Quantum Chemistry by Levine

LuMg

Sep 2023

1 Chapter 1 The Schrodinger Equation

1.1
(a) F.
$E = h\nu$
(b) T.
$c = \nu\lambda$
(c) F.
Energy has different level. in quantumized way.

1.2
(a)$E = h\nu = h * \frac{c}{\lambda} = 6.626 * 10^{-34} * 3 * 10^8/1064 * 10^{-9} = 1.867 * 10^{-19}J$
(b)$n = \frac{5*10^6*2*10^{-8}}{E} = 5 * 10^{17}$

1.3
Energy of 1 mol photon:
$E = \frac{hc}{\lambda} * N = \frac{6.02*10^{23}*6.626*10^{-34}*3*10^8}{300*10^{-9}} = 399kJ$

1.4
(a) $T = \frac{hc}{\lambda} - \Phi = \frac{6.626*10^{-34}*3*10^8}{200*10^{-9}} - 2.75 * 1.602 * 10^{-19} = 5.53 * 10^{-19}J$
(b) It only needs to give energy as large as Φ:
$\lambda = \frac{hc}{E} = \frac{6.626*10^{-34}*3*10^8}{2.75*1.602*10^{-19}} = 451nm$
(c) $T = E - \Phi$
The left kinetic energy is larger than pure Na.

1.5
(a)Planck's blackbody equation:
$B_\nu(\nu, T) = \frac{2h\nu^3}{c^2} * \frac{1}{exp(\frac{h\nu}{\nu_B T})-1}$
Get its derivitive to ν:
$\frac{dB_\nu(\nu,T)}{d\nu} = 3(e^u - 1) - ue^u$
where:
$u = \frac{h\nu}{k_B T}$
At peak wavelength:
$3(e^u - 1) - ue^u = 0$

then:
$\nu = \frac{2.8214 k_B T}{h}$
(b)$e^u = 1 + u$

1.6
$\lambda = \frac{h}{mV} = \frac{6.626*10^{-34}}{9.109*10^{-28}*\frac{1}{137}*3*10^8} = 0.332nm$

1.7
$x = -\frac{1}{2}gt^2 + (gt_0 + v_0)t + C$

1.8
Using Schrondinger equation:
$-\frac{\hbar}{i} * \frac{\partial \Phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Phi}{\partial x^2} + V\Phi$
Given:
$\Phi = ae^{-ibt}e^{-bmx^2/\hbar}$
$V = 2b^2mx^2$

1.9
(a) F.
Not all has a phase term. Not separable. Not stationary.
(b) F.
Not all Ψ can be separated to $F(x)G(\psi)$

1.10
Given the postulation of E: $-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi = E\Psi$
$E = \frac{3\hbar^2 c}{m}$

1.11
Only time-dependent

1.12
(a) The infinitesimal is small enough:
$Prob = |\Psi|^2 dx = 3.29 * 10^{-6}$
(b) The distance is not small enough:
$Prob = \int_0^{2nm} |\Psi|^2 dx = 0.0753$
(c)$x = 0$
(d)$\int_{-\inf}^{\inf} |\Psi|^2 dx = 1$

1.13
The infinitesimal is small enough not to use integral:

$|\Psi|^2 dx = 0.000216$

1.14
force to use integral:
$\int_{15nm}^{1.5001nm} |\Psi|^2 dx = 4.978 * 10^{-6}$
Almost the same

1.15
(a) not real
(b) negative
(c) can find a plausible b

1.16
(a)Not independent: $\frac{1}{3}$
(b)Independent: $\frac{1}{2}$

1.17
the prob of 138 peak:
0.9889^2
the peak of 139 is $C_{12}C_{13}F_6$
$: 0.9889 * 0.0111 * 2/(0.9889 * 0.9889) * 100 = 2.24$
the peak of 140 is $C_{13}^2 F_6$:
$0.0111^2/(0.9889 * 0.9889) * 100 = 0.0126$

1.18
26 cards of 2 spade, 24 non-spade:
one getting 13 non-spade:
$\frac{24}{26} * \frac{23}{25} * \cdots * \frac{12}{14} = \frac{6}{25}$
the prob of getting one spade to each person is:
$1 - \frac{6}{25} * 2 = \frac{13}{25}$

1.33
(a) T.
prob density always positive.
(b) F.
function can have negative value.
(c) F.
function can have imaginary value, like oscillating.
(d) T.

(e) F.
To all normalized system.
(f) T.