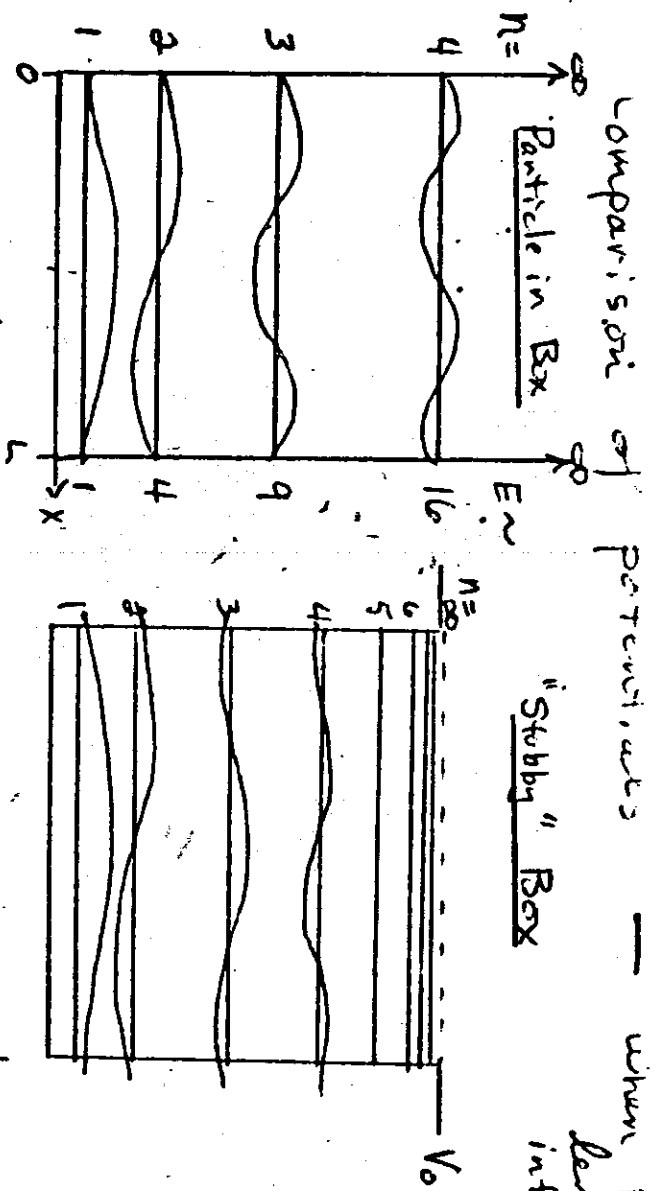
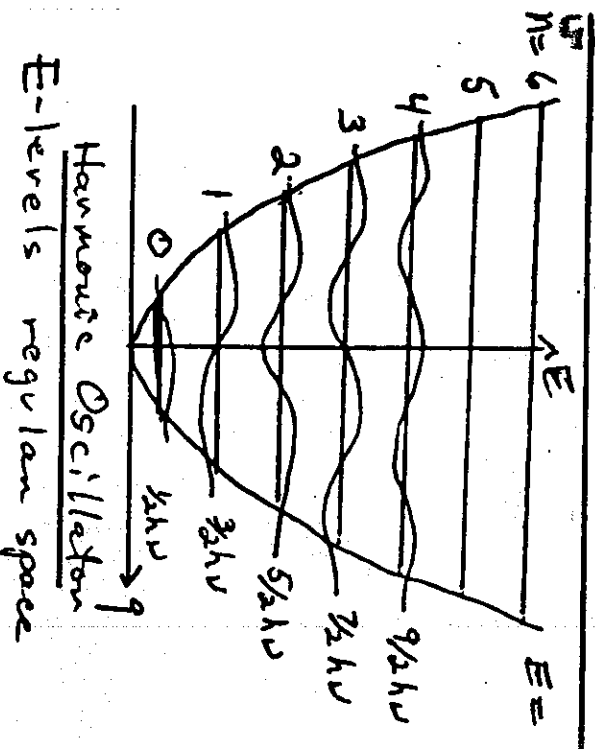


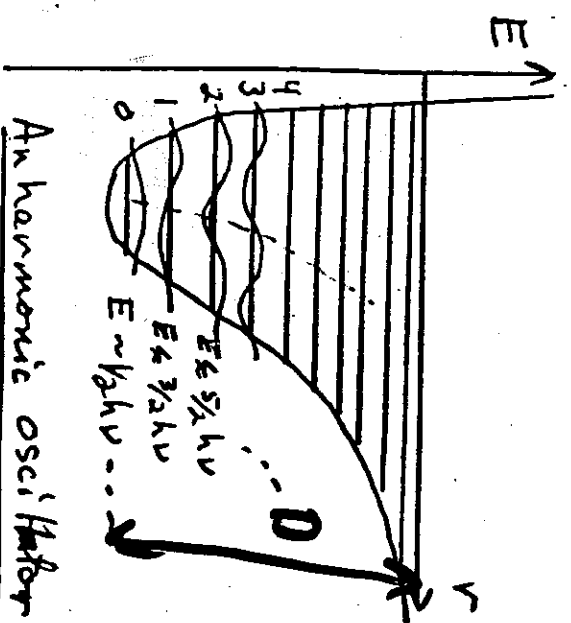
when potential NOT infinite, levels collapse, when sides not infinite and vertical w/f penetrates the potential well



E-levels expand
 $\Delta E \sim n$
 At top, E-levels collapse



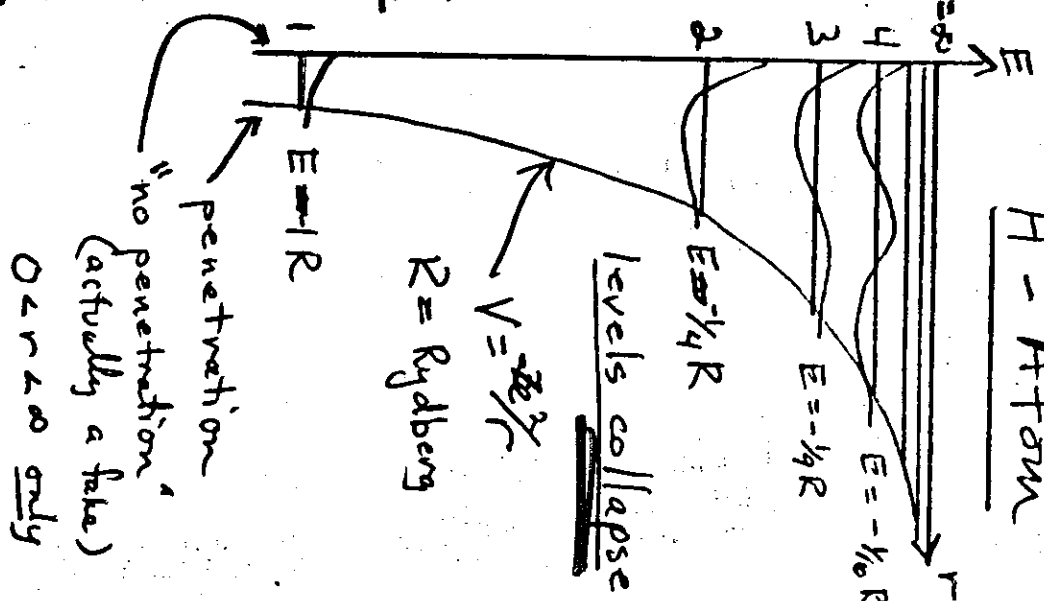
Harmonic Oscillator
 E-levels regular space
 $\Delta E = h\nu$ - constant



Anharmonic oscillator
 E-levels collapse

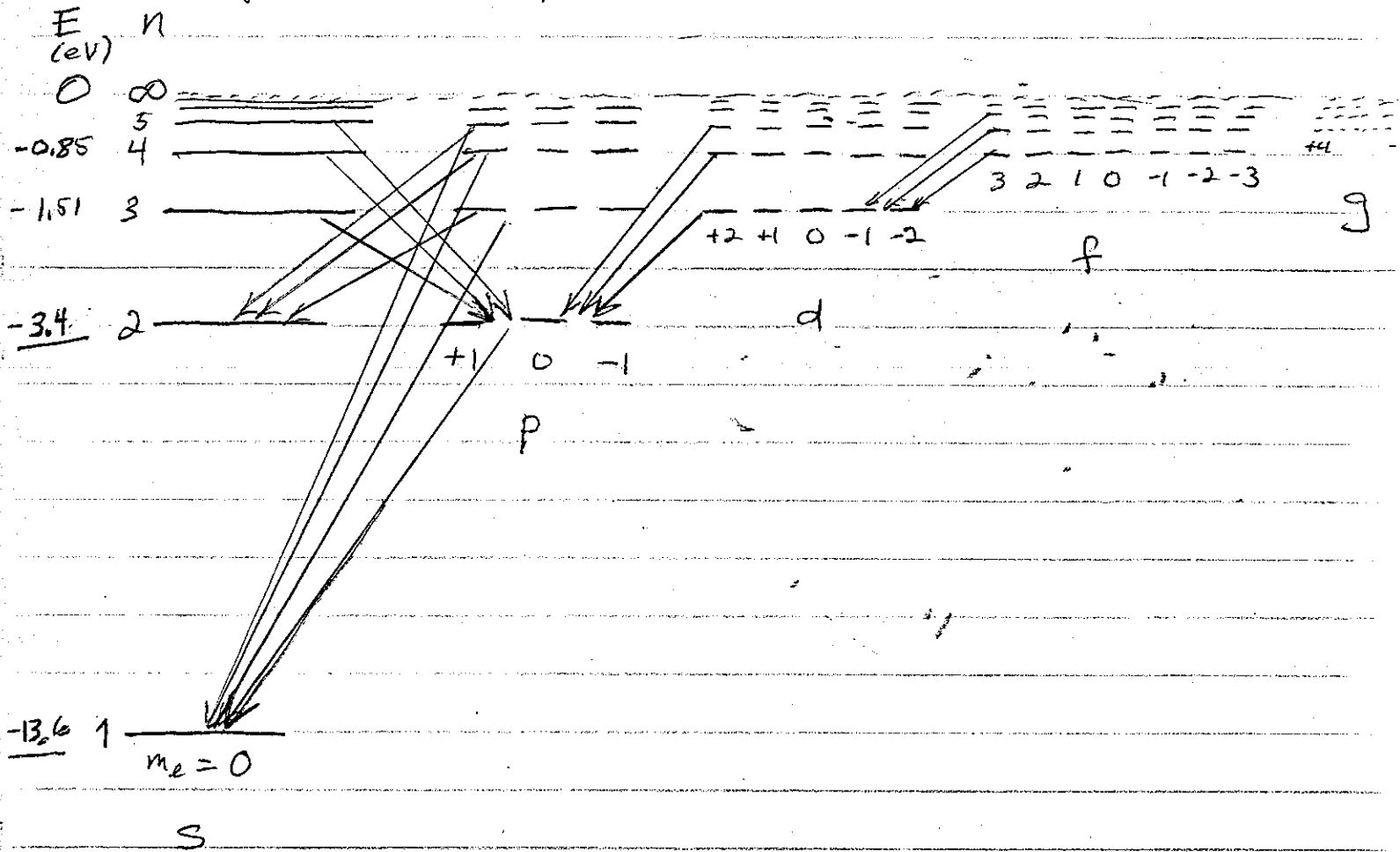
$Q = 0$
 $g \frac{dQ}{dt}$

H-Atom



$R = \text{Rydberg}$
 $V = -\frac{e^2}{r}$
 "no penetration" (actually a fake)
 $0 < r < \infty$ only

Energy level diagram - H-atom



Spectral transitions match Balmer series
 but also must account for Θ, Φ functions
 allowed — any n change: $\Delta n \neq 0$

— l, m_l as before: $\Delta l = \pm 1$

$\Delta m_l = 0, \pm 1$

$n \rightarrow n'=1$ — Lyman must start p orb

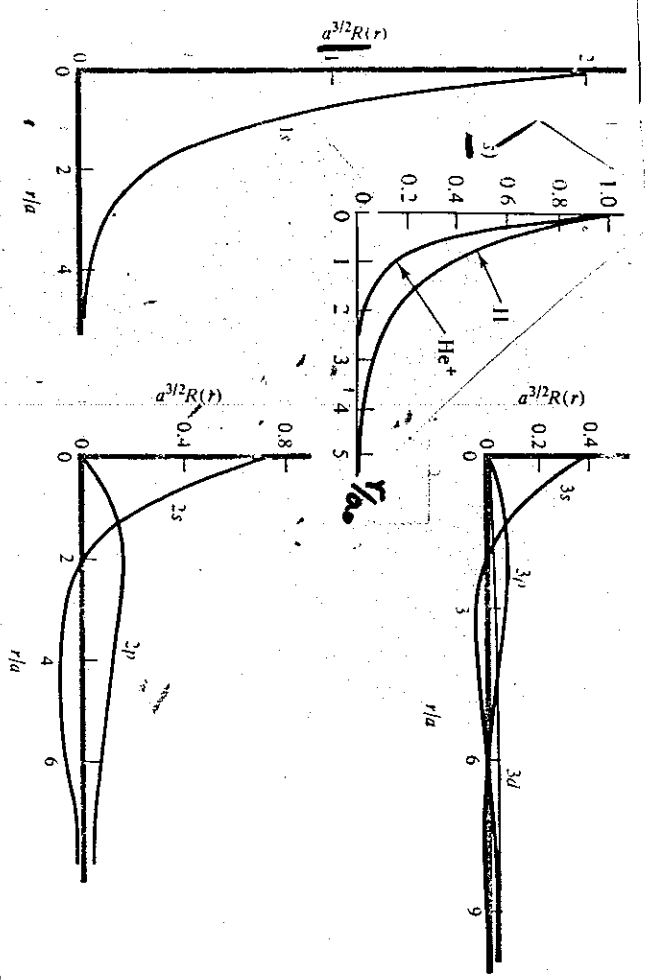
$n \rightarrow n'=2$ — Balmer must start d or s orb \rightarrow p

or p orb \rightarrow s

etc.

Test with Zeeman effect — $m_l \beta H = E'$ added E due to fields

From I. Levine Physical Chemistry
(McGraw-Hill, 1978)



Some different representation
of Hydrogen orbitals.

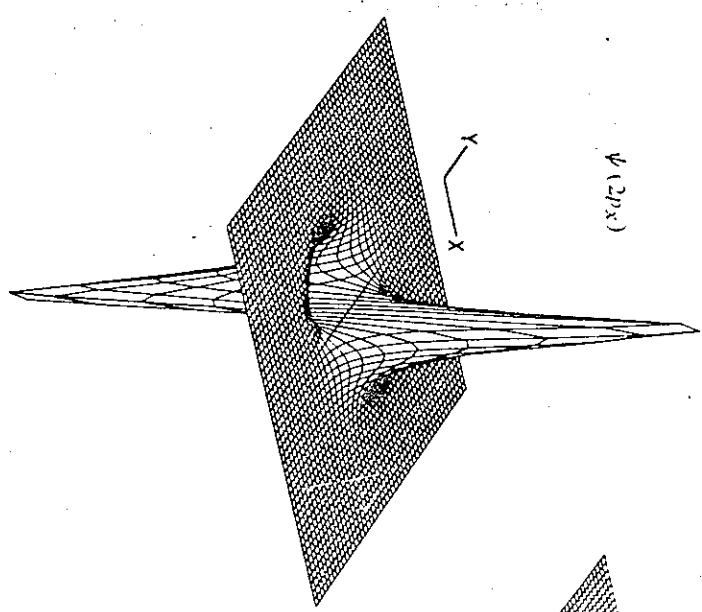
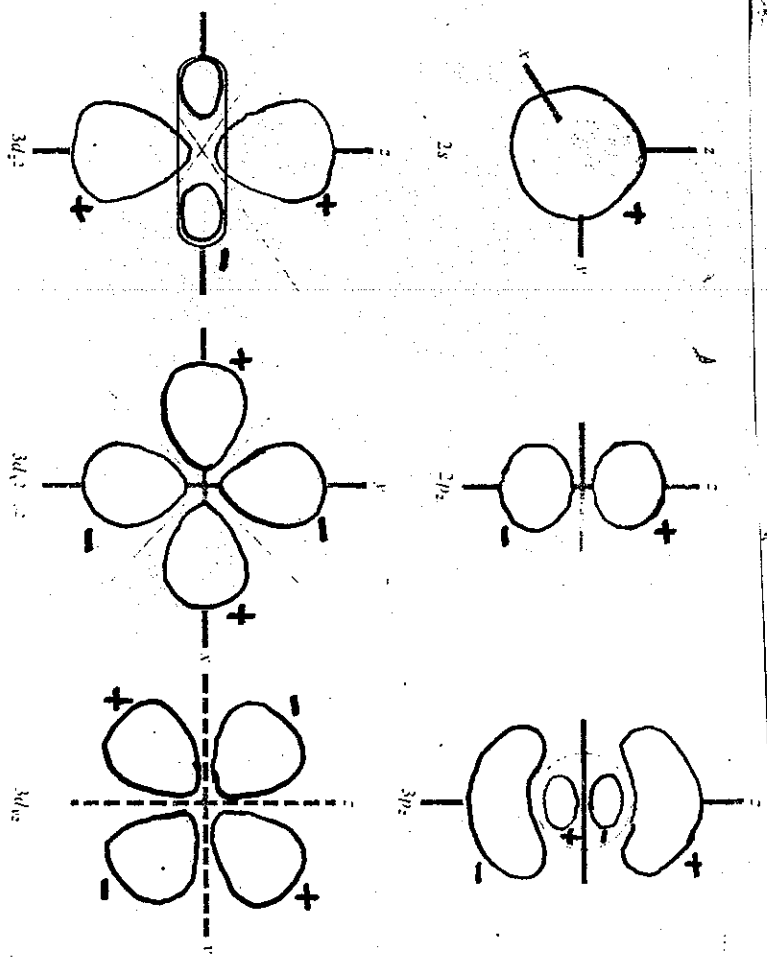


Figure 19.6

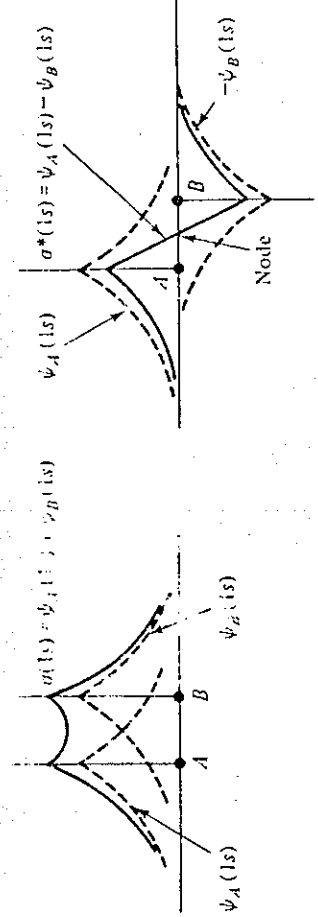
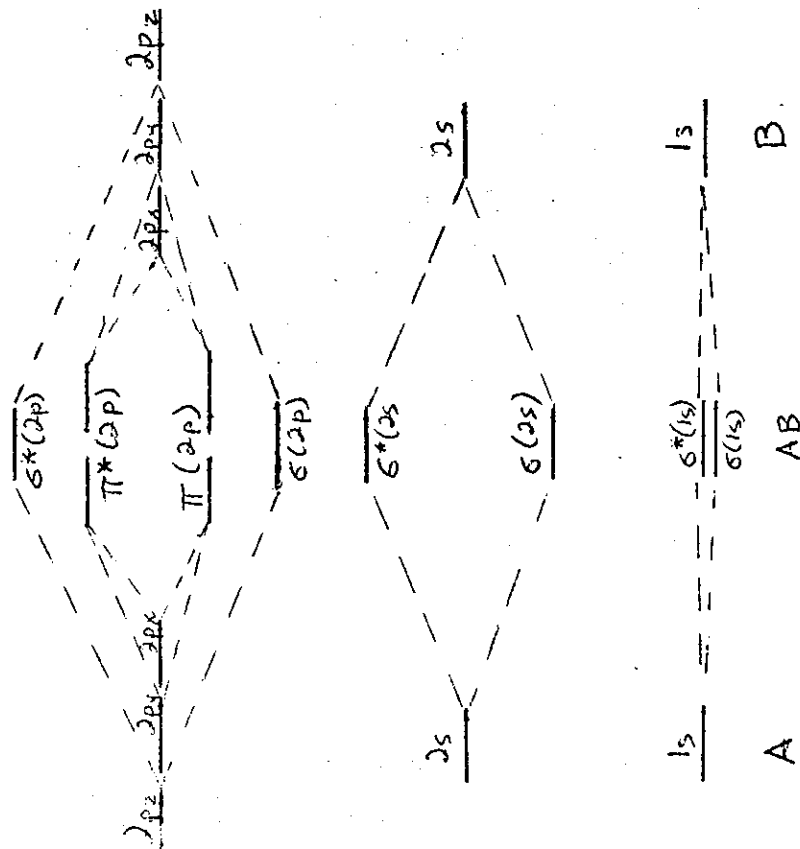
Shapes of some hydrogen-atom orbitals. (Not drawn to scale.) Note the different orientation of the axes in the $3d_{x^2-y^2}$ figure compared with the others. Not shown are the $3d_{xy}$ and $3d_{zx}$ orbitals; these have their lobes between the x and y axes and the x and z axes, respectively.



Nodal surfaces indicated by dotted line - - - .

Fig. 9.15 Computer plots of $\psi(1s)$, $\psi(2s)$, and $\psi(2p_x)$. ψ is plotted in perspective in the x - y plane. The marked line in front of the grid is of length $10a_0 = 5.29 \text{ \AA}$. [From A. Streitwieser, Jr., and P. H. Owens, *Orbital and Electron Density Diagrams*, Macmillan, New York, 1973. Copyright 1973 by Macmillan Publishing Co., Inc.]

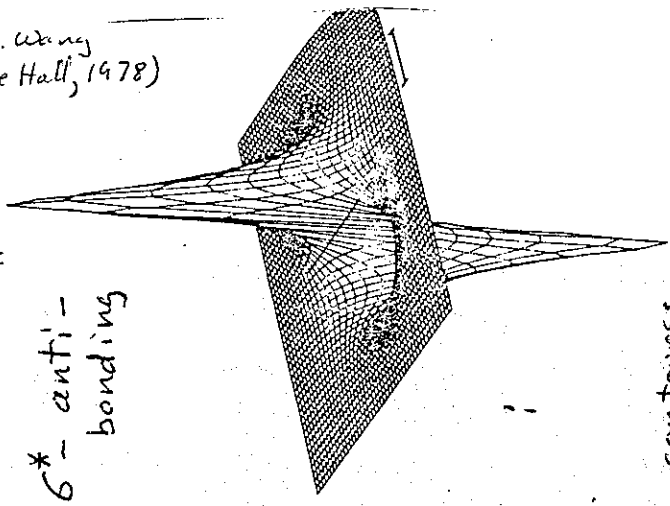
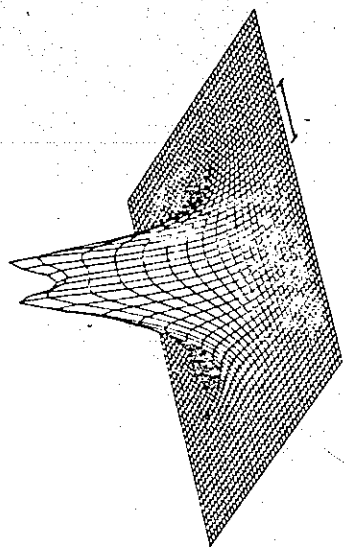
Homonuclear diatomic MO scheme



H_2 lowest energy molecular orbitals

$\sigma(1s)$ bonding

$\sigma^*(1s)$ anti-bonding



Electron density contours:

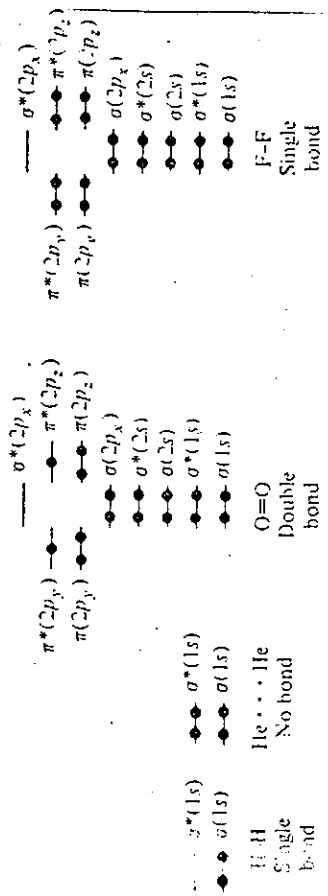
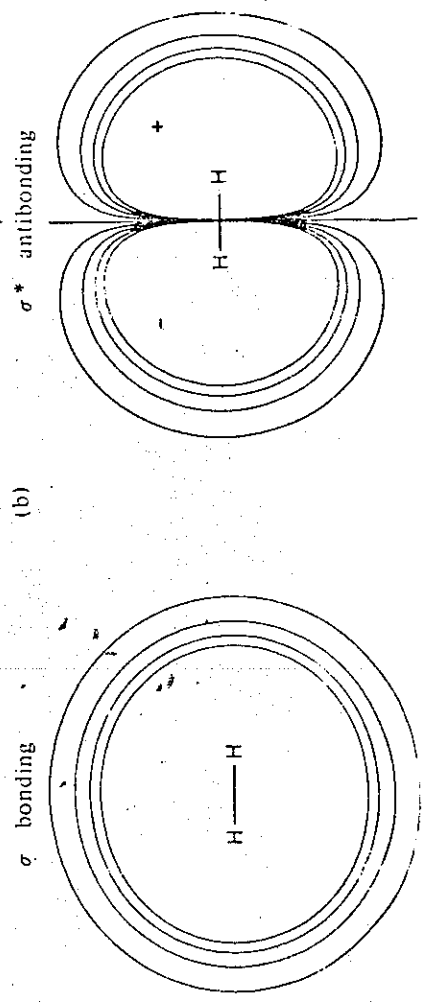


Fig. 9.21 Typical energy-level pattern for a homonuclear diatomic molecule. The type of bonding and the change in bonding on exciting, ionizing, or capturing an electron can be understood for the first 10 elements.

From A. Tomasco, K. Sauer, J.C. Wang
Physical Chemistry (Prentice Hall, 1978)

π-bonding and antibonding orbitals for diatomics

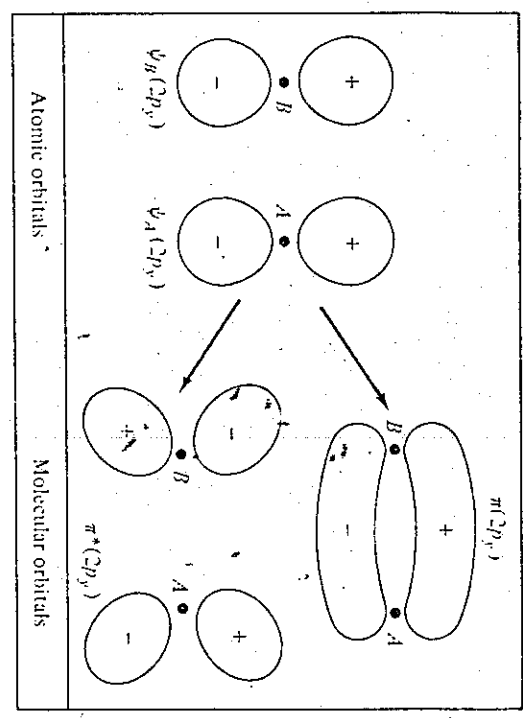
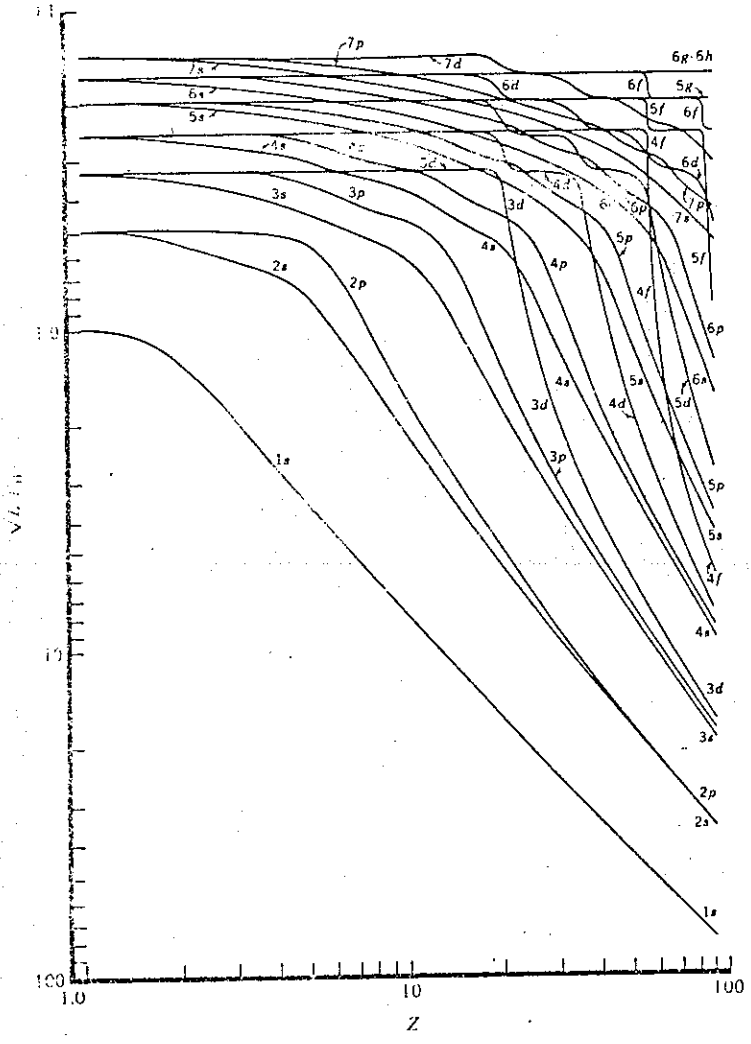
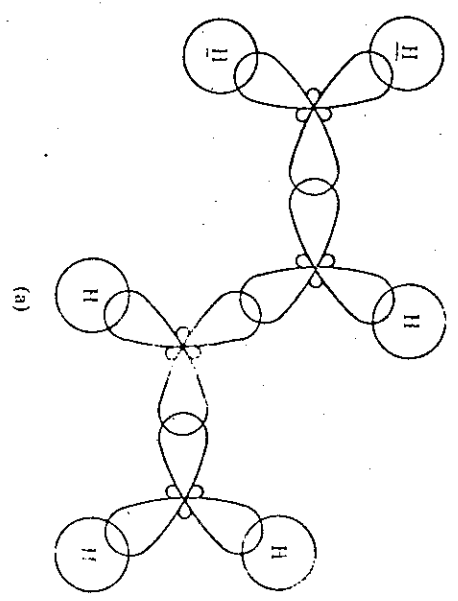


Fig. 9.20 Combination of two $2p_y$ atomic orbitals into a bonding π and antibonding π^* molecular orbital. The drawings represent the angular distributions of the electron densities; the signs + and - specify the phases of the wavefunction.

Orbital Energy vs. Atomic Number for neutral atoms. $E_H = -13.6 \text{ eV}$. (Levine)



Butadiene σ -bonding (hybrids)



π -MO's: Atomic orbitals \rightarrow π Molecular orbitals

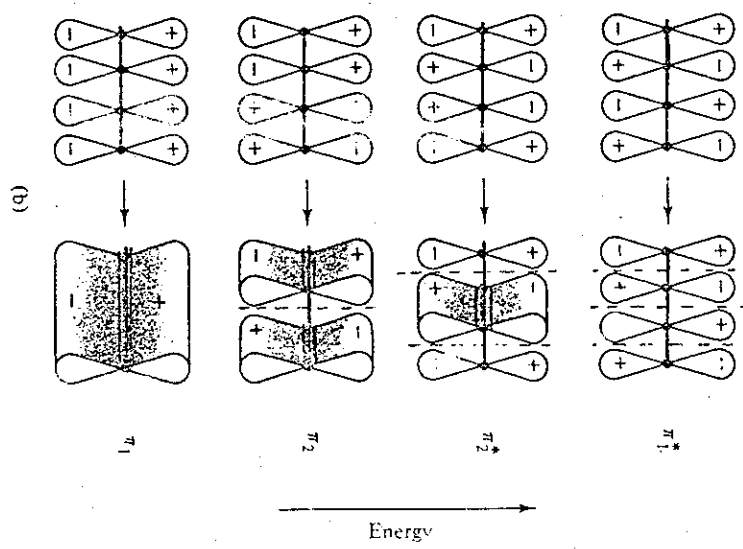


Fig. 9.24 (a) The σ bonds in butadiene $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$. (b) The π molecular orbitals in butadiene. The four π electrons occupy the two bonding orbitals, π_1 and π_2 . The dots (•) represent the positions of the carbon atoms. (dashed lines indicate nodes)