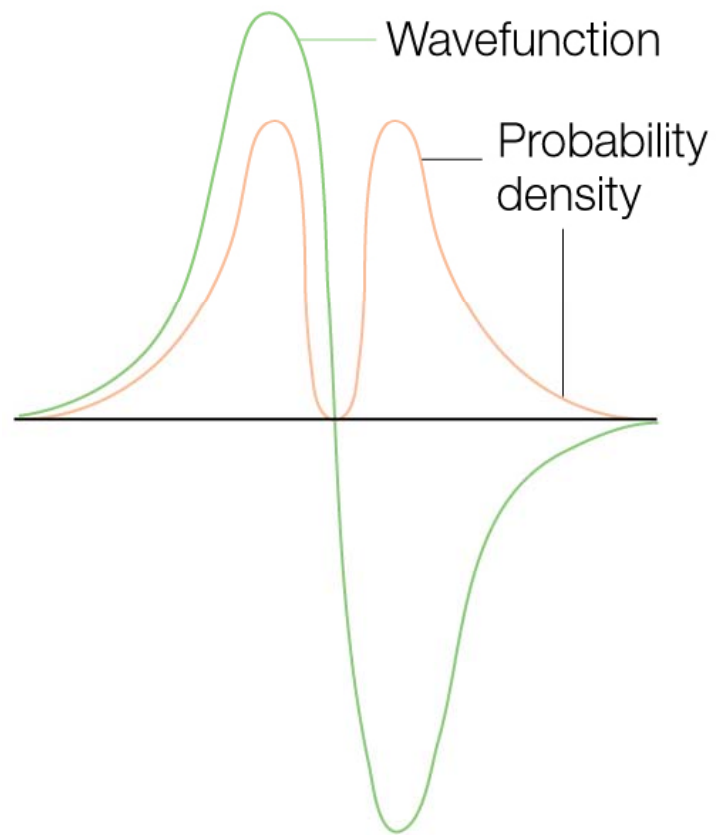
Table 10.1 Operators for various observables and their classical counterparts^a

Observable	Operator	Classical counterpart
Position	$\hat{x} = x \cdot$ And so forth for coordinates other than x	x
Momentum (linear)	$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ And so forth for coordinates other than x	$p_x = mv_x$
Momentum (angular)	$\hat{L}_x = -i\hbar \left(\hat{y} \frac{\partial}{\partial z} - \hat{z} \frac{\partial}{\partial y} \right)$	$L_x = yp_z - zp_y$
Kinetic energy, 1-D ^b	$\hat{K} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$	$K = \frac{1}{2}mv_x^2 = \frac{p_x^2}{2m}$
Kinetic energy, 3-D ^b	$\hat{K} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$	$K = \frac{1}{2}m(v_x^2 + v_y^2 + v_z^2)$ $= \frac{p_x^2 + p_y^2 + p_z^2}{2m}$
Potential energy:		
Harmonic oscillator	$\hat{V} = \frac{1}{2}kx^2 \cdot$	$V = \frac{1}{2}kx^2$
Coulombic	$\hat{V} = \frac{q_1 \cdot q_2}{4\pi\epsilon_0 r}$	$V = \frac{q_1 \cdot q_2}{4\pi\epsilon_0 r}$
Total energy	$\hat{H} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \hat{V}$	$H = \frac{p^2}{2m} + V$

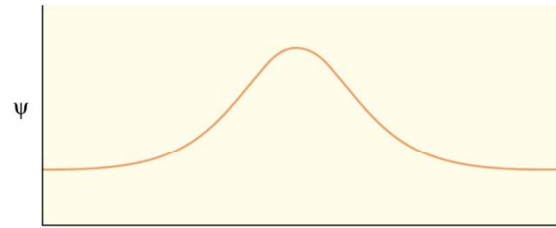
^aOperators expressed in x , y , and/or z are Cartesian operators; operators expressed in r , θ , and/or ϕ are spherical polar operators.

^bThe kinetic energy operator is also symbolized by \hat{T} .

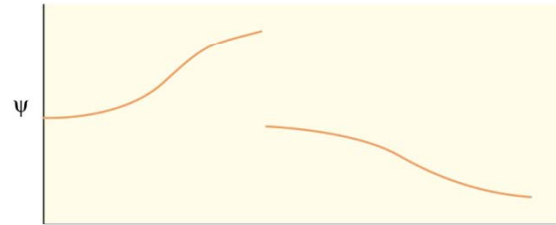
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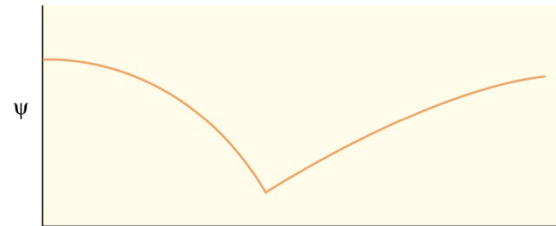
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Allowed



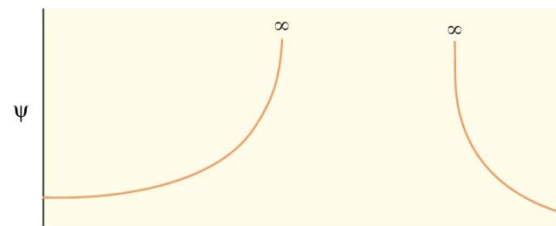
Not allowed
Discontinuous



Not allowed
Derivative
Not continuous



Not allowed
Multiple values



Not allowed
Infinite

x

ε Presentation

物理



物質

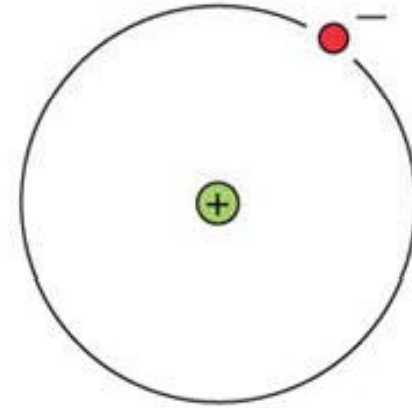
表面上是粒子，
實際上是波動。

波

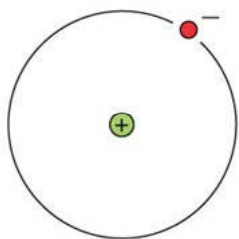
力

表面上是粒子。

能量描述



- 受到作用力
- 位能



Schrödinger equation for hydrogen atom

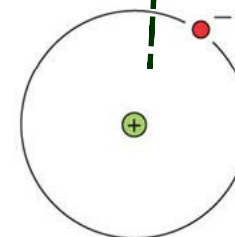
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

E

ψ

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Name	Charge	Mass (amu)	Mass (grams)
Electron (e)	-1	5.4×10^{-4}	9.1095×10^{-28}
Proton (p)	+1	1.00	1.6725×10^{-24}
Neutron (n)	0	1.00	1.6750×10^{-24}

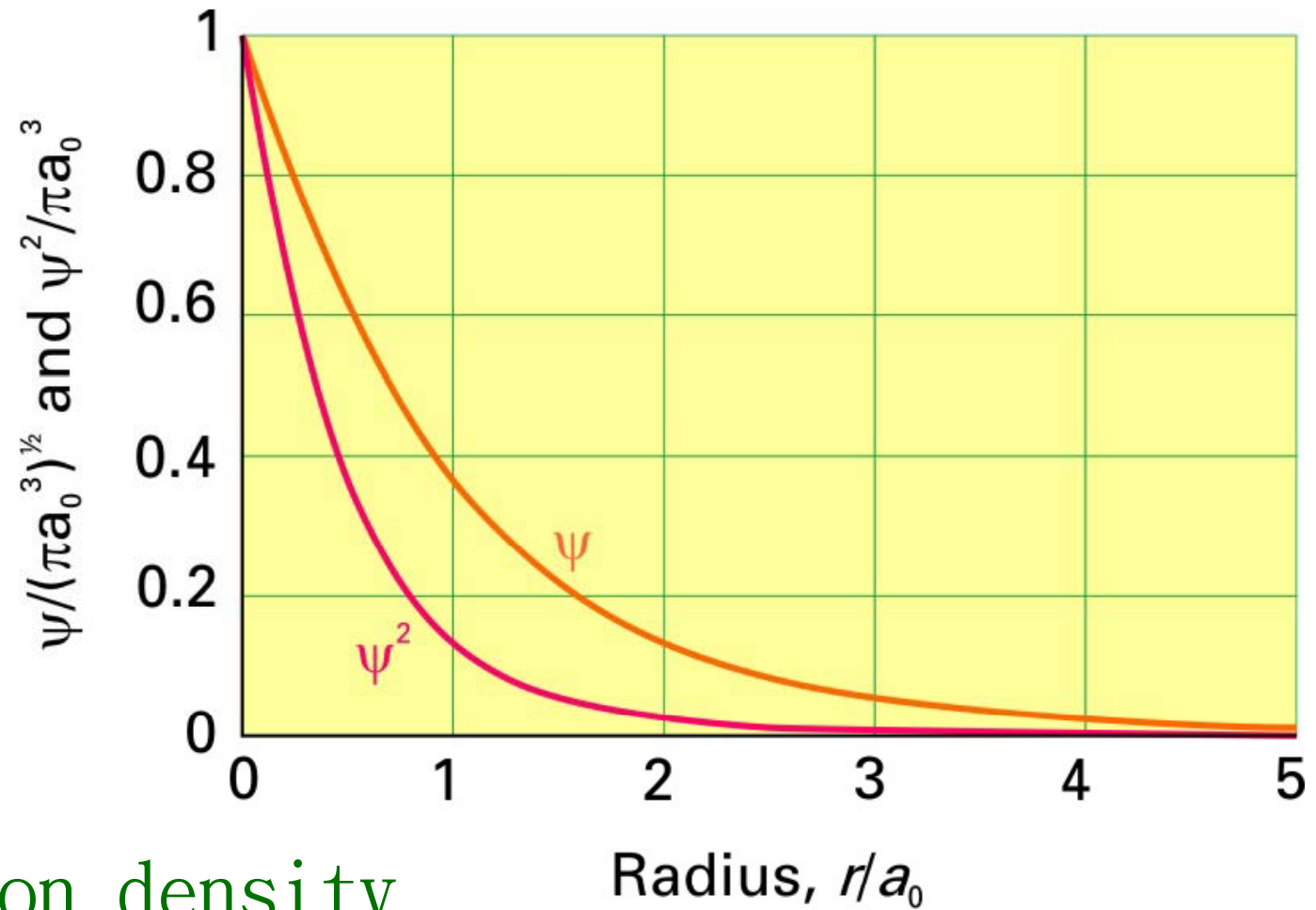


Solution of Schrödinger equation for hydrogen atom

- n, l, m_l
 $n = 1, 2, 3, \dots$
 $l = 0, 1, 2, 3, \dots, n-1$
 $m_l = 0, \pm 1, \pm 2, \pm 3, \dots, \pm l$
- E_n
- Ψ_{n,l,m_l}

The shapes of atomic orbitals

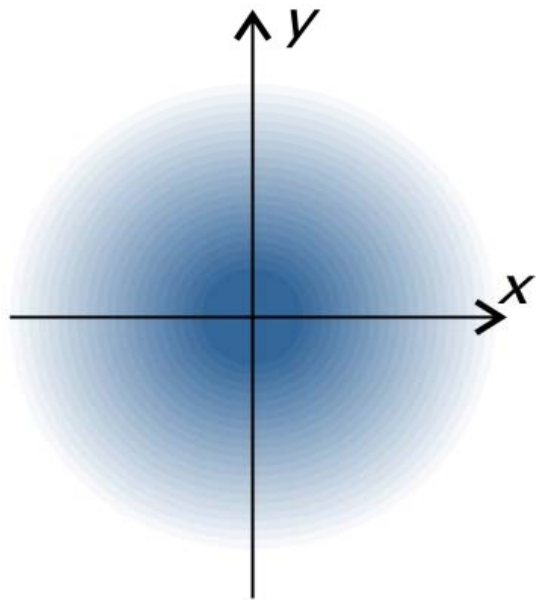
1s



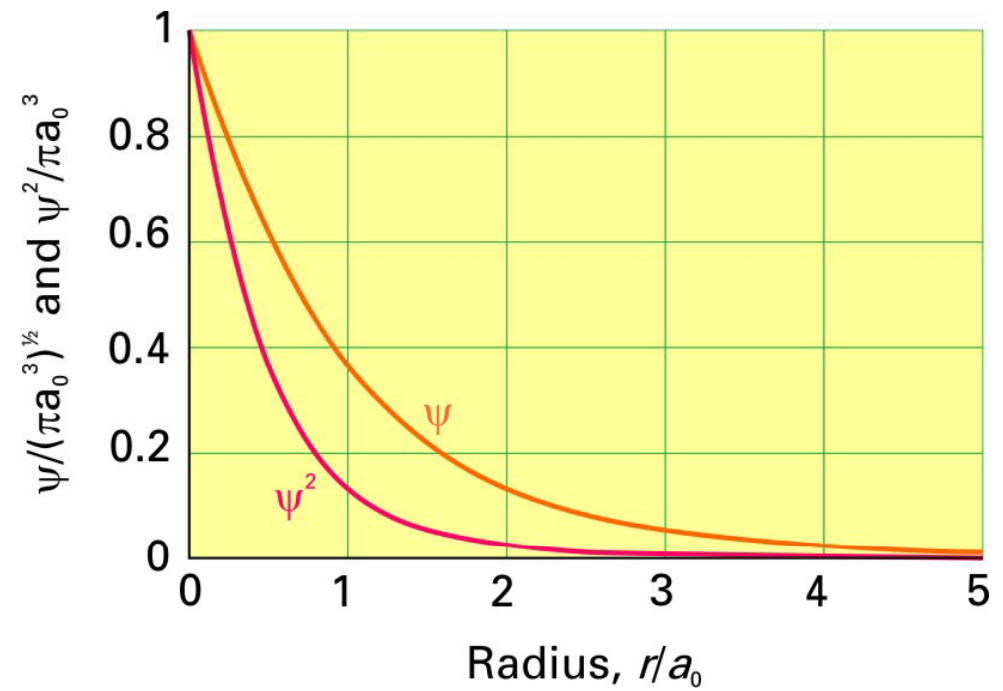
ψ^2 : electron density

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1s

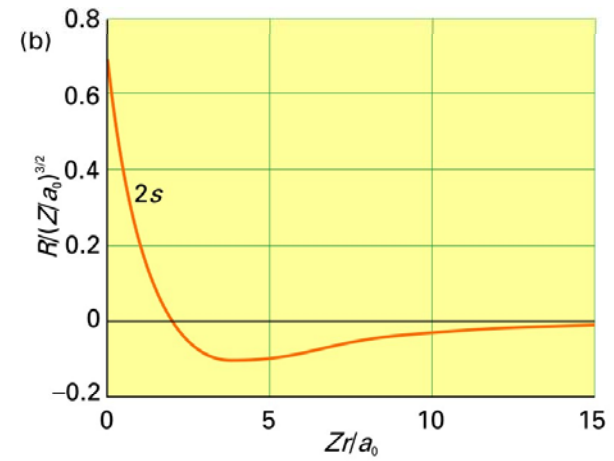
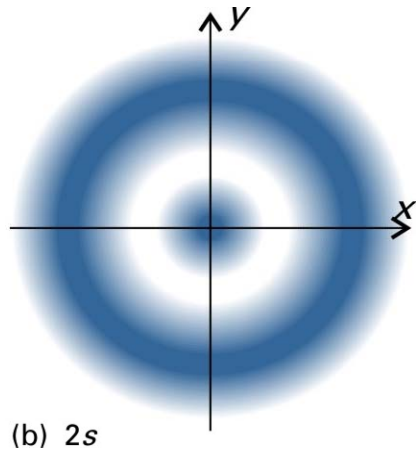


(a) 1s



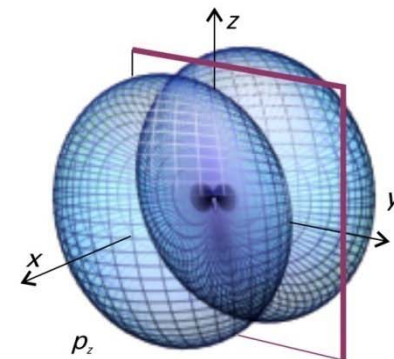
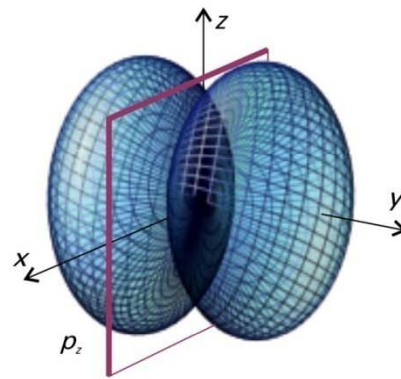
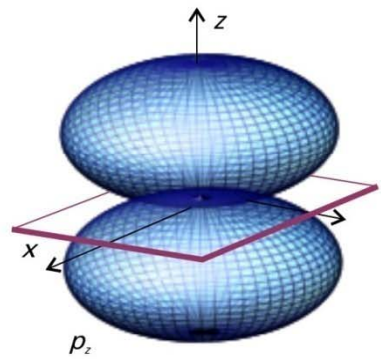
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2s



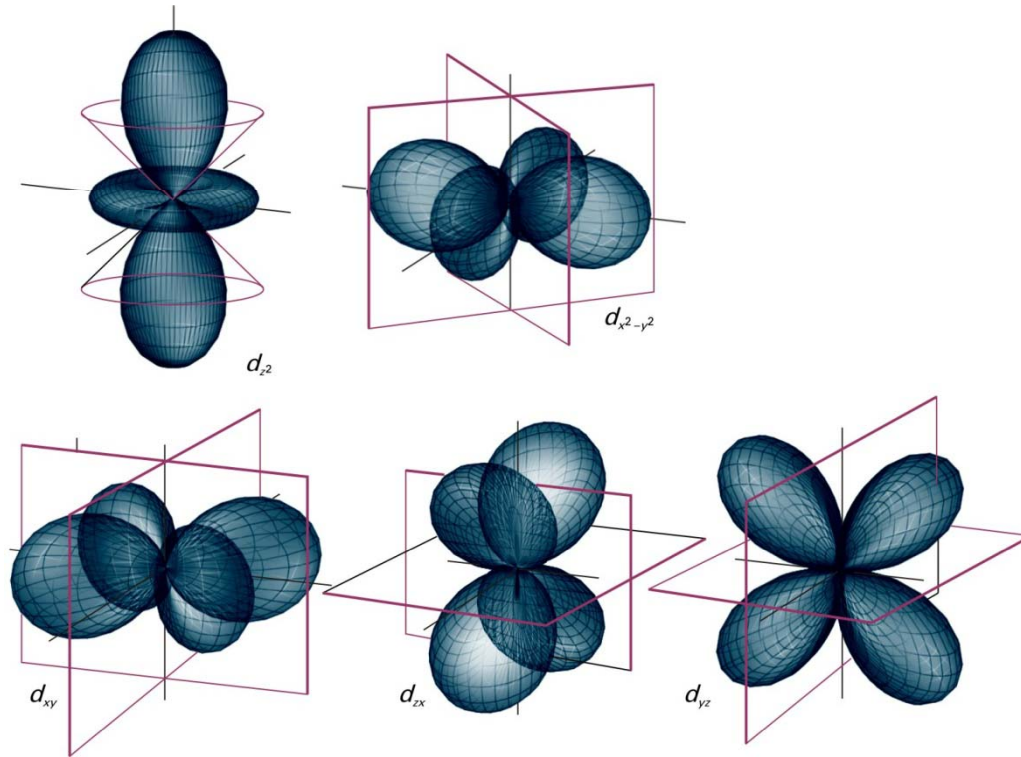
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2p



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3d



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REPRESENTATIVE ELEMENTS

Metals (main-group)
Metals (transition)
Metals (inner transition)
Metalloids
Nonmetals

REPRESENTATIVE ELEMENTS

Period	1	1A (1)	TRANSITION ELEMENTS										REPRESENTATIVE ELEMENTS					8A (18)	
	1	1											2					2	
		H 1.008											He 4.003						
	2	3	4											5	6	7	8	9	10
		Li 6.941	Be 9.012											B 10.81	C 12.01	N 14.01	O 16.00	F 19.00	Ne 20.18
	3	11							12	13	14	15	16	17	18				
		Na 22.99							Mg 24.31	Al 26.98	Si 28.09	P 30.97	S 32.07	Cl 35.45	Ar 39.95				
4	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	
	K 39.10	Ca 40.08	Sc 44.96	Ti 47.88	V 50.94	Cr 52.00	Mn 54.94	Fe 55.85	Cobalt (58.93)	Ni 58.71	Cu 63.55	Zn 65.39	Ga 69.72	Ge 72.61	As 74.92	Se 78.96	Br 79.90	Kr 83.80	
5	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	
	Rb 85.47	Sr 87.62	Y 88.91	Zr 91.22	Nb 92.91	Mo 95.94	Tc (98)	Ru 101.1	Rh 102.9	Pd 106.4	Ag 107.9	Cd 112.4	In 114.8	Sn 118.7	Sb 121.8	Te 127.6	I 126.9	Xe 131.3	
6	55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	
	Cs 132.9	Ba 137.3	La 138.9	Hf 178.5	Ta 180.9	W 183.9	Re 186.2	Os 190.2	Ir 192.2	Pt 195.1	Au 197.0	Hg 200.6	Tl 204.4	Pb 207.2	Bi 209.0	Po (209)	At (210)	Rn (222)	
7	87	88	89	104	105	106	107	108	109	110	111	112		114		116			
	Fr (223)	Ra (226)	Ac (227)	Rf (263)	Db (262)	Sg (266)	Bh (267)	Hs (277)	Mt (268)	Ds (281)	Rg (272)	(285)		(289)		(292)			

$n = 1, 2(1)^2 = 2$

$n = 2, 2(2)^2 = 8$

$n = 3, 2(3)^2 = 18$

$n = 4, 2(4)^2 = 32$

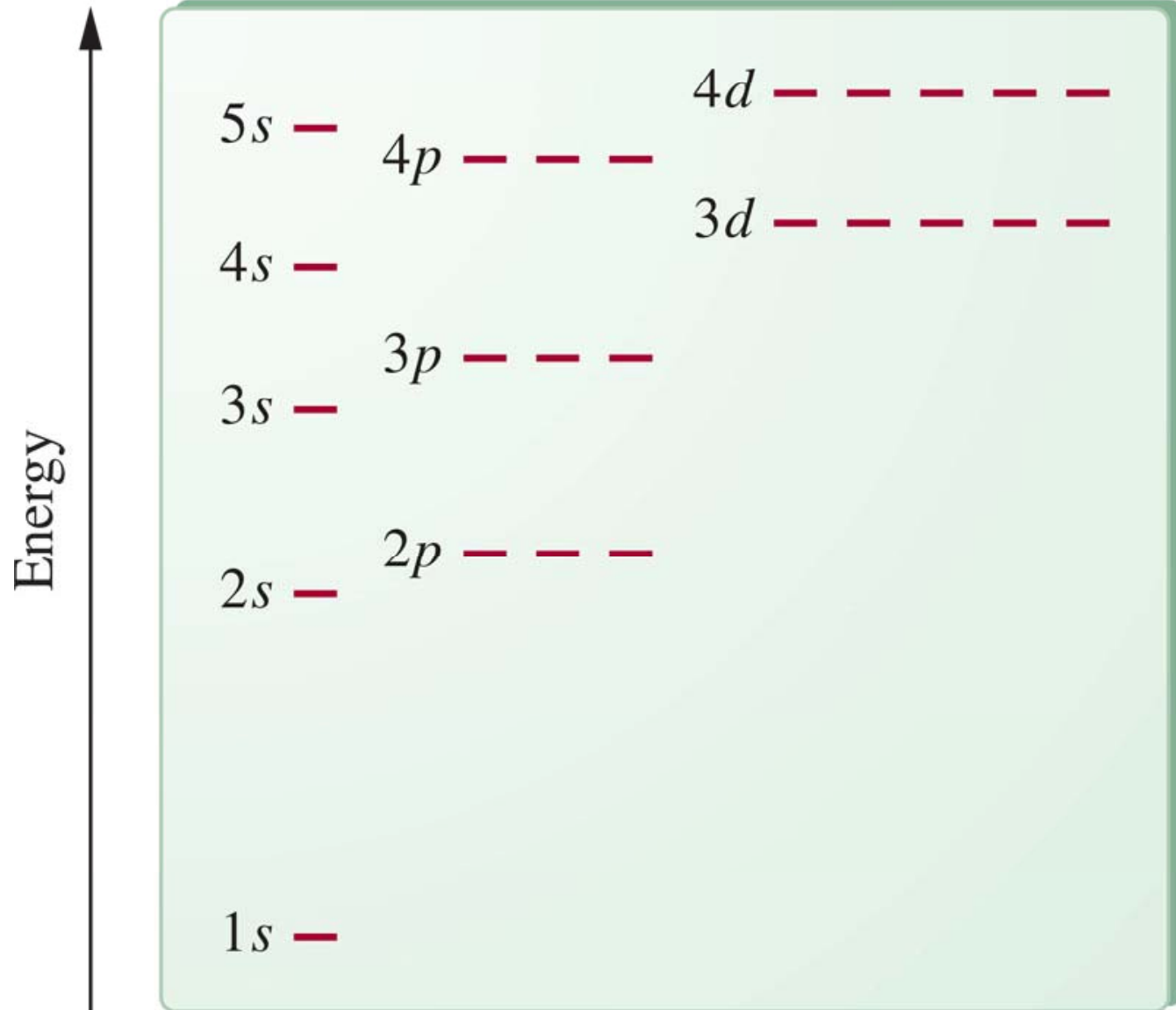
INNER TRANSITION ELEMENTS

6	Lanthanides	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
7	Actinides	90 Th 232.0	91 Pa (231)	92 U 238.0	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

212

Orbital Energy-level Diagram

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tion

Different Systems

(Chapter 14 ~ Chapter 18)

- 不同的系統，
有不同的 Schrödinger equation 的解

Y. J. Lin's Presentation

Schrödinger equation 的解，
是 Orthogonal。

$$\int_{-\infty}^{\infty} \psi_i^*(x) \psi_j(x) dx = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases} \quad (13.21)$$

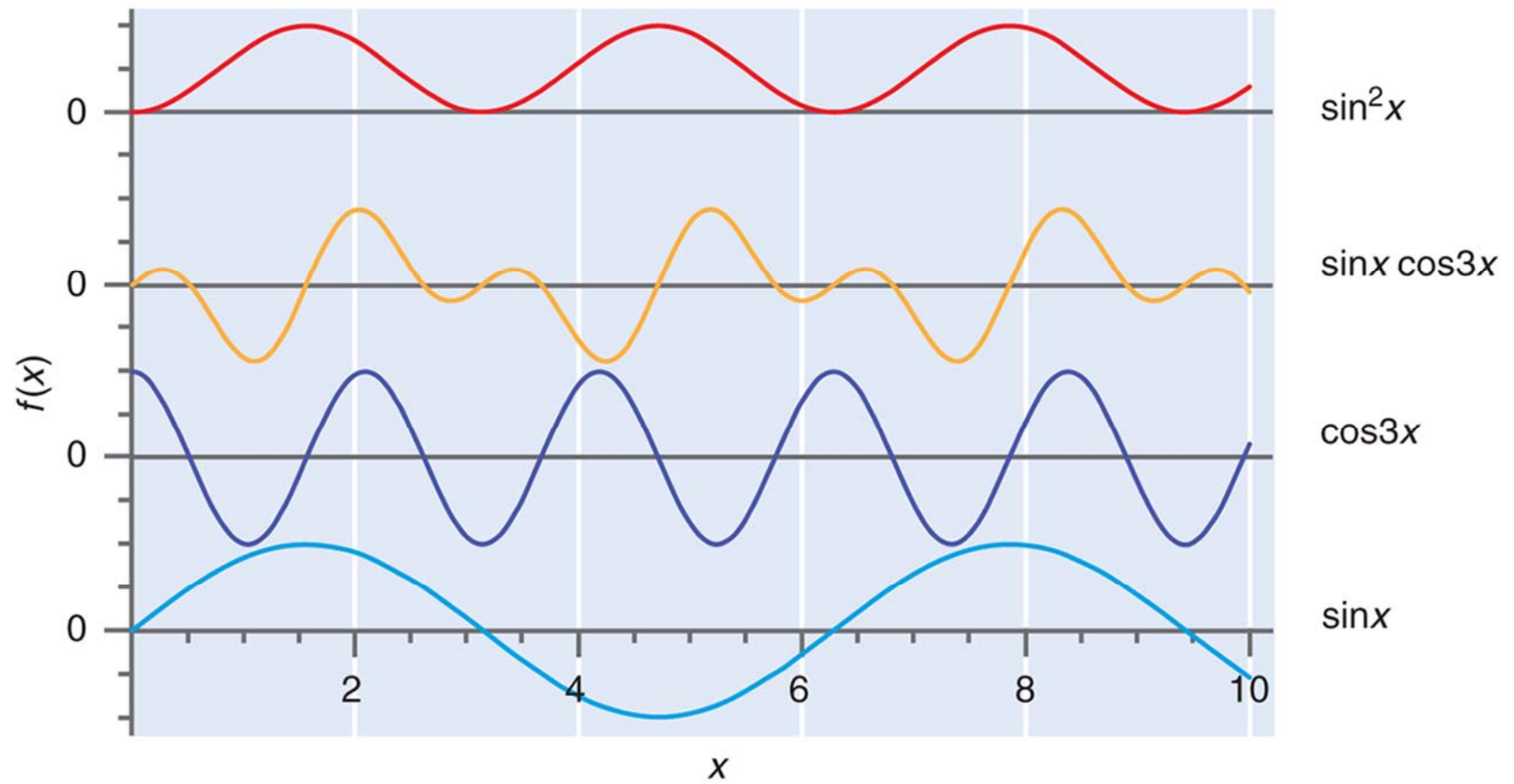


Figure: 13-02EP

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The Free Particle

Chapter 14.1, Physical Chemistry for the Life Sciences (Engel, Drobný and Reid)

Y. J. Lin's Presentation

The Heisenberg Uncertainty Principle

$$\Delta p \Delta x \geq \frac{\hbar}{2}$$



A ball in a box – what happened?



Potential of wall

$$V = \infty$$

Y. J. Lin's Presentation

The Particle in a One-Dimensional Box

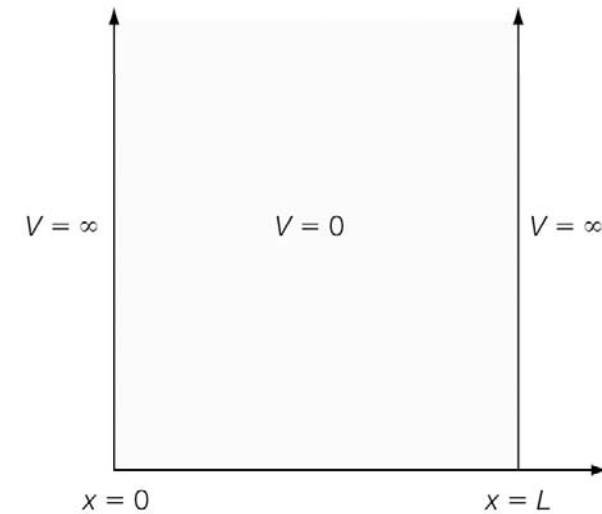
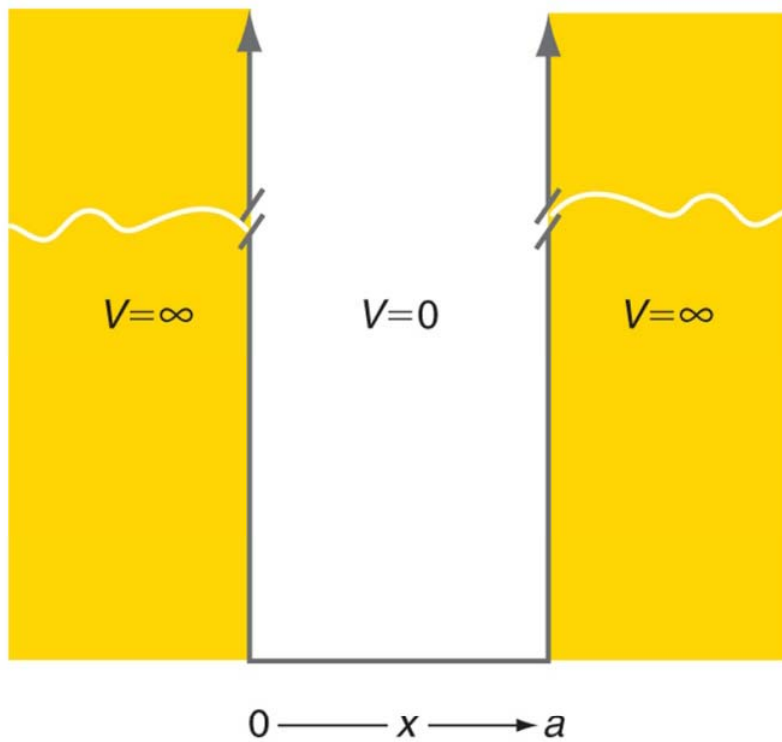


Figure: 14-01

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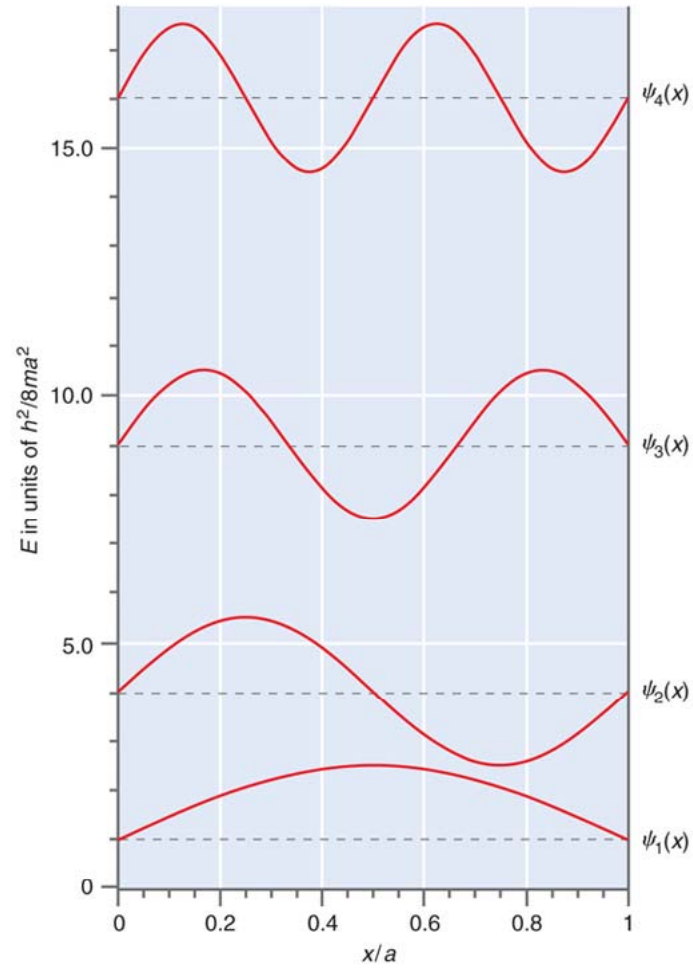
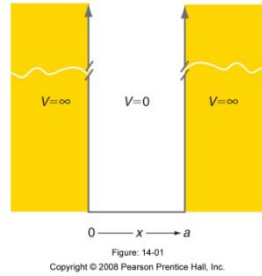


Figure: 14-02

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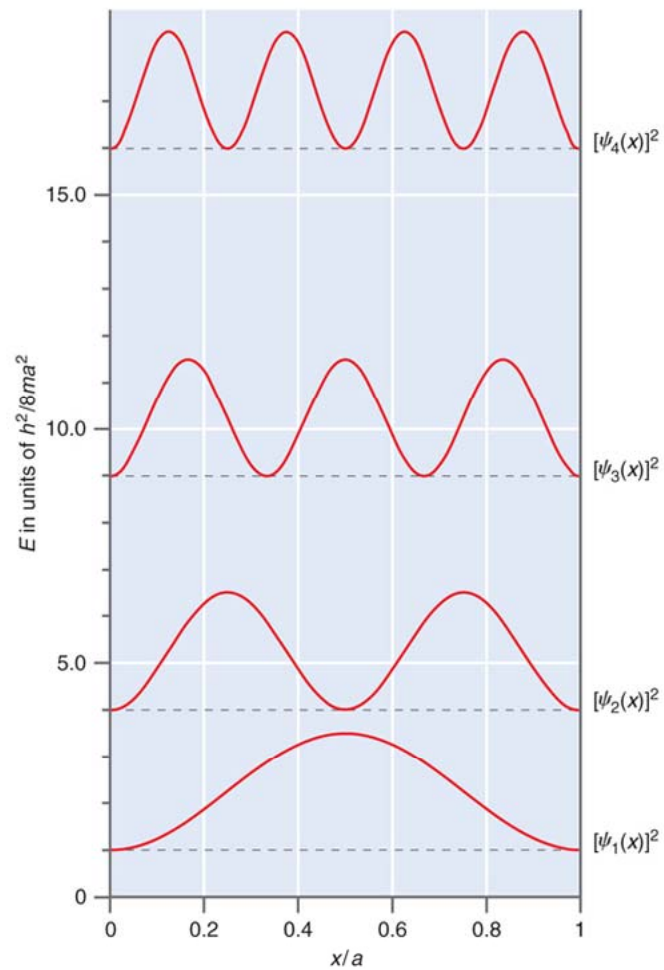
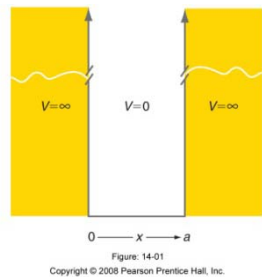
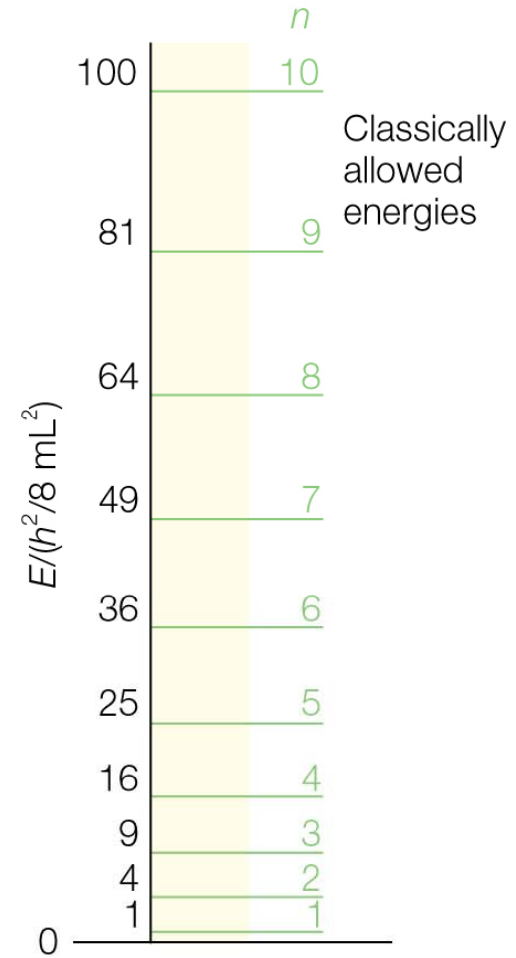
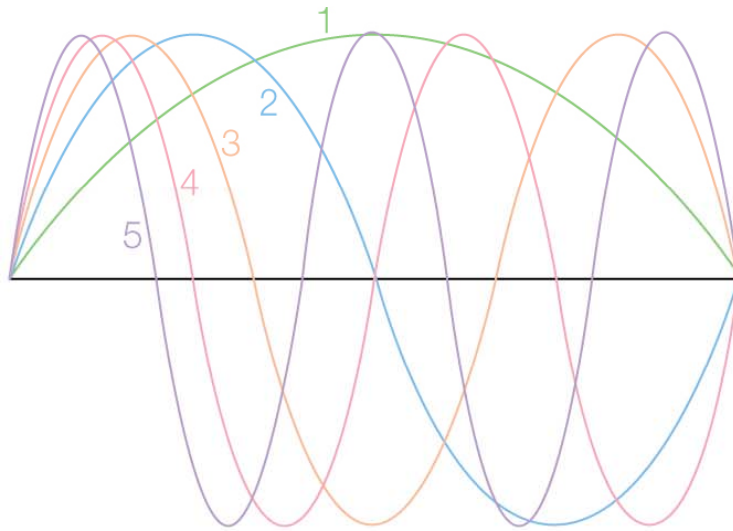
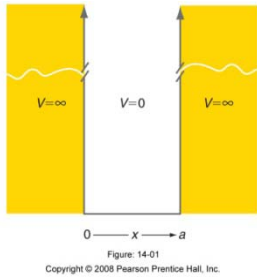


Figure: 14-03

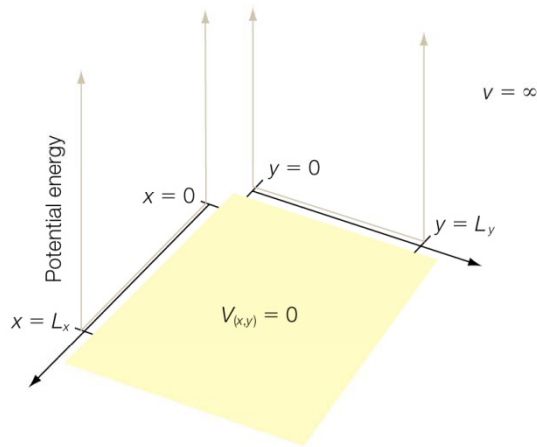
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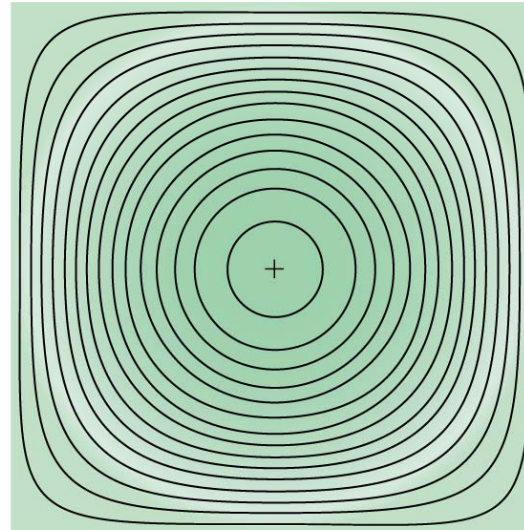


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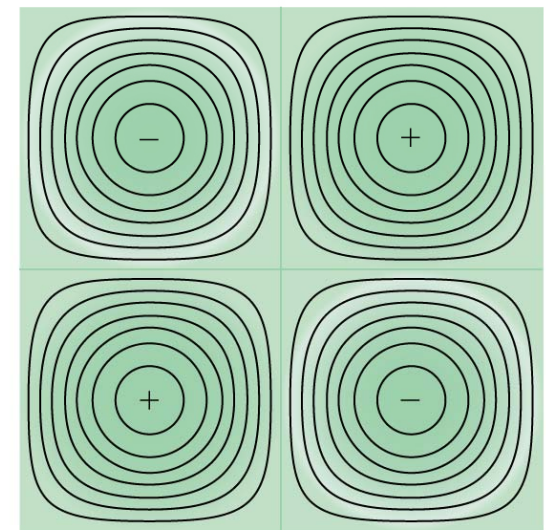
Two-Dimensional Box



$$n_x = n_y = 1$$



$$n_x = n_y = 2$$



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Three-Dimensional Box



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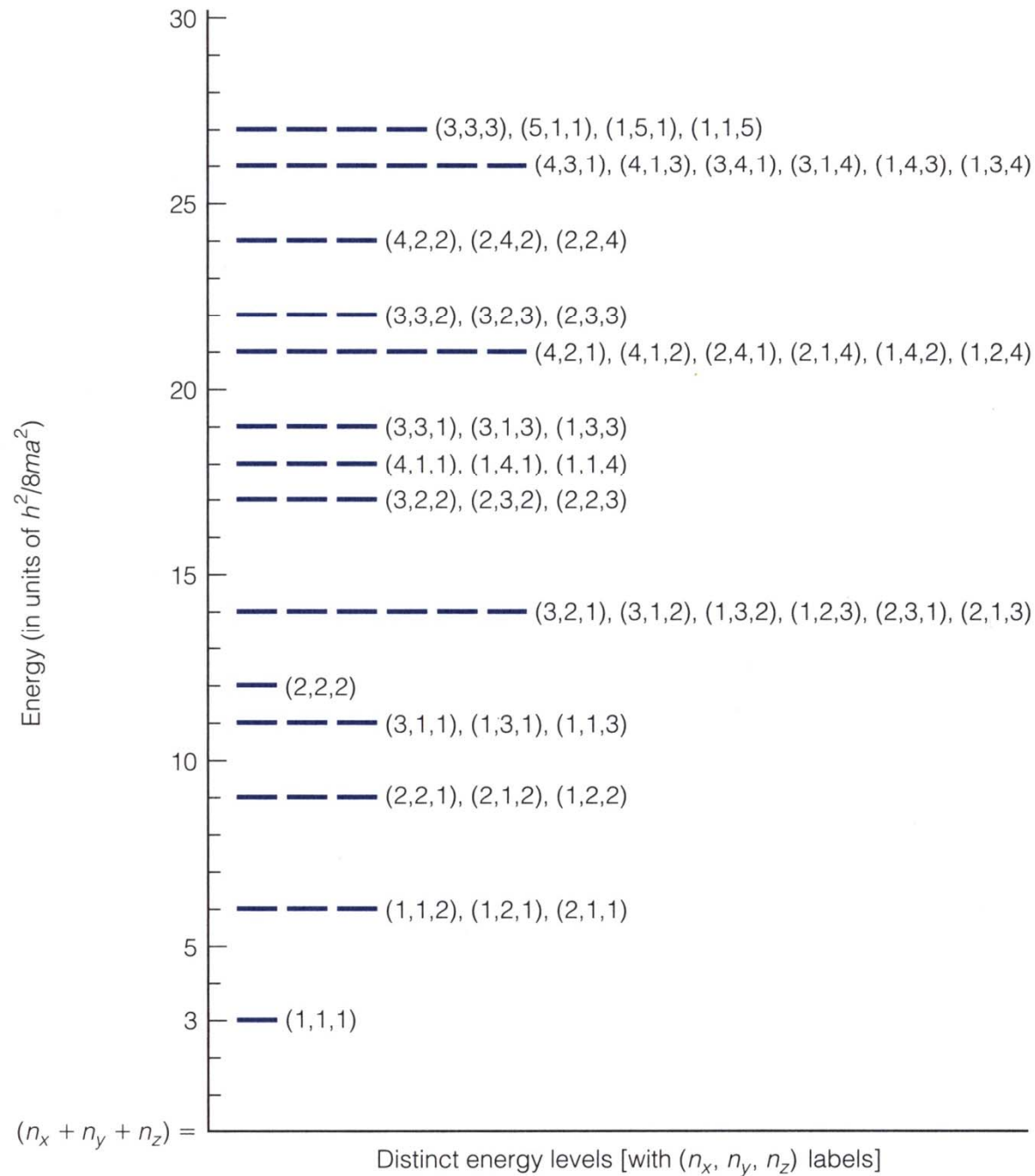


Figure 10.13 The energy levels of the 3-D particle-in-a-(cubical)-box. In this system, different wavefunctions can have the same energy. This is an example of degeneracy.

The Particle in the Finite Depth Box



Potential of wall

$$V = V_0$$

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The Particle in the Finite Depth Box

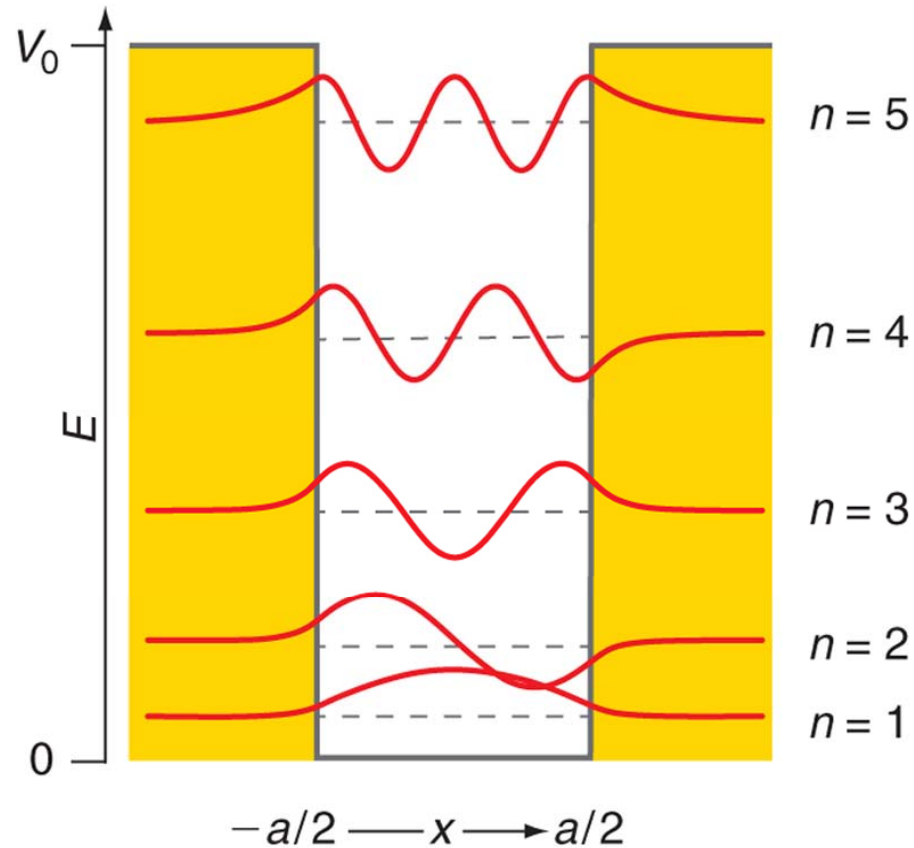


Figure: 14-04

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Tunneling

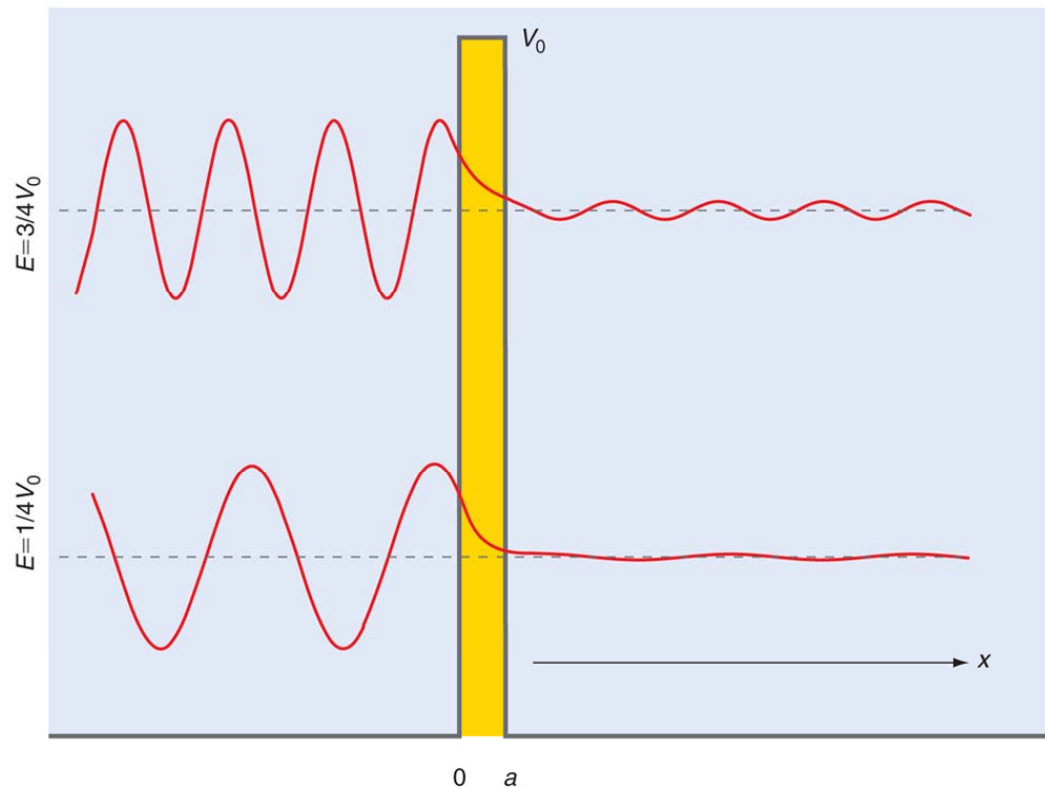
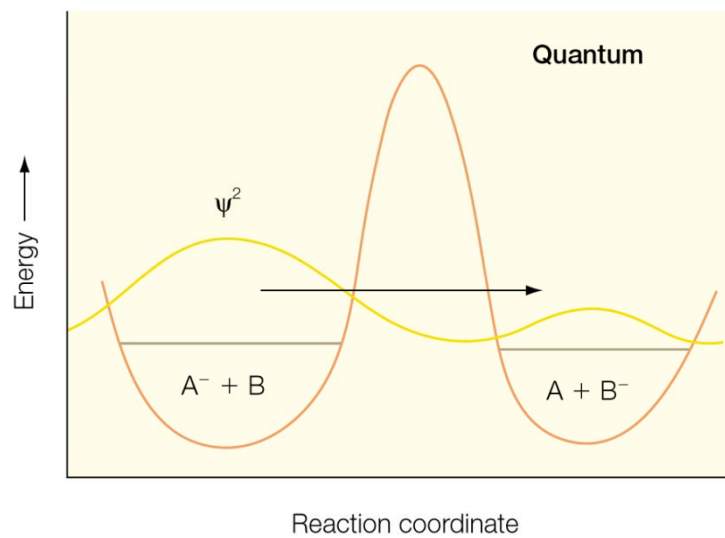
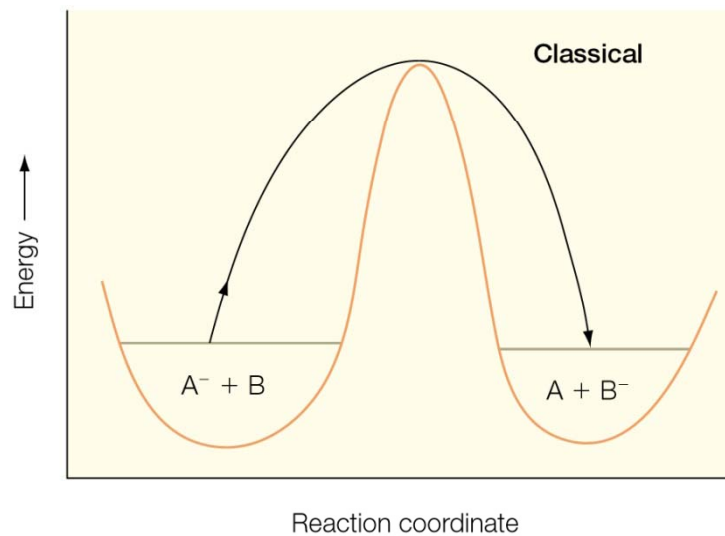


Figure: 14-09

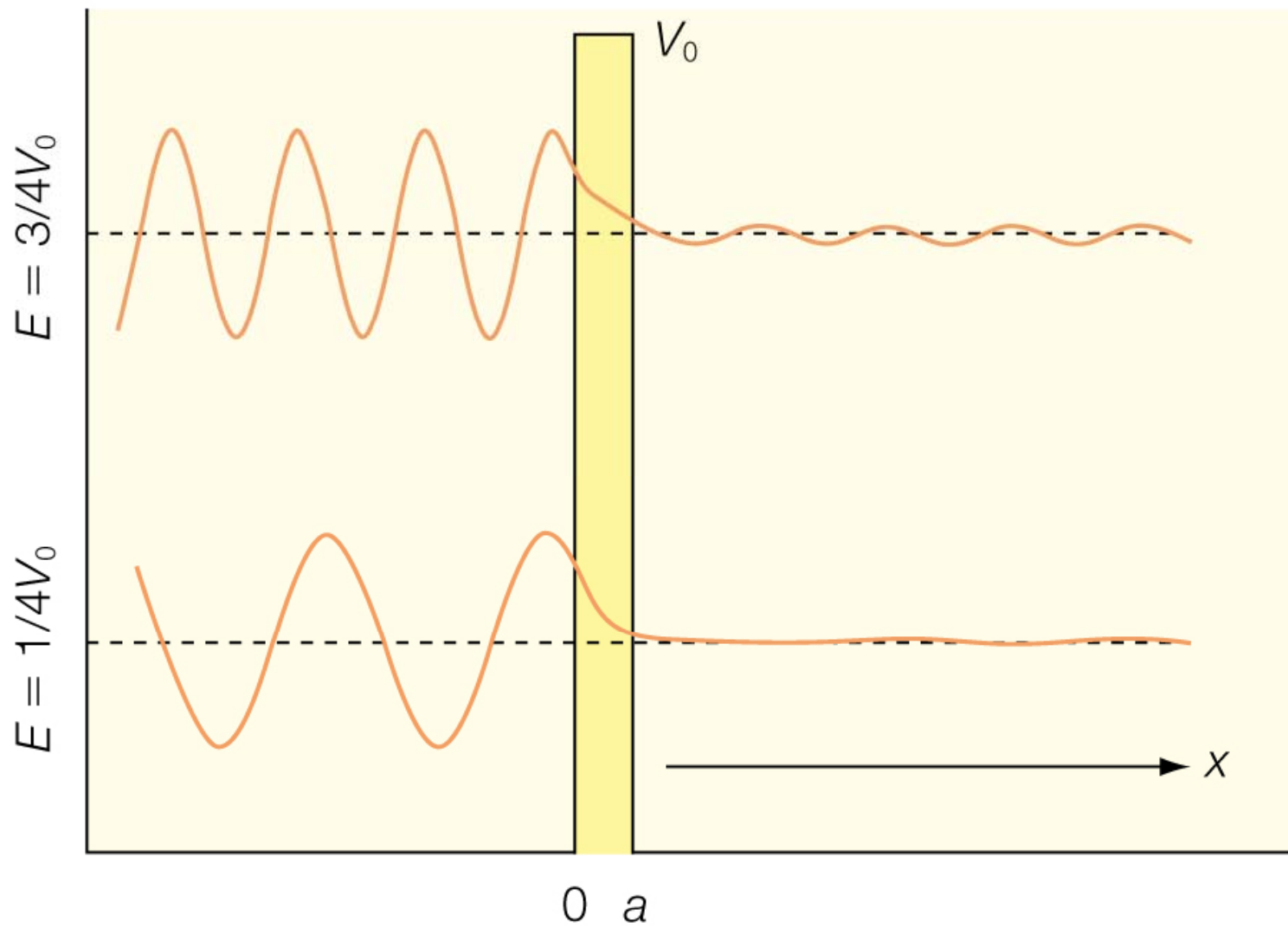
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Tunneling

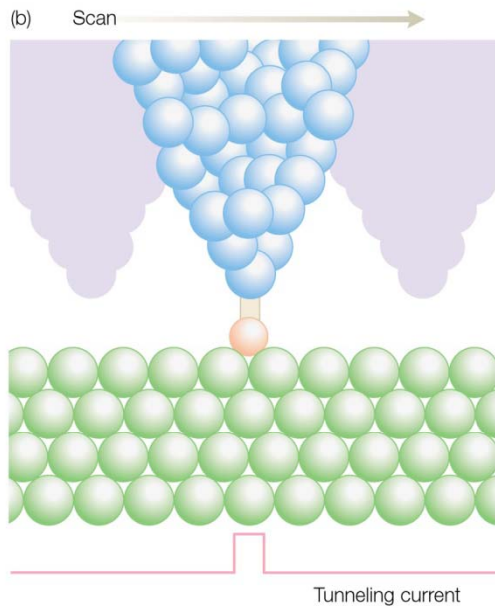
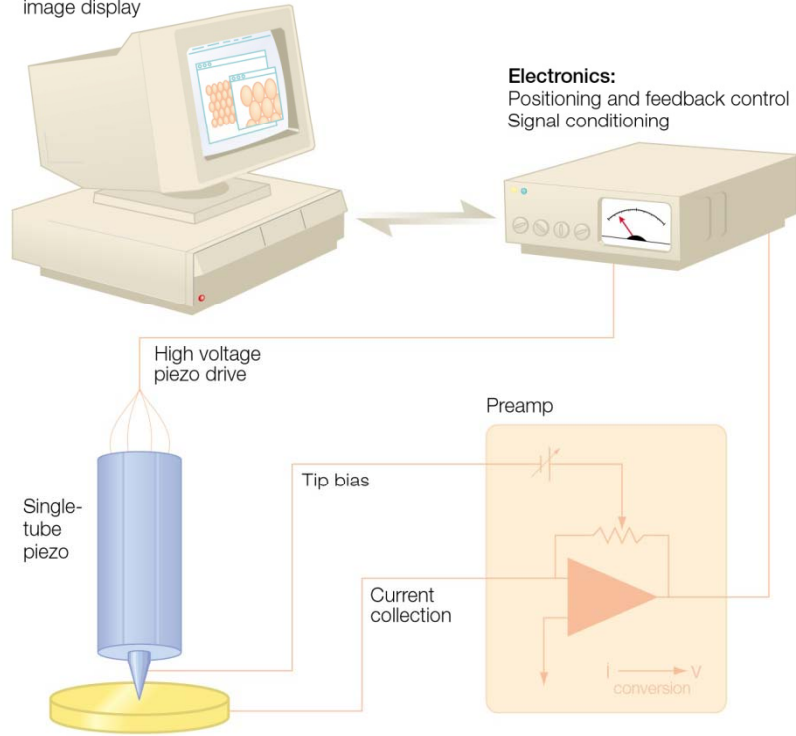


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(a) **Computer:**
Scan generation and
image display



Scanning Tunneling Microscopy (STM)

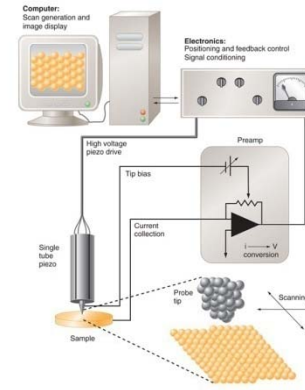


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Scanning Tunneling Microscopy

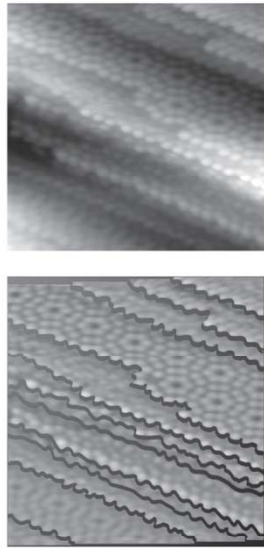


Figure: 14-12

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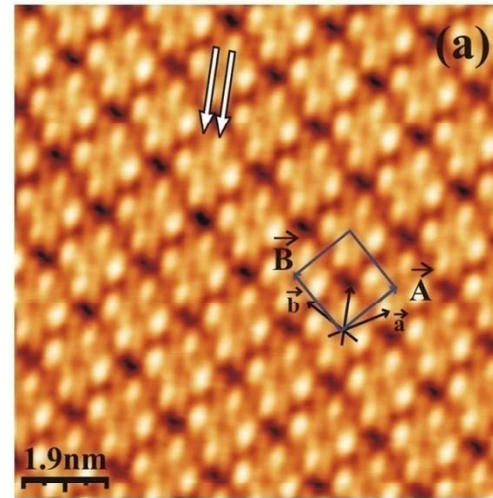


Figure: 14-13TOP

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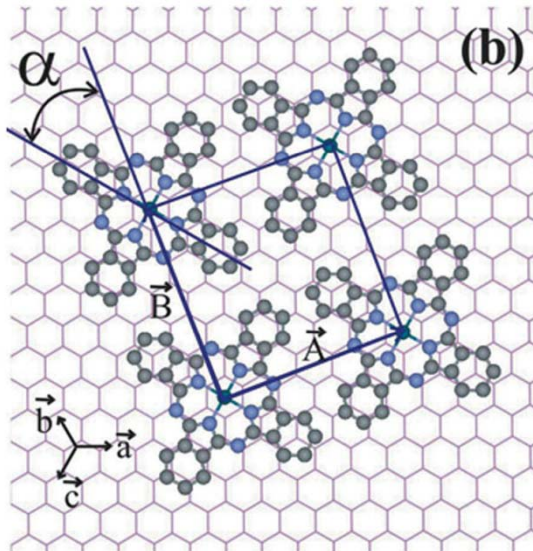


Figure: 14-13BOTTOM

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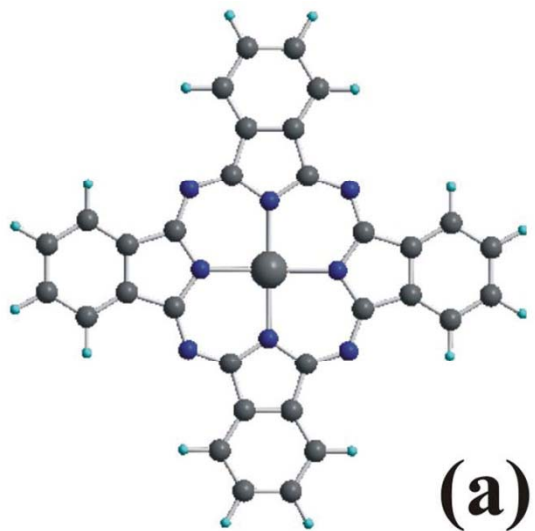


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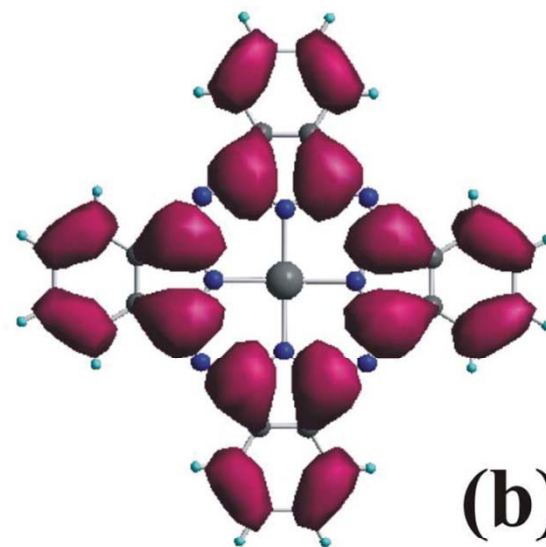


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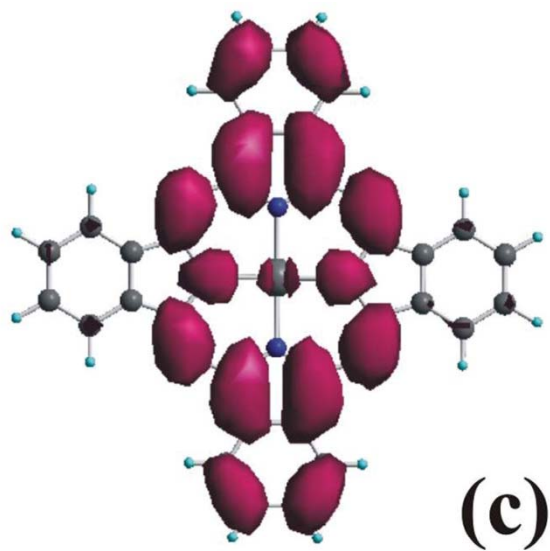


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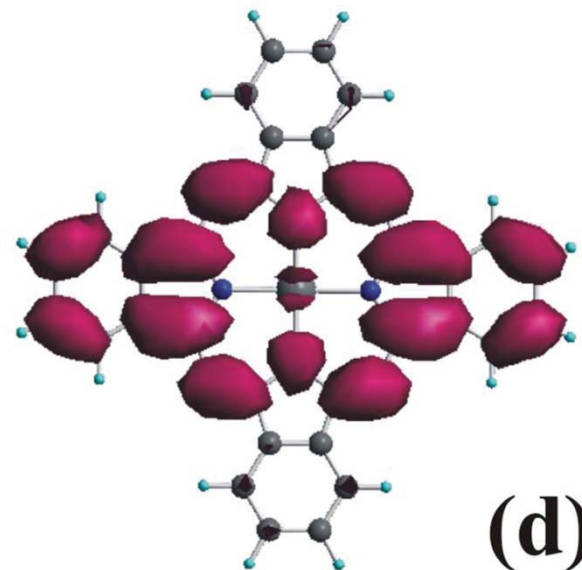


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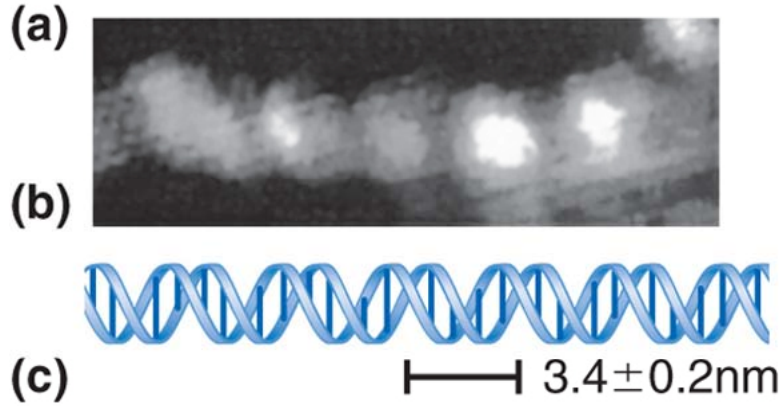
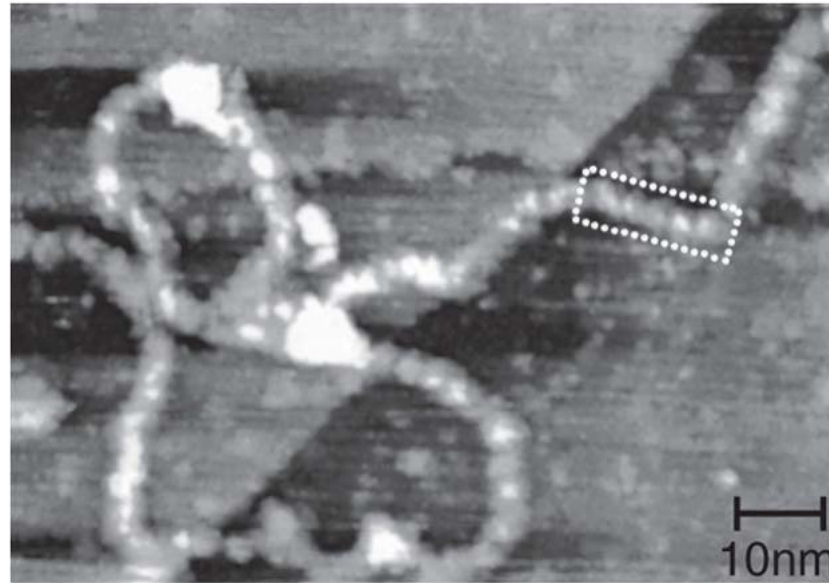


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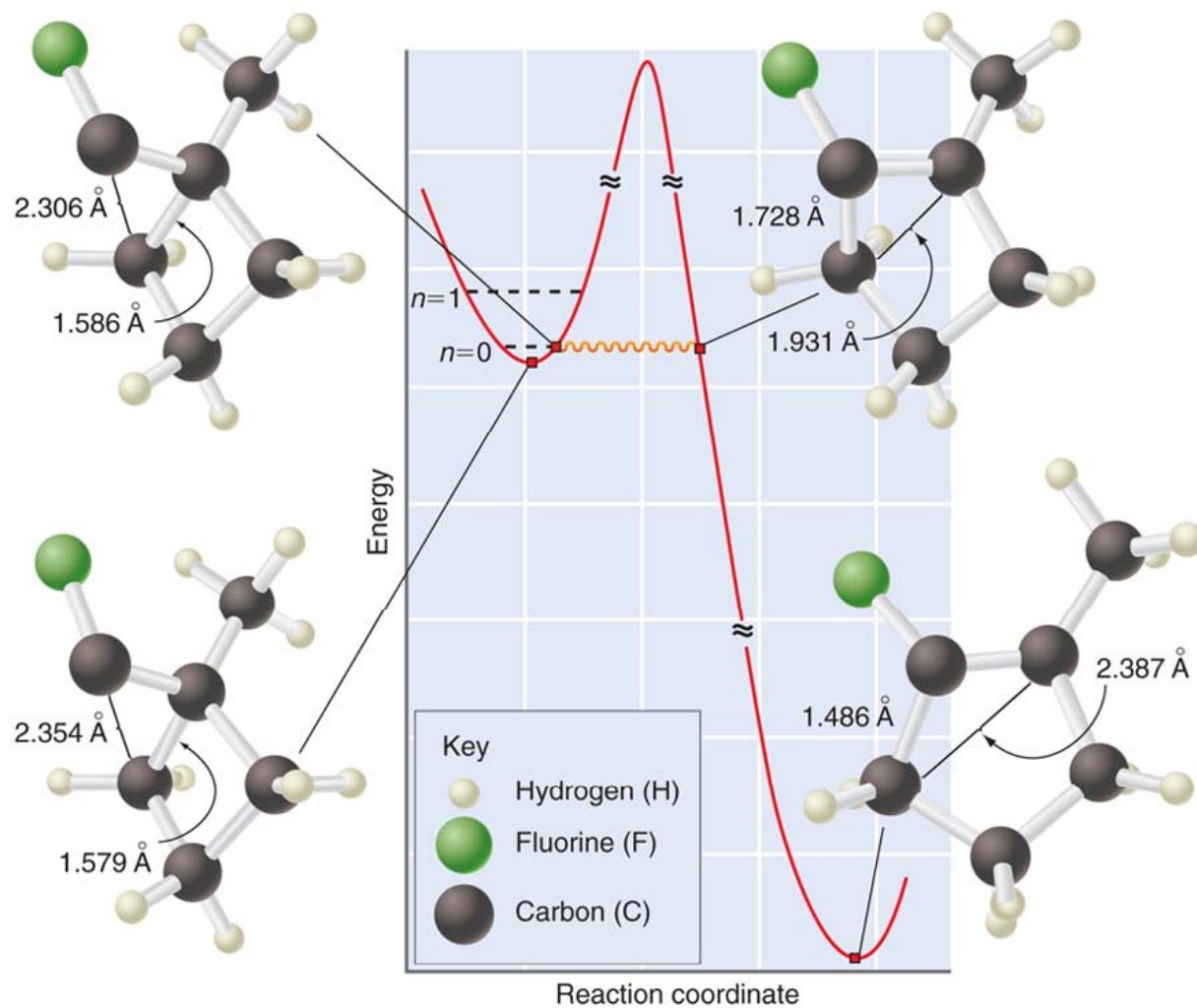
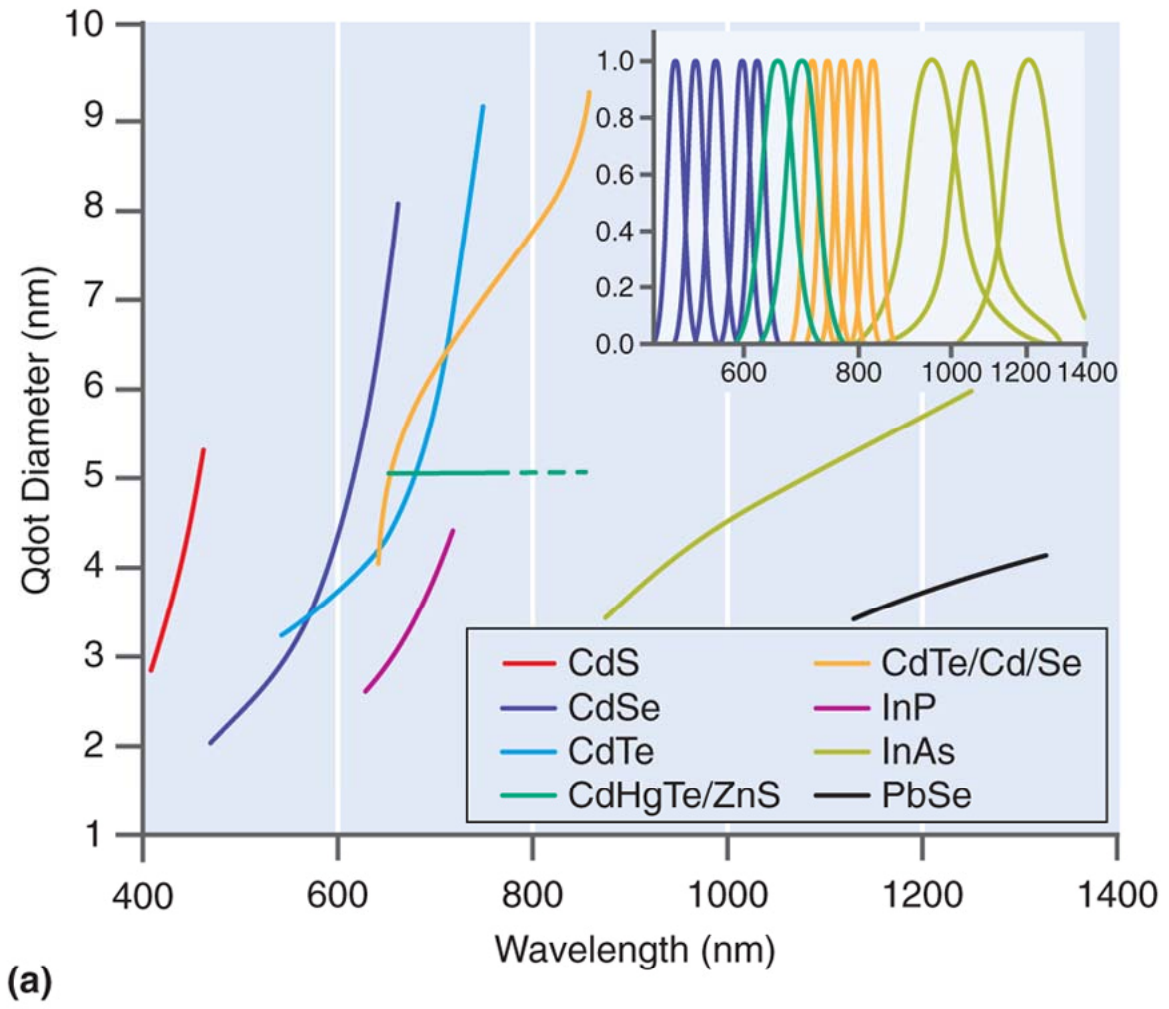


Figure: 14-16

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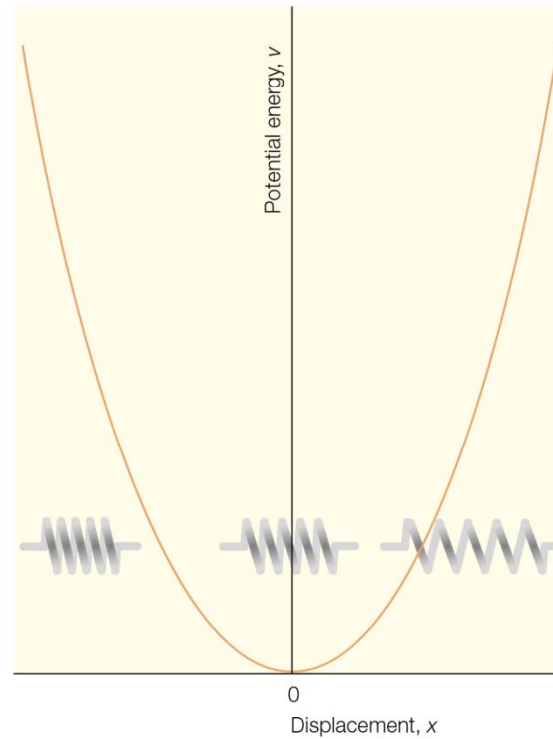
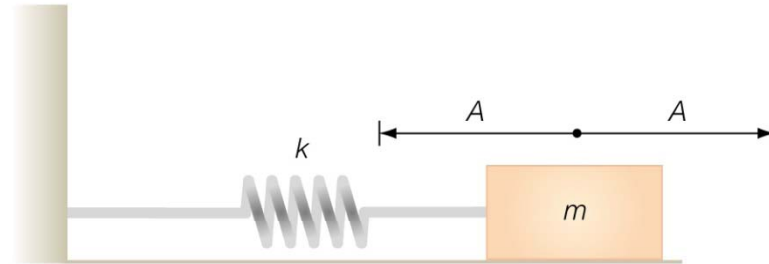
Quantum dots



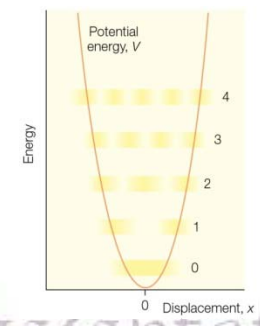
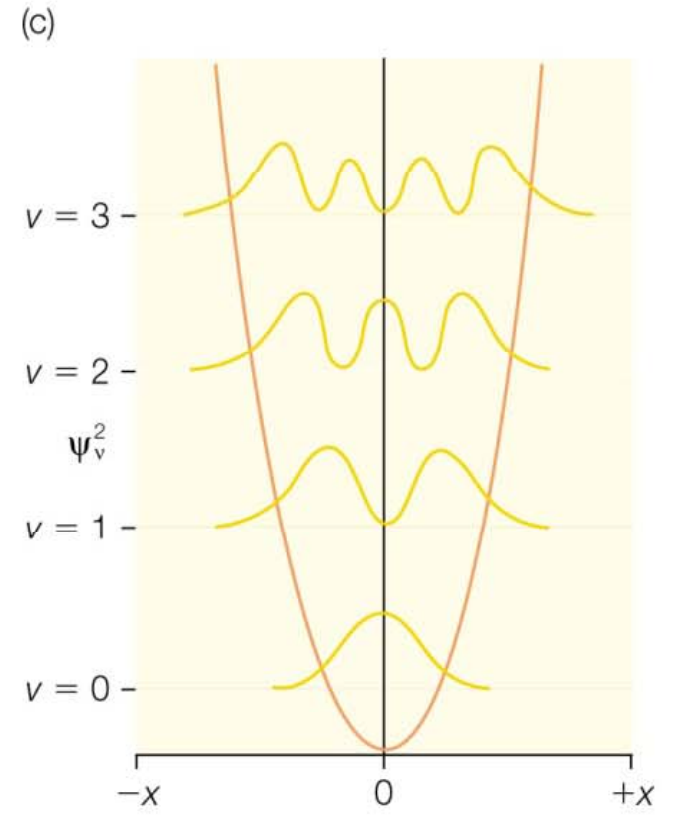
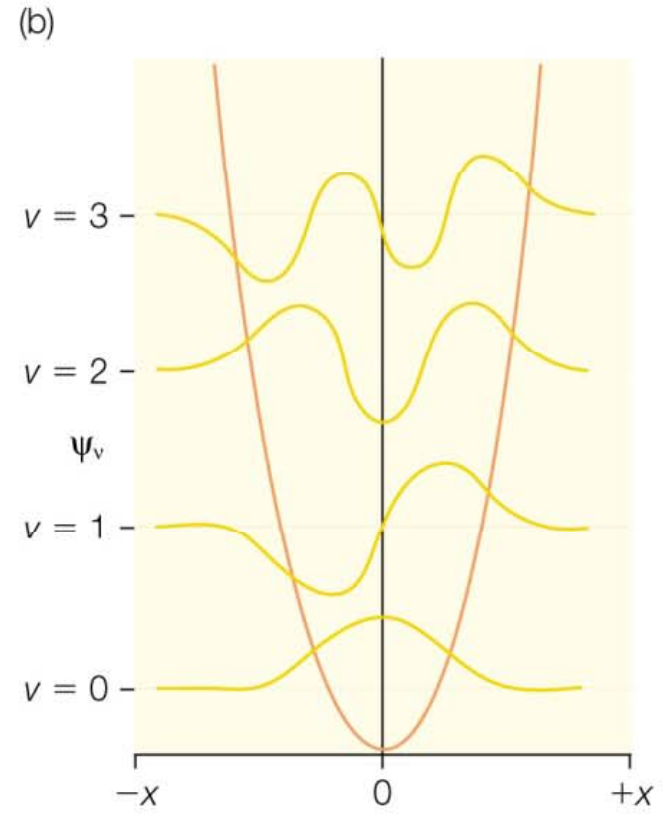
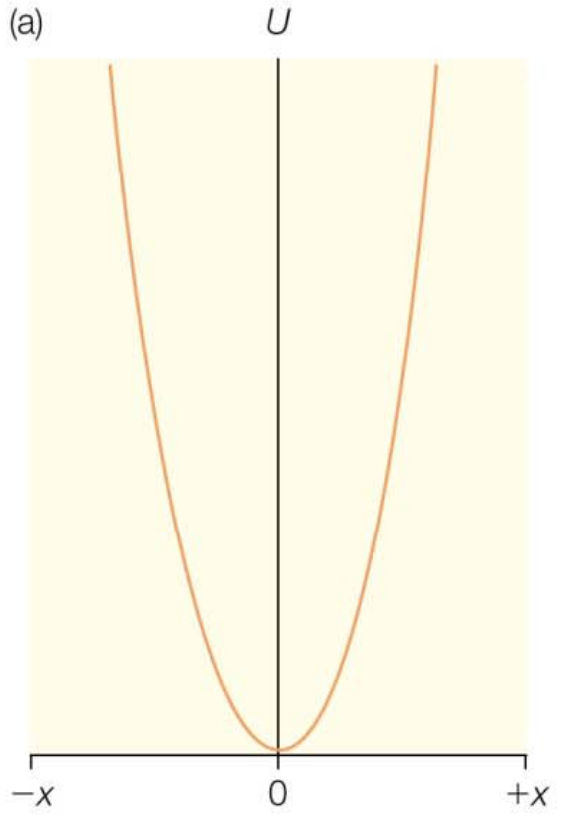
(a)

Figure: 14-17A

Harmonic Oscillator



y. win's Presentation



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Rotational Energy Levels

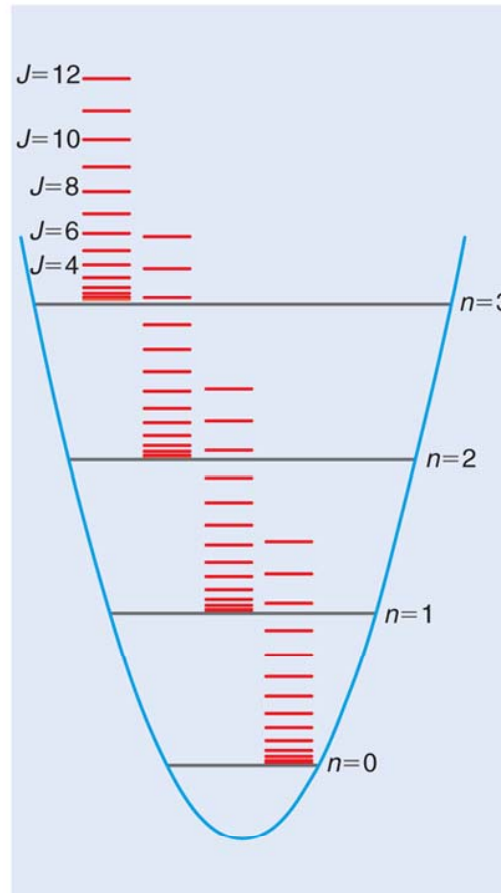


Figure: 18-08

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CO₂

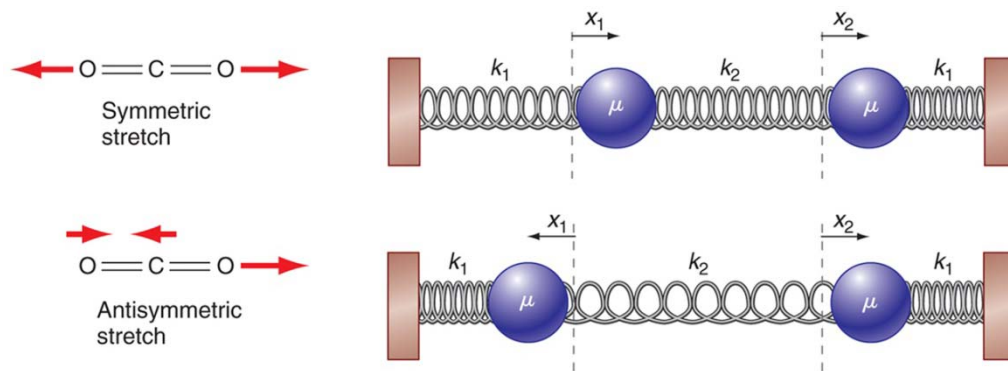
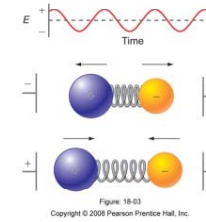
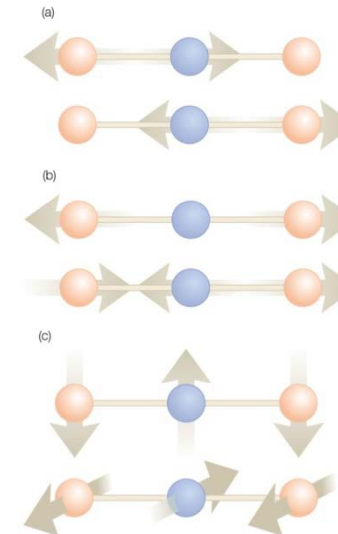


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H₂O

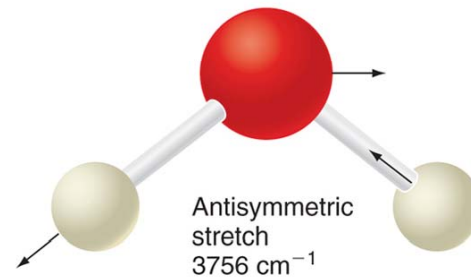
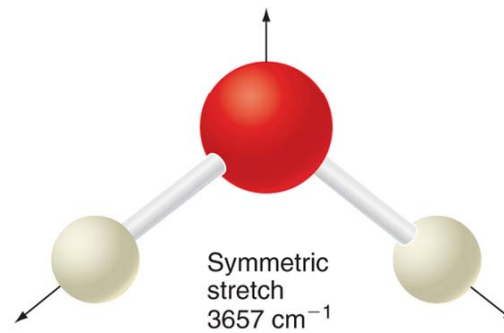


Figure: 18-12

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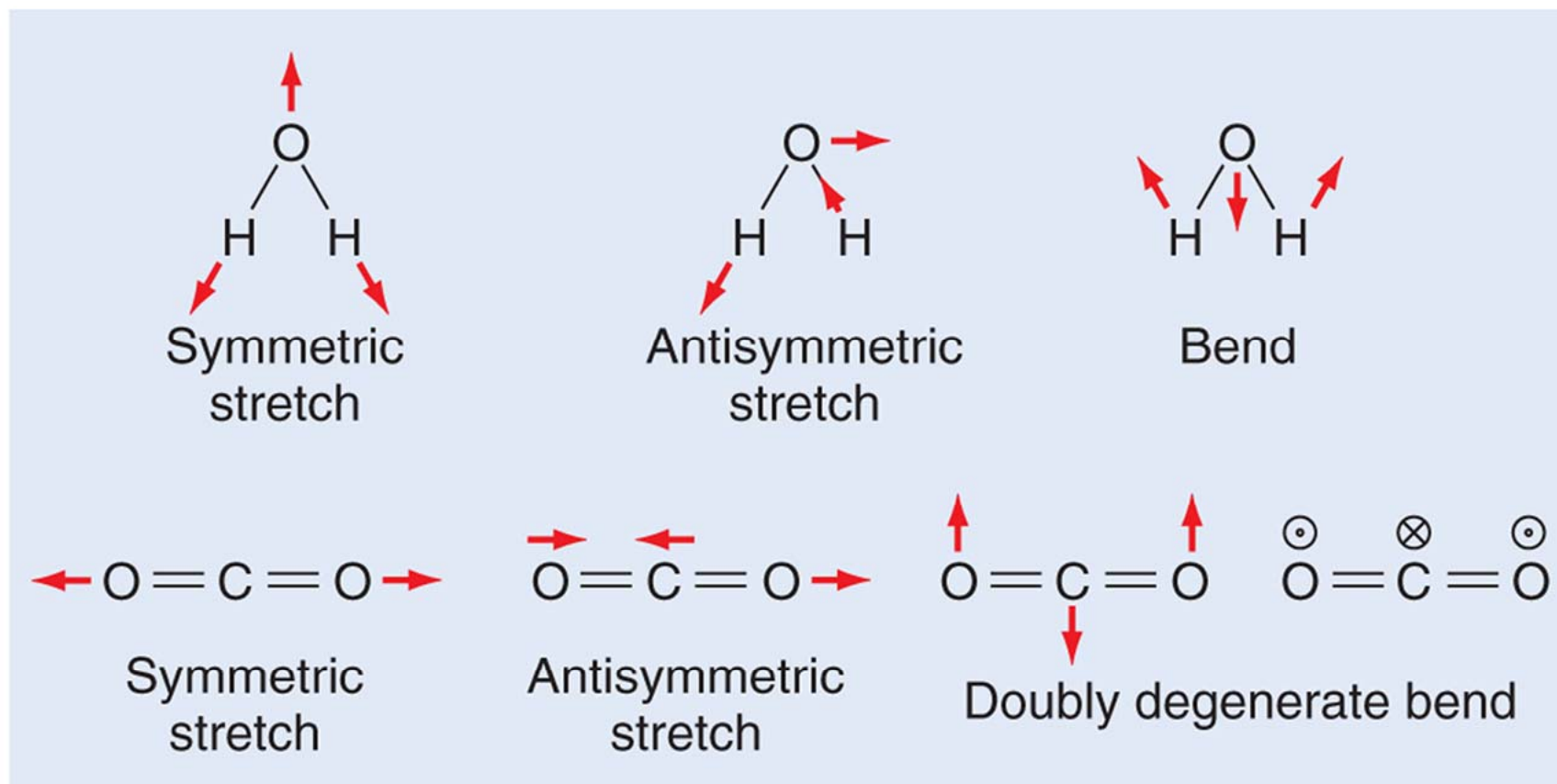


Figure: 18-14P

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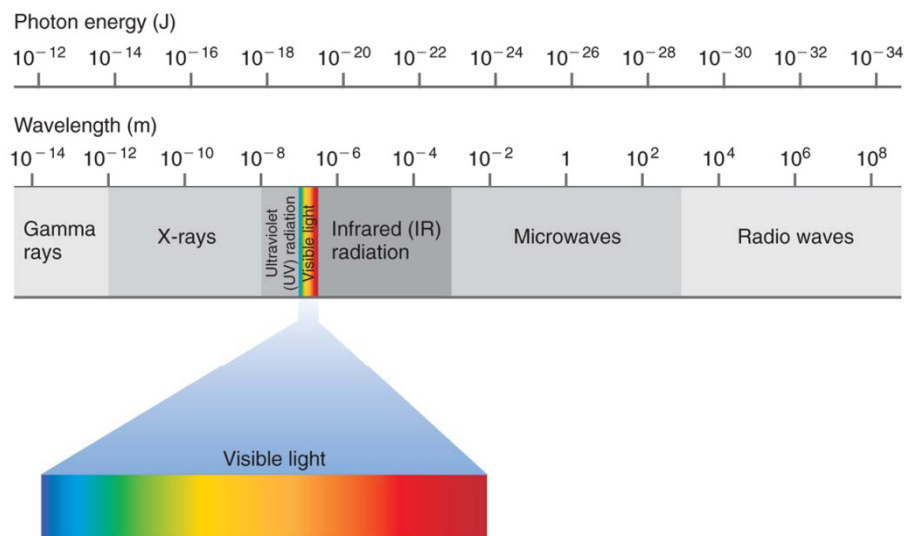


Figure: 18-01

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TABLE 18.1 Important Spectroscopies and Their Spectral Range

Spectral Range	λ (nm)	$\nu/10^{14}$ (Hz)	$\tilde{\nu}$ (cm) $^{-1}$	Energy (kJ/mol)	Spectroscopy
Radio	$\sim 1 \times 10^9$	$\sim 10^{-6}$	~ 0.01	$\sim 10^{-8}$	NMR
Microwave	$\sim 100,000$	$\sim 10^{-2}$	~ 100	$\sim 10^{-2}$	Rotational
Infrared	~ 1000	~ 3.0	$\sim 10,000$	$\sim 10^3$	Vibrational
Visible (red)	~ 700	~ 4	$\sim 14,000$	$\sim 10^5$	Electronic
Visible (blue)	~ 450	~ 6	$\sim 22,000$	$\sim 3 \times 10^5$	Electronic
Ultraviolet	< 300	> 10	$> 30,000$	$> 5 \times 10^5$	Electronic

Table: 18_01

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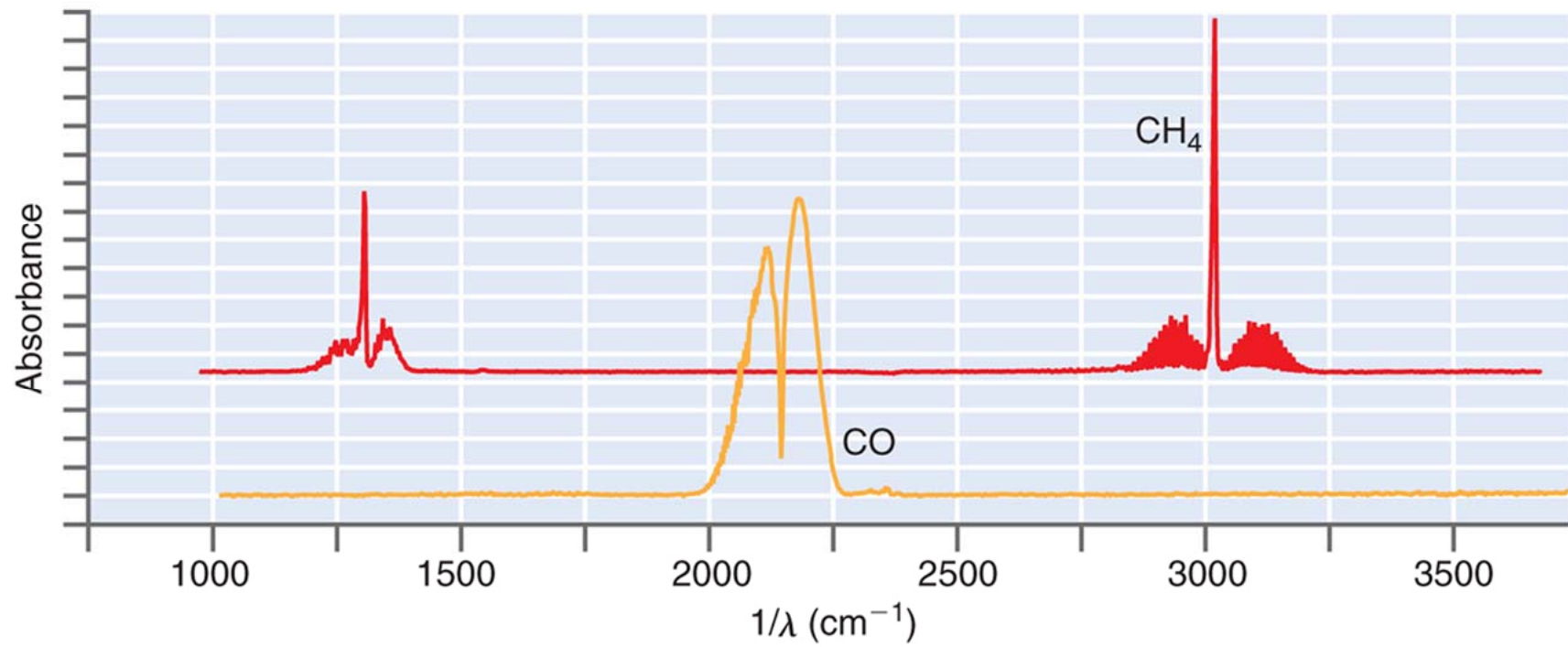
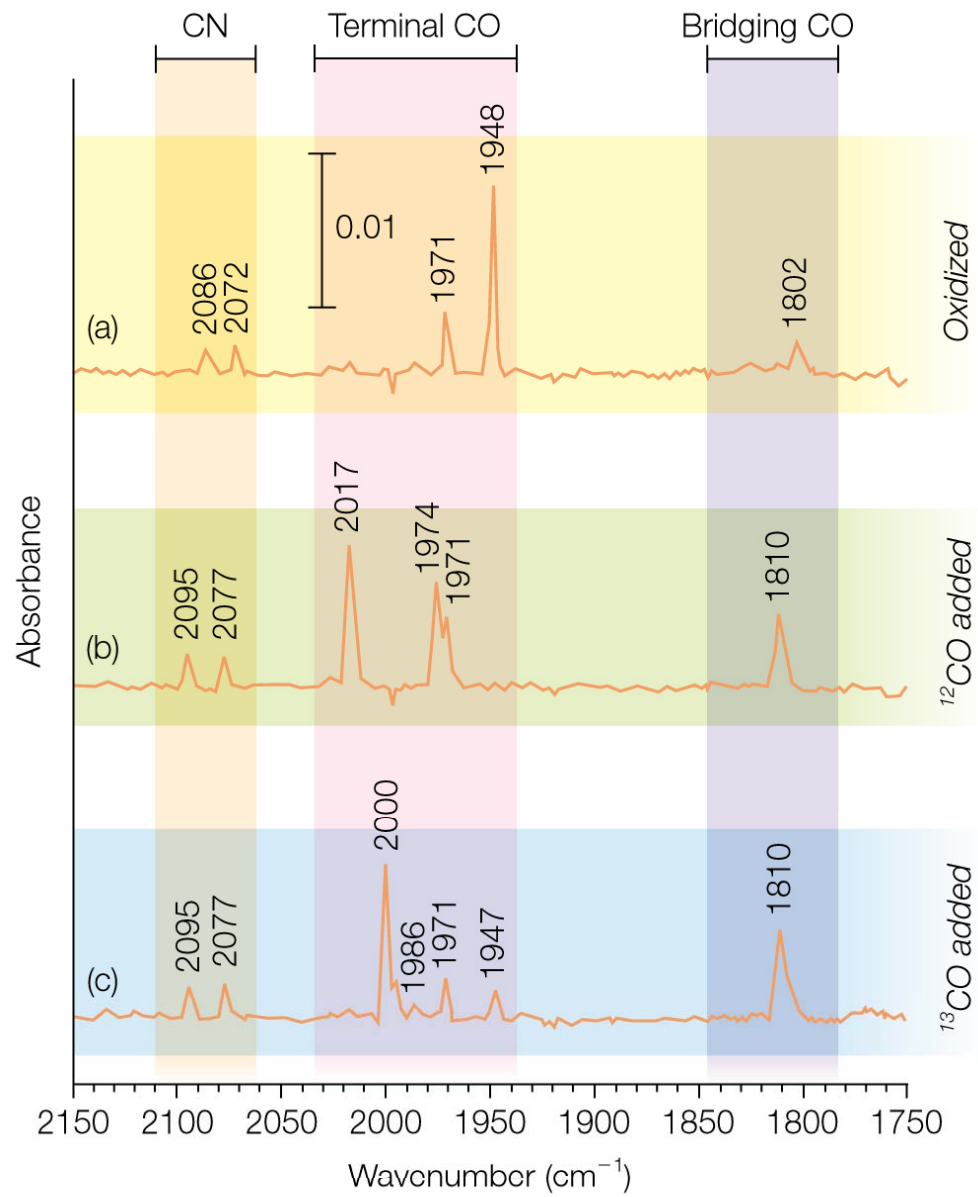


Figure: 18-10

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TABLE 18.2 Vibrational State Populations for Selected Diatomic Molecules

Molecule	$\tilde{\nu}$ (cm ⁻¹)	ν (s ⁻¹)	N_1/N_0 for 300 K	N_1/N_0 for 1000 K
H—H	4400	1.32×10^{14}	6.88×10^{-10}	1.78×10^{-3}
H—F	4138	1.24×10^{14}	2.42×10^{-9}	2.60×10^{-3}
H—Br	2649	7.94×10^{13}	3.05×10^{-6}	2.21×10^{-2}
N≡N	2358	7.07×10^{13}	1.23×10^{-5}	3.36×10^{-2}
C≡O	2170	6.51×10^{13}	3.03×10^{-5}	4.41×10^{-2}
Br—Br	323	9.68×10^{12}	0.213	0.628

Table: 18_02

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TABLE 18.4 Selected Group Frequencies

Group	Frequency (cm ⁻¹)	Group	Frequency (cm ⁻¹)
O—H stretch	3600	C=O stretch	1700
N—H stretch	3350	C=C stretch	1650
C—H stretch	2900	C—C stretch	1200
C—H bend	1400	C—Cl stretch	700

Table: 18_04

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End of Lecture

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