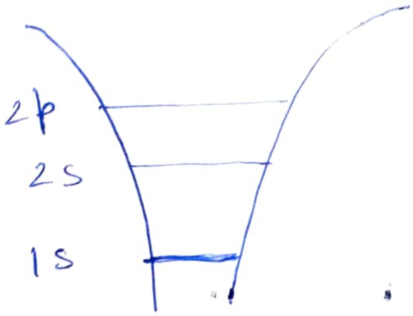
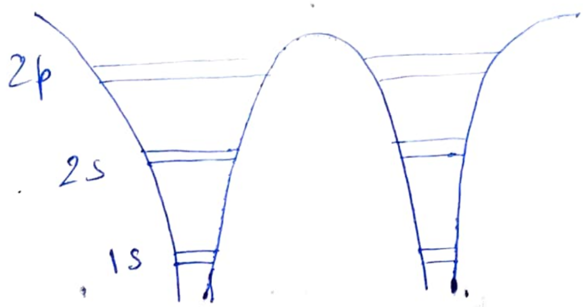
--Do--

Note Band theory of solids

(13) Energy Spectra in atoms, molecules, and solids

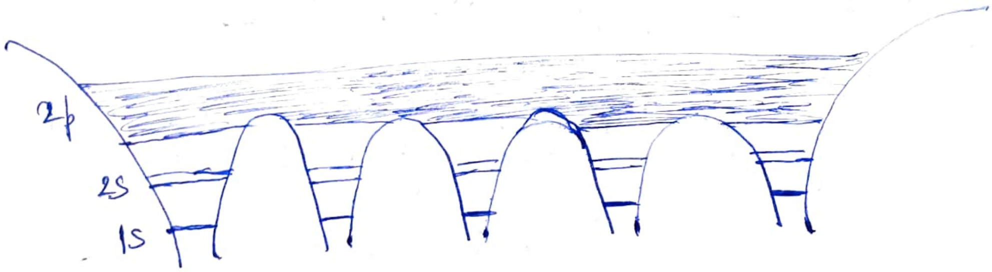


Li atom



Li_2 molecule

(double well potential)



Solid

Energy band is formed

Many atoms comes close together

⇓

bands form

The energy spectrum is comprised of a set of discrete doublets.

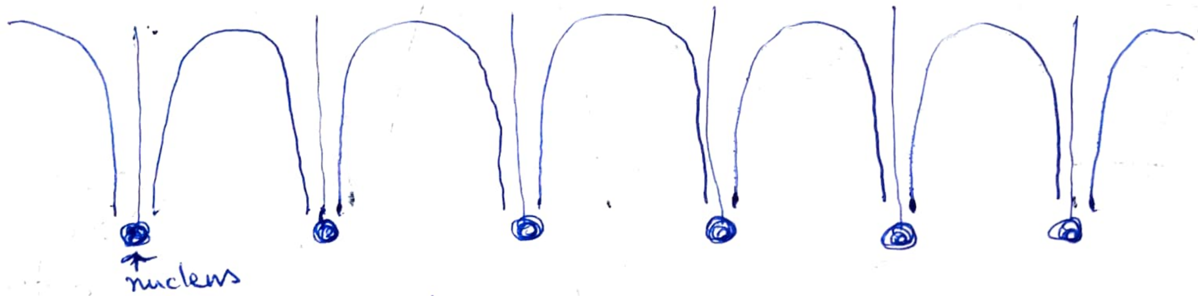
Because of interaction between a two atomic potentials.

Each atomic level splits into two.

Energy Bands in Solids

The Block theorem

Assume a crystalline solid:



Crystal potential seen by electron

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(\vec{r})\right]\psi(\vec{r}) = E(\vec{r})$$

[time independent Schrödinger equation in 3D 'T.I.S.E.']

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \quad \text{--- (1)}$$

$V(\vec{r})$ is periodic

It has same translational symmetry as the lattice

$$V(\vec{r}+\vec{R}) = V(\vec{r})$$

$\vec{R}$ is lattice vector

According ~~the~~ to Block theorem the solution of T.I.S.E. can be expressed as

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r}) \qquad (2)$$

where $u_k(\vec{r})$ has same translational symmetry

$$u_{\vec{k}}(\vec{r}+\vec{R}) = u_k(\vec{r})$$

This part is free electron solution (when $V=0$)

$\boxed{\vec{p} = \vec{k}\hbar}$

Put (2) into (1)

$$\left[-\frac{\hbar^2}{2m}(\nabla + i\vec{k})^2 + V(\vec{r})\right] u_{\vec{k}}(\vec{r}) = E_{\vec{k}}\, u_{\vec{k}}(\vec{r})$$

Easy to plot solutions in 1-D lattice