Nuclear physics → approx. methods

° How do we write down electron wave f^{n}'s for $z \geq 3$ atoms consistent w/ Fermi statistics

° Strange features of Helium

° Notation for atomic states

A one particle quantum state
→ uniquely specified energy eigenstate

for atoms → hydrogen like but w/ general z — z protons — charge z
$\psi_{nlm}(\vec{r})|+\rangle$

2 energy eigenstate $\psi_0(\vec{r})$ $\psi_1(\vec{r})$

spin ½ particle

4 one particle states:

$$\varphi_1 = \psi_0(\vec{r}) \otimes |+\rangle$$
$$\varphi_2 = \psi_0(\vec{r}) \otimes |-\rangle$$
$$\varphi_3 = \psi_1(\vec{r}) \otimes |+\rangle$$
$$\varphi_4 = \psi_1(\vec{r}) \otimes |-\rangle$$

Atomic physics: have N spin ½ particles

$\varphi_j(i)$ = i^{th} fermion in j^{th} one particle state

$\varphi_3(2) = \psi_1(\vec{r}_2) \otimes |+\rangle_2$ second fermion

N spin ½ fermions → $\mathcal{H} = (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)_1 \otimes (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)_2 \otimes \dots \otimes (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)_N$

Slater Determinant

$$\Psi(1,2,\dots,N) = \frac{1}{N!} \begin{vmatrix} \varphi_1(1) & \varphi_1(2) & \dots & \varphi_1(N) \\ \varphi_2(1) & \varphi_2(2) & & \varphi_2(N) \\ \vdots & \vdots & & \vdots \\ \varphi_N(1) & \varphi_N(2) & \dots & \varphi_N(N) \end{vmatrix}$$

expand – but w/ $\otimes$

exchange 1st 2 particles (to check if antisymmetric)

exchange 1st 2 columns

exchange columns for det( ) changes sign

Li: $(1s)^2(2s)$

3 electrons → put in 3 1 particle states

$\varphi_1 = \psi_{100}(\vec{r}) \otimes |+\rangle$

$\varphi_2 = \psi_{100}(\vec{r}) \otimes |-\rangle$

$\varphi_3 = \psi_{200}(\vec{r}) \otimes |+\rangle$ for $|-\rangle$

$$\psi(1,2,3) = \frac{1}{3!} \begin{vmatrix} \varphi_1(1) & \varphi_1(2) & \varphi_1(3) \\ \varphi_2(1) & \varphi_2(2) & \varphi_2(3) \\ \varphi_3(1) & \varphi_3(2) & \varphi_3(3) \end{vmatrix}$$

$$= \frac{1}{3!}\Big(\varphi_1(1)\big(\varphi_2(2)\varphi_3(3) - \varphi_2(3)\varphi_3(2)\big)$$

$$- \varphi_1(2)\big(\qquad \big)$$

$$+ \varphi_1(3)\big(\qquad \big)\Big)$$

$\varphi_1(1)\varphi_2(3)\varphi_3(2)$

$$= \frac{1}{3!}\Big(\psi_{100}(\vec{r}_1)\otimes|+\rangle_1 \big(\psi_{100}(\vec{r}_2)\otimes|-\rangle_2 \cdot \psi_{300}(\vec{r}_3)\otimes|+\rangle_3 - \qquad \big)\ldots$$

.... +5 more terms

include all possible states of 1 particle

He $(1s)^2$ – 2 electrons in 1s states in ground states

Excited states:

$$E_{n_1,n_2} = (-13.6\text{eV}) \cdot 4 \cdot \left(\frac{1}{n_1^2} + \frac{1}{n_2^2}\right)$$

3^2 energy of 1st electron energy of 2^{nd} electron

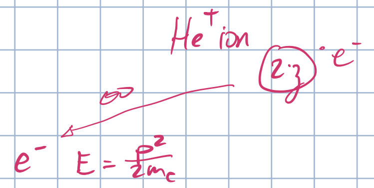
E_{grnd}: $E_{1,1} = \underline{-108.8\text{eV}}$ ground

$E_{1,n_2} = -54.4\text{eV}\left(1 + \frac{1}{n_2^2}\right) \geq \underline{-54.4\text{eV}}$ 1 excited, ground

$E_{2,2} = -54.4\text{eV}\left(\frac{1}{4} + \frac{1}{4}\right) = \underline{-27.2\text{eV}}$ both in 2^{nd} excited state remove 2 electrons, put e ∞

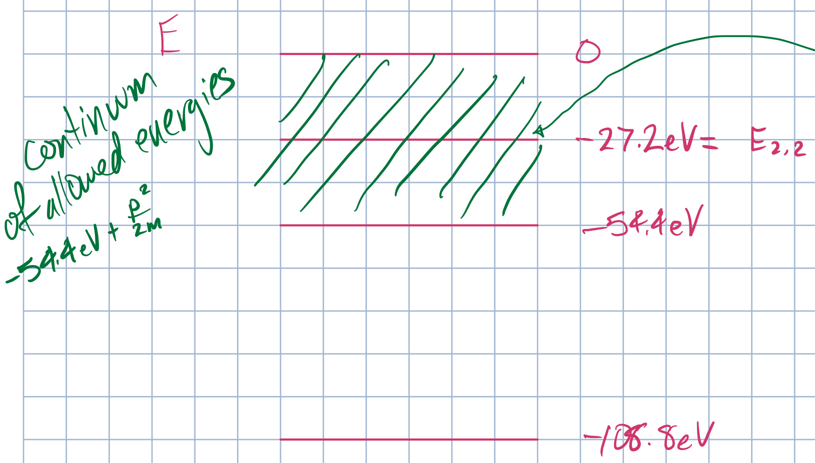
takes energy $-108.8\,eV$

remove 1 electron e ∞



$$E^{He^+}_{grnd} = -54.4\,eV$$

$$E = E^{He^+}_{grnd} + \frac{p_e^2}{2m_e}$$



but we have @ bound state in continuum!

bound state w/ higher energy than where continuum starts

when looking @ bound & scattering in 1-D, found bound states & scattering states
E could vary continuously, can adjust KE of what was being scattered

here, continuum starts @ $-54.4\,eV$ b/c if we remove one e^- to ∞ w/ some KE, then E of combined system is binding energy of He ion + KE part ☆