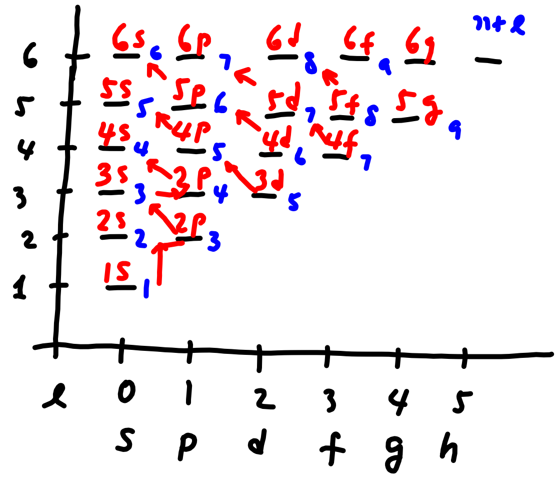
Complex atoms + Periodic table

Energy level Rules:

1) higher n higher energy

n

2) higher n+ℓ has higher energy



atomic shell model

$-\frac{Ze^2}{r}$

energy levels	1S	2S 2P	3S 3P	4S 3d 4P	5S 4d 5p	6s 4f 5d 6p	7s 5f 6d 7p
# electrons	(2)	(2 6)	(2 6)	(2 10 6)	(2 10 6)	(2 14 10 6)	(2 14 10 6
	2	8	8	18	18	32	32
	↑	↑	↑	↑	↑	↑	↑
	1st row	2 row	third	4th	5th	6th	7th

For neon : $1s^2 2s^2 2p^6$

Chapter 9: Scattering Theory for finite-range potential

(not Coulomb)

A wave packet

$$\psi(\vec{r},t_0) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} a_k(t_0)$$

$a_k \sim e^{-\frac{1}{2a}(\vec{k}-\vec{k}_0)^2}$

$\psi \sim e^{i\vec{k}_0\cdot\vec{r}} e^{-\frac{1}{2}ar^2}$ Expand in terms of the exact solution ψ_k

$$\Big(\underbrace{\frac{\hbar^2\nabla^2}{2m}}_{= -H_0} + E_k\Big)\psi_k = V(r)\psi_k(r) \qquad E_k > 0$$

$$E_k = \frac{\hbar^2 k^2}{2m} > 0$$

The generate time-dependent solution is then

$$\psi(\vec{r},t_0) = \int \frac{d^3k}{(2\pi)^3} \psi_k(r) A_k$$

$$\hookrightarrow \psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^3} \psi_k(r) A_k e^{-iE_k(t-t_0)/\hbar}$$

This then means that

$$|\psi_k\rangle = \frac{1}{-H_0+E_k} V|\psi_k\rangle + |\phi_0\rangle$$

such that $(-H_0+E)|\phi_0\rangle = 0$

The wave function

$$\langle r|\psi_k\rangle = \int d^3\vec{r}\,' \underbrace{\langle r|\frac{1}{-H_0+E_k}|r'\rangle}_{G(r,r';k)} \langle r'|V|\psi_k\rangle + \langle r|\phi_0\rangle$$

$e^{-it(H-E)/\hbar}$

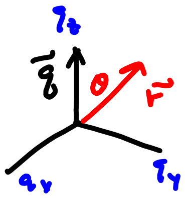
$$E_k = \frac{\hbar^2 k^2}{2m}$$

$$\psi_k(r) = \int d^3\vec{r}\,' G(\vec{r},\vec{r}\,';k) V(\vec{r}\,')\psi_k(\vec{r}\,') + \phi_0(r)$$

To compute the resolvent $\langle \vec r | \frac{1}{E_k - H_0} | \vec r'\rangle$

$$G(\vec r, \vec r'; k) = \int \frac{d^3q}{(2\pi)^3} \langle \vec r | \frac{1}{E_k - H_0}|q\rangle\langle q|\vec r'\rangle$$

q, k wave #



$$= \int \frac{d^3q}{(2\pi)^3}\frac{2m}{\hbar^2}\frac{1}{k^2-q^2} e^{i\vec q\cdot(\vec r' - \vec r)}$$

$E_k = \frac{\hbar^2k^2}{2m}$

$\vec r$ temporarily $\parallel \hat y$

$$= \frac{2m}{\hbar^2}\frac{2\pi}{(2\pi)^3}\int_0^\pi \sin\theta\, d\theta\, q^2 dq \frac{-1}{q^2-k^2} e^{iqr\cos\theta}$$

$$= \frac{2m}{\hbar^2}\frac{2\pi}{(2\pi)^3}\int_0^\infty q^2dq\left(\frac{-1}{q^2-k^2}\right)\int_{-1}^1 dx\, e^{iqrx}$$

$x=\cos\theta$
$dx=-\sin\theta\, d\theta$

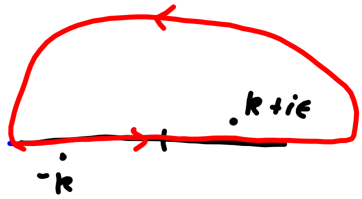
$$= \frac{2m}{\hbar^2}\frac{2\pi}{(2\pi)^3}\int_0^\infty q^2dq\left(\frac{-1}{q^2-k^2}\right)\frac{1}{iqr}\left[e^{iqr}-e^{-iqr}\right] \qquad \frac{e^{iqrx}}{iqr}\Big|_{-1}^{1}$$

$$= \frac{2m}{\hbar^2}\frac{\cancel{2\pi}}{(2\pi)^{\cancel{3}\,2}}\int_{-\infty}^\infty q^{\cancel{2}}\,dq\, \frac{-1}{q^2-k^2}\,\frac{1}{i\cancel{q}r}\,e^{iqr}$$

$\int_0^\infty q^2dq\left(-e^{-iqr}\right)$

$\int_0^{-\infty} -q'^2 dq' \qquad q=-q'$

$$= \frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\frac{-1}{ir}\int_{-\infty}^\infty q\, dq\, \frac{1}{q^2-k^2}\,e^{iqr}$$



$$\frac{1}{(q-k)(q+k)}$$

$$= \frac{\cancel{2}m}{\hbar^2}\frac{1}{(2\pi)^{1}}\frac{-1}{ir}\,\cancel{2\pi}(i)\,\frac{\cancel{k}}{\cancel{2k}}\,e^{ikr}$$

$$G(\vec r, \vec r'; k) = -\frac{m}{\hbar^2}\frac{1}{2\pi}\frac{1}{r}e^{ikr} = -\frac{m}{\hbar^2}\frac{1}{2\pi}\frac{1}{|\vec r-\vec r'|}e^{ik|\vec r-\vec r'|}$$

$$\boxed{\psi_k(\vec r) = e^{i\vec k\cdot\vec r} - \frac{m}{2\pi\hbar^2}\int d^3r'\,\frac{e^{ik|\vec r-\vec r'|}}{|\vec r-\vec r'|}\,V(\vec r')\,\psi_k(\vec r')}$$

$\phi_0(r) = e^{i\vec k\cdot\vec r}$