PHYS261 Atomic Physics and Physical Optics

Lecture Tuesday 7. October 2008

Topics:

Helium; Final touch

Helium; Excited States, Doubly excited states

Autoionizing states – also Auger Effect

Comment:

Revised version;

The Perturbation Theory (see next slide – work)

$$\left[-\frac{\hbar^2}{2m_e}\nabla_{r_1}^{2} - \frac{Z\,e^2}{r_1} - \frac{\hbar^2}{2m_e}\nabla_{r_2}^{2} - \frac{Z\,e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\right]\Psi(\mathbf{r}_1,\mathbf{r}_2) = E\,\Psi(\mathbf{r}_1,\mathbf{r}_2)$$

Repulsion expectation Value

Evaluation of the repulsion term using the multipole expansion

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} = \sum_{LM}\frac{4\pi}{2L+1}\,\frac{r_<^L}{r_>^{L+1}}\,Y_{LM}^{\star}(\hat{r}_1)\,Y_{LM}(\hat{r}_2)$$

where

$$r_< = r_1,\quad r_> = r_2 \quad \text{for} \quad |\mathbf{r}_1| < |\mathbf{r}_2|$$

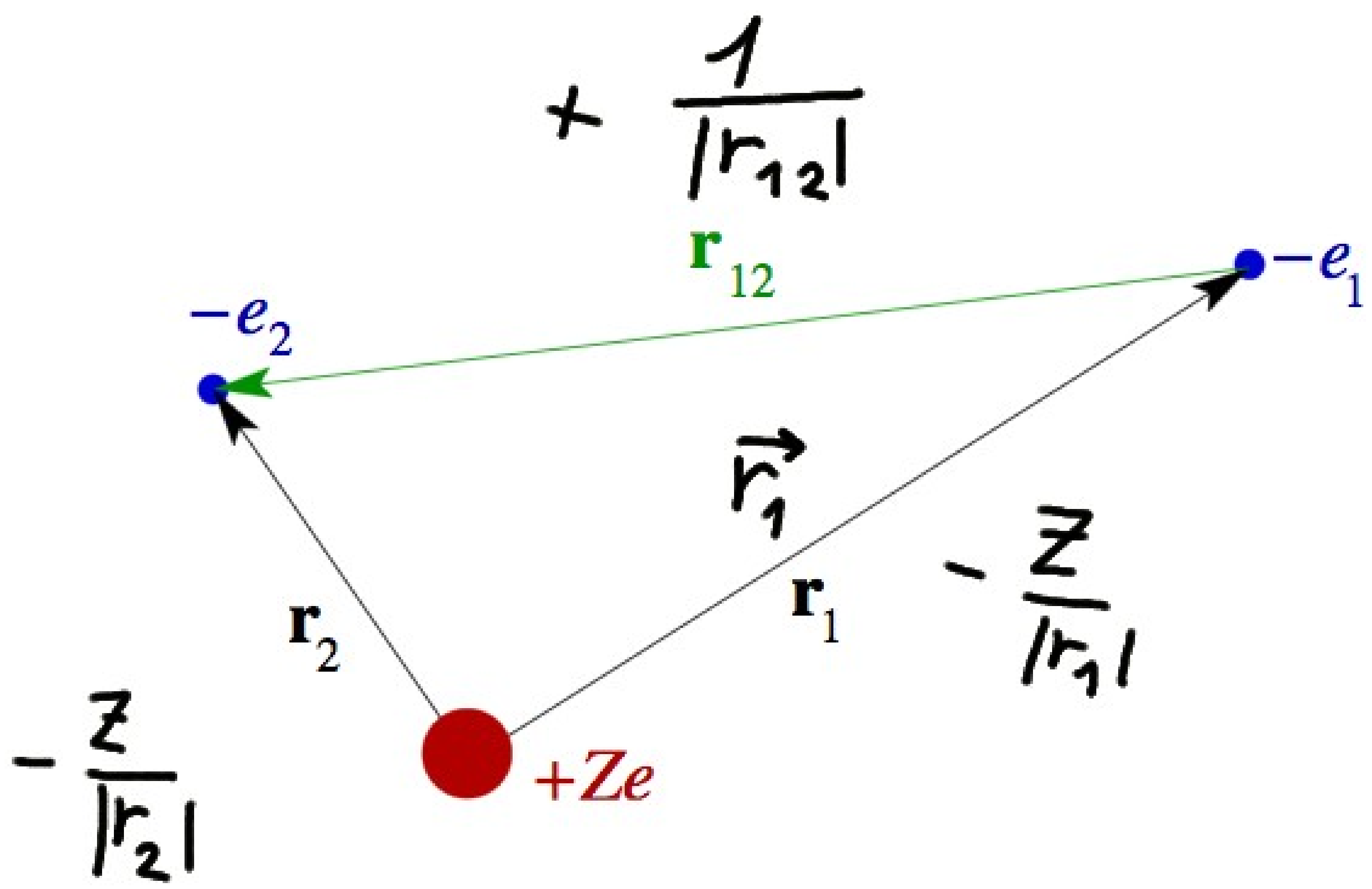
$$r_< = r_2,\quad r_> = r_1 \quad \text{for} \quad |\mathbf{r}_1| > |\mathbf{r}_2|$$

Perturbation theory result:

$$\int d^3\mathbf{r}_1\int d^3\mathbf{r}_2\;\psi_{100}^{\star}(\mathbf{r}_1)\,\psi_{100}^{\star}(\mathbf{r}_2)\,\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\,\psi_{100}(\mathbf{r}_1)\,\psi_{100}(\mathbf{r}_2) = \frac{5}{8}\frac{Ze^2}{a_0}$$

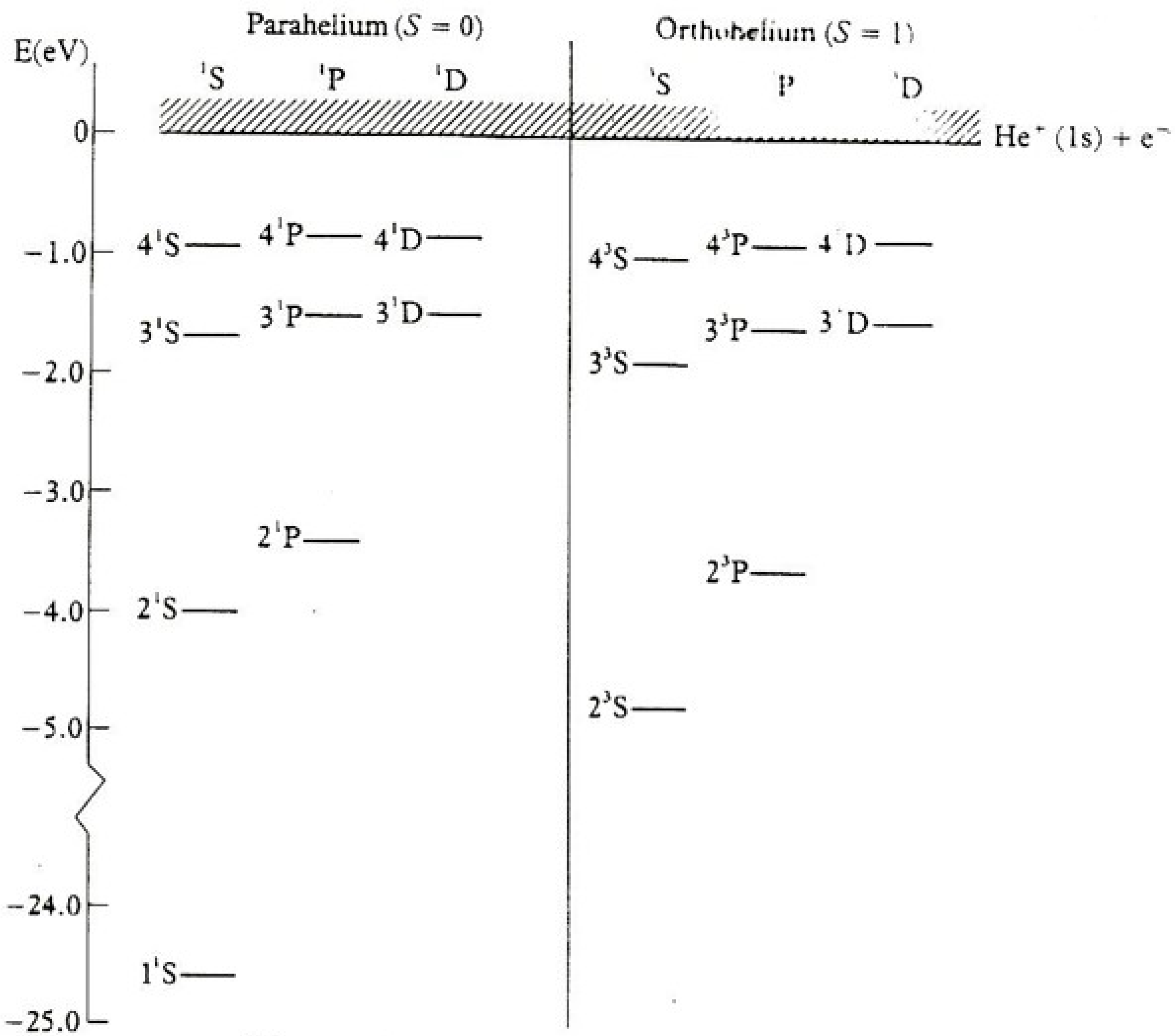
$$E(Z,1s,1s) = -\frac{1}{2}Z^2 - \frac{1}{2}Z^2 + \frac{5}{8}Z \quad [a.u.]$$

The Variational Method



H minus is also possible
Negative ion of
hydrogen

Experiment – Level scheme for Helium



The experimental values of the lowest energy levels of helium.
$E = 0$ corresponds to the ionisation threshold.

Variational Method basics

$H\varphi = E\varphi$ $\qquad u(\vec{x}, \alpha)$ $\qquad \alpha$ - parameter

$e^{-\alpha r} \cdot N(\alpha)$

"best possible α"

i.e. gives best approximation to ??

ENERGY E

$\langle u(\alpha) | H | u(\alpha) \rangle \cong E(\alpha)$?

for which α $E(\alpha)$ closest to E.

$u(\vec{x}, \alpha) = \sum_i c_i \varphi_i(\vec{x})$ $\quad | \quad H\varphi_i = E_i \varphi_i$

E_0 (or E_{1s} in H)

$\sum_i c_i^* \sum_j c_j \int \varphi_i^*(x) H(x) \varphi_j(x) \, d\tau$ $\quad$ ($H(x)\varphi_j(x) \to E_j \delta_{ij}$)

$\langle E \rangle = \langle H \rangle = E_j \sum_i \sum_j c_i^* c_j \delta_{ij} = \sum_i |c_i|^2 E_i \geq \sum_i |c_i|^2 E_0$ $\quad$ ($\sum_i |c_i|^2 = 1$)

$E_\alpha \to \langle E \rangle = \langle H \rangle \geq E_0$

$\langle u(\alpha) | u(\alpha) \rangle = \sum_i c_i^* \sum_j c_j \langle \varphi_i | \varphi_j \rangle$ $\quad$ ($\langle \varphi_i | \varphi_j \rangle = \delta_{ij}$)

$= \sum_i |c_i|^2 = 1$

normalized

$$E(z) = \left(z^2 - 2z Z + \frac{5}{8} z\right) E_0$$

find z by $\frac{\partial E(z)}{\partial z} = 0$

$$2z - 2Z + \frac{5}{8} = 0$$

$$z = Z - \frac{5}{16}$$

≈ 0.3

$$z = Z - 0.3$$

Derivation of "EXTREMUM"

$$E(\varphi) \geq E(\varphi_0)$$

$$\varphi = \sum_i c_i \varphi_i$$

To remember ...... in preliminary version

Carousel (pictures t include??)
Flogiston - Look it up

The joke about Who wrote Hamlet - for remembering
Stern-Gerlach (see wikipedia)

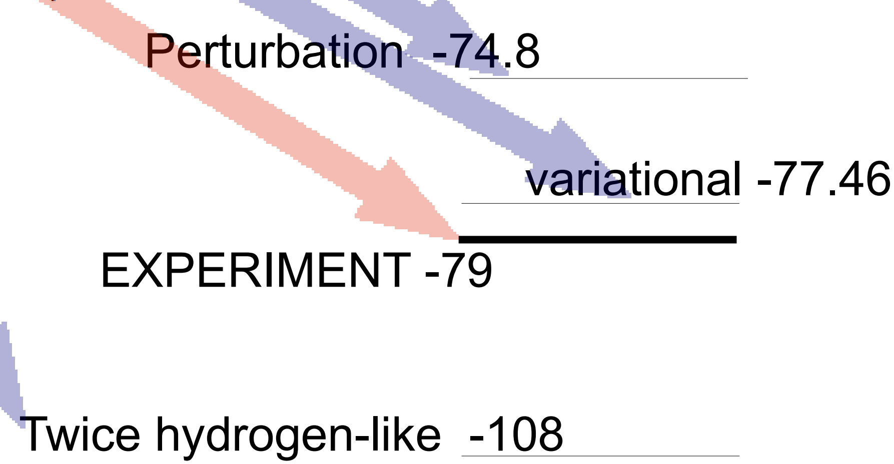
Quantiki (Quantum wiki) - very bad QM intro
Quantum Computation

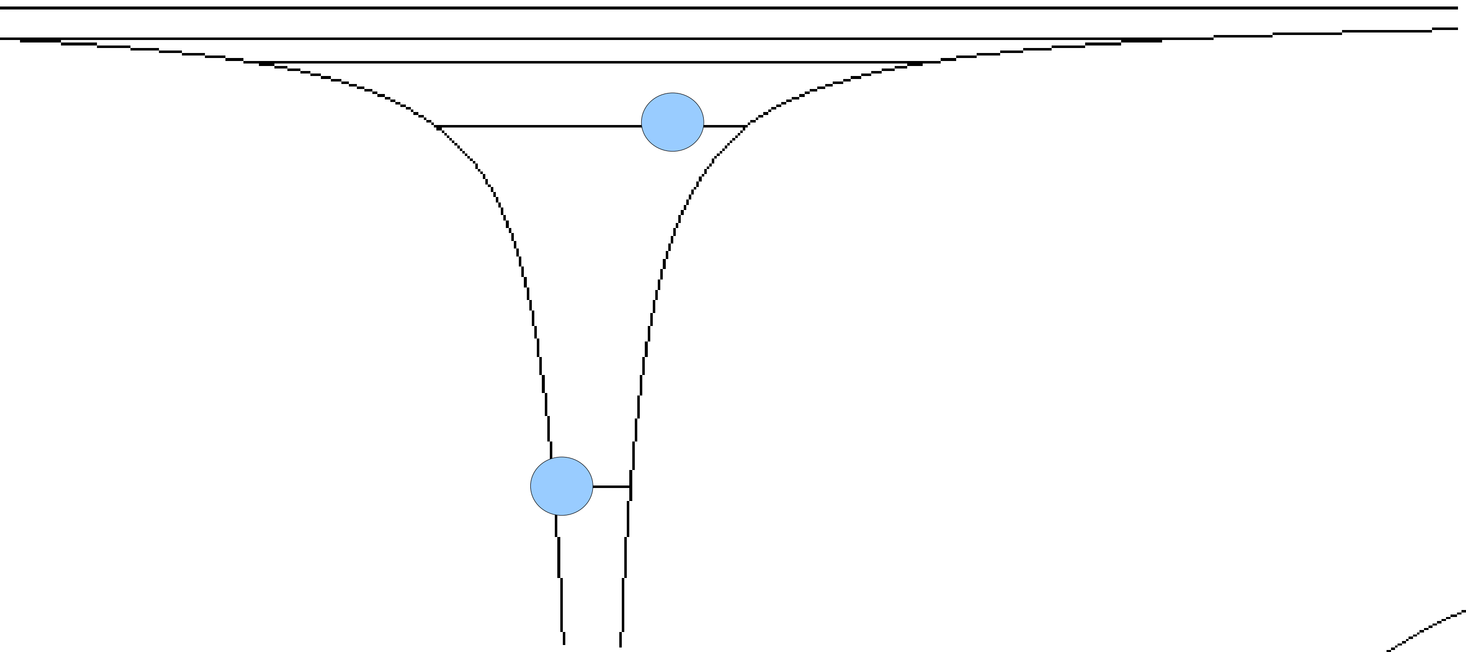
	H^-	He	Li^+	Be^{++}	$B^{(3+)}$	$C^{(4+)}$
Z	1	2	3	4	5	6
Ion.pot.[au]	0,757	24,60	75,62	153,95	259,49	392,22
2.Ion.pot	13,600	54,40	122,40	217,60	340,00	489,60
EXP.BindEner	-14,357	-79,00	-198,02	-371,55	-599,49	-881,82
$2\,E_{1s}$	-27,200	-108,80	-244,80	-435,20	-680,00	-979,20
$2\,E_{1s} + 5/8\,Z$	-10,200	-74,80	-193,80	-367,20	-595,00	-877,20
Variational	-12,856	-77,46	-196,46	-369,86	-597,66	-879,86
EXP.BindEner	-14,357	-79,00	-198,02	-371,55	-599,49	-881,82

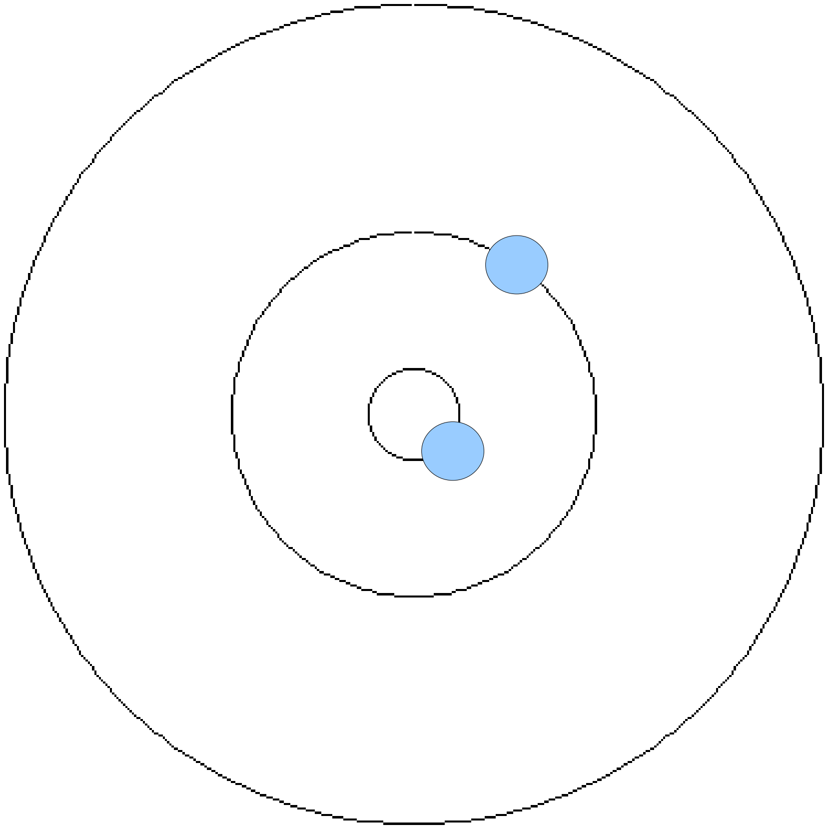
Ion.pot. Ionization potential: The energy to remove the first electron

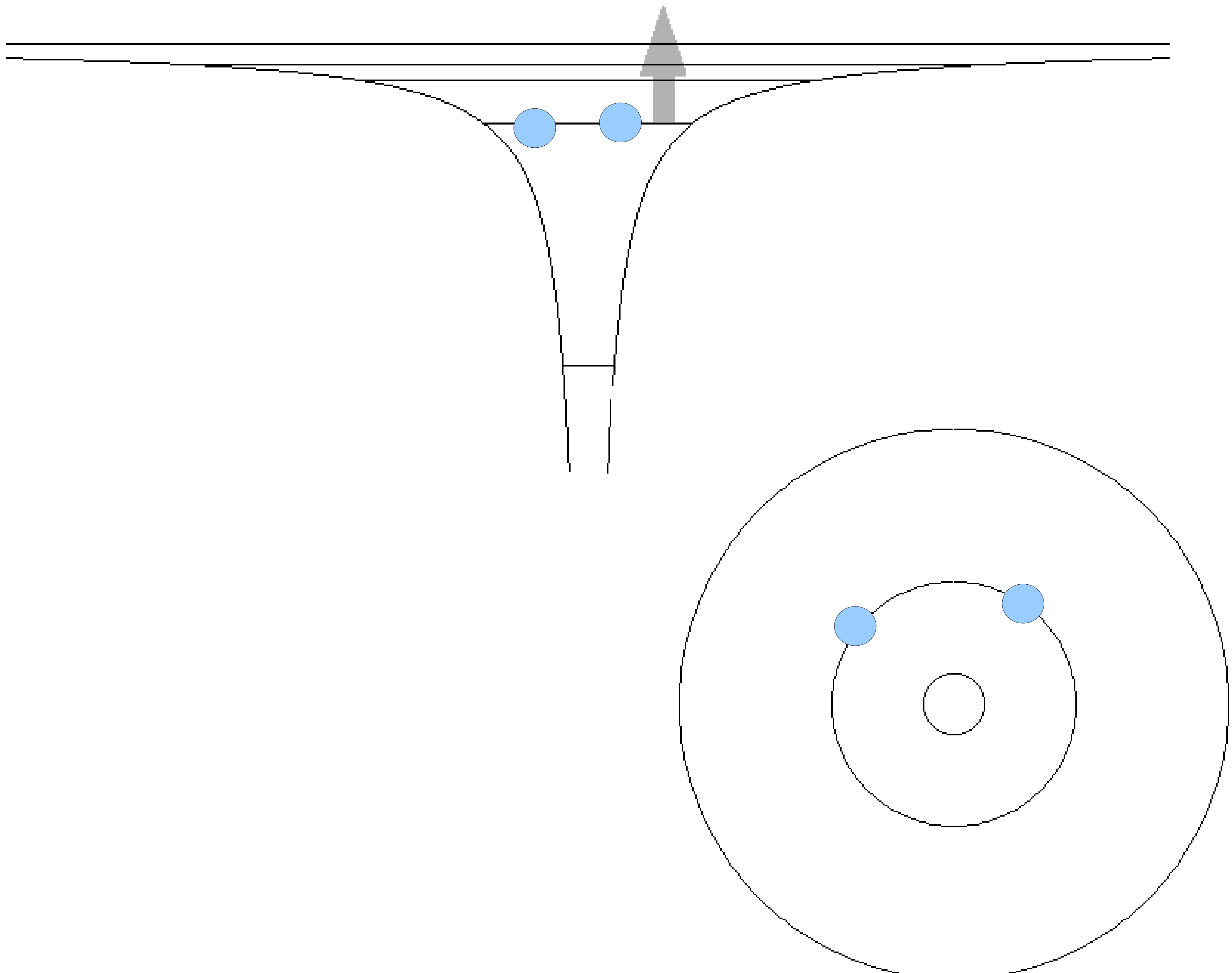
2.Ion.pot Second Ionization potential: The energy to remove the second electron

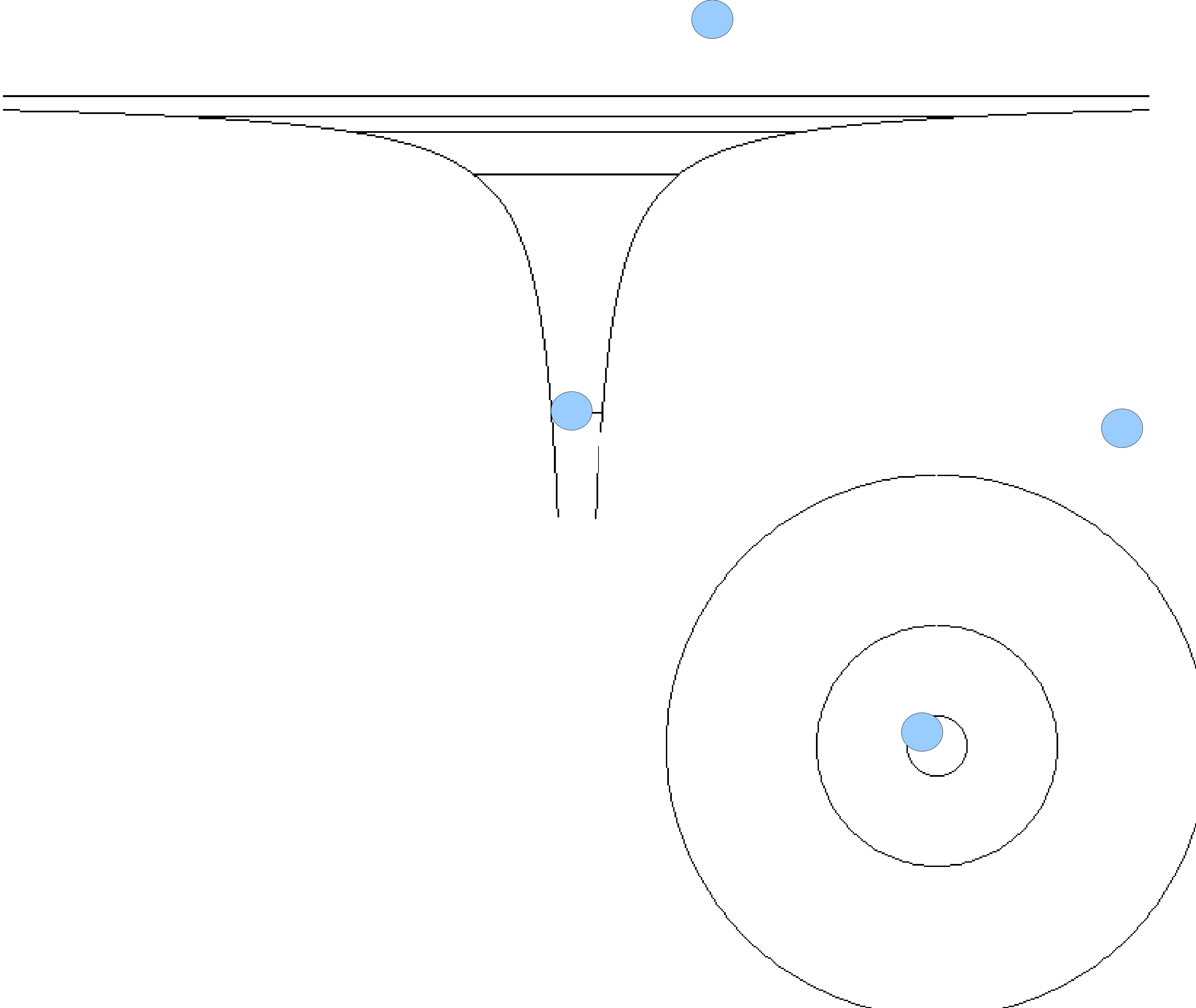
EXP.BindEner The experimental binding energy is sum of the two ionization potentials











Variational methods $e^{-\alpha r}$

effective Z

More parameters one sees Z_1, Z_2 Antisym

$\psi_Z(\vec{r}_1 \vec{r}_2) = \varphi_Z(r_1)\,\varphi_Z(r_2)$ independent

IMPROVEMENTS: not independent

$\psi(r_1, r_2) \propto \varphi_\alpha(r_1)\varphi_\alpha(r_2)\, f(r_{12})$

$\psi(r_1, r_2) \propto \varphi_\alpha(r_1)\varphi_\alpha(r_2)\, f'(r_{12})$

- More than 1 parameter
- more terms ....

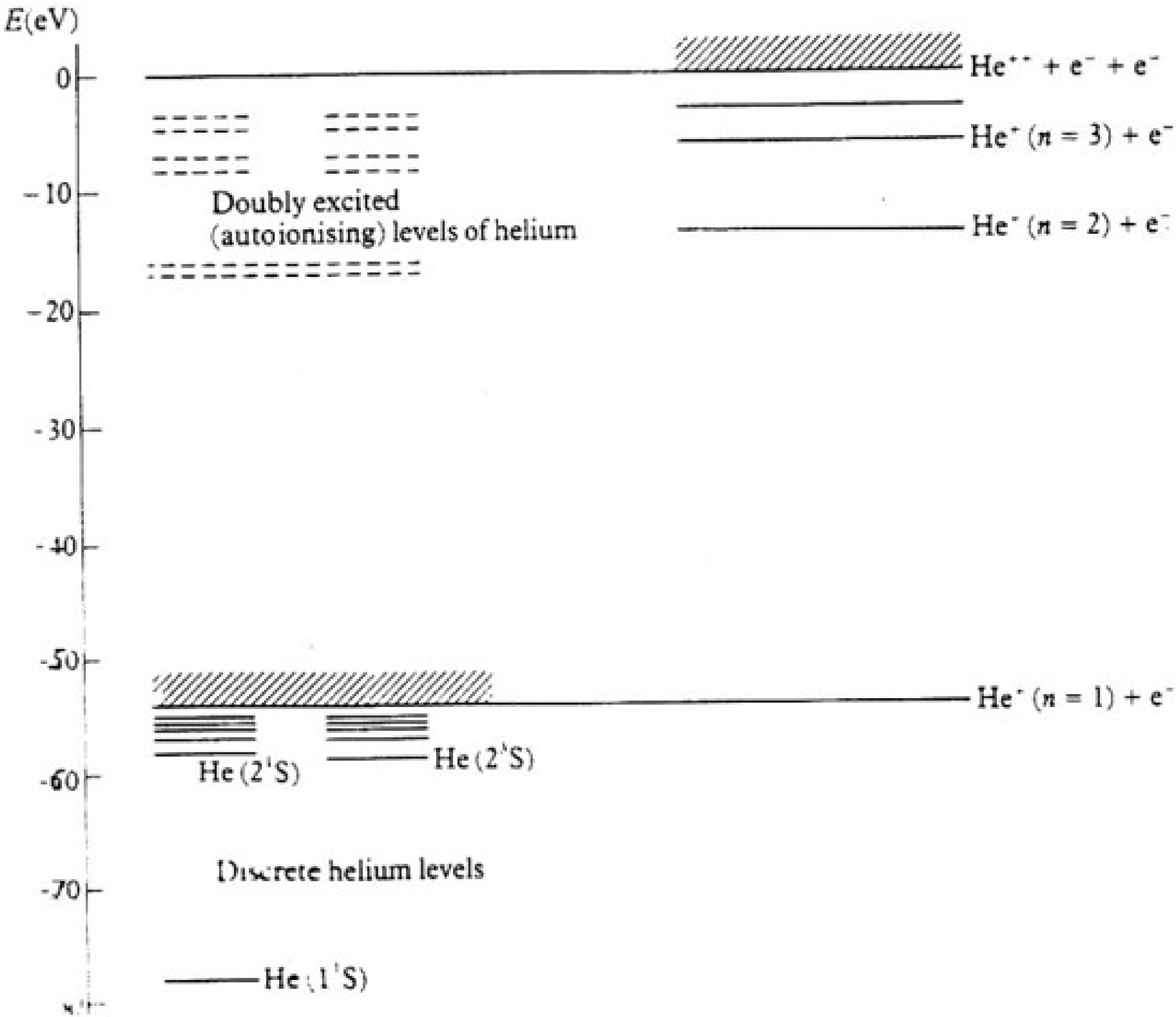
Hylleraas wavefunctions 1935

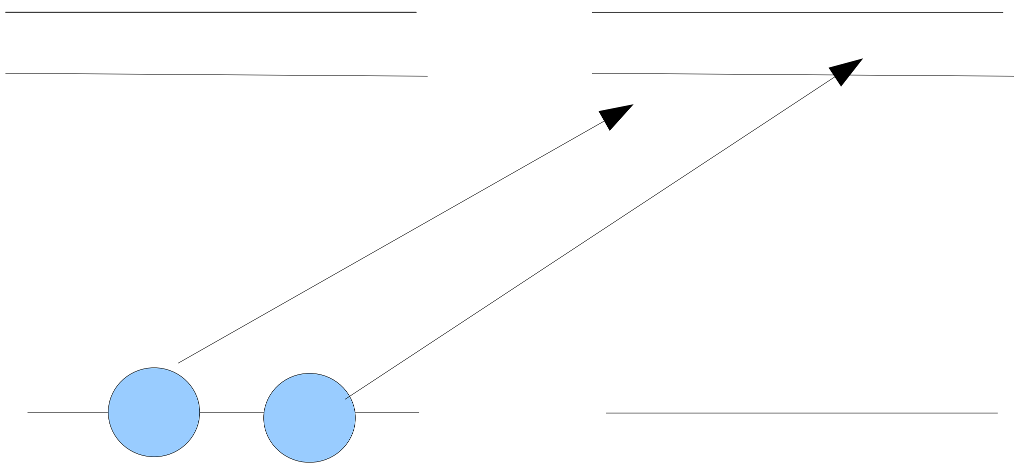
IN BERGEN

Most modern wavefunctions

over 1000 parameters

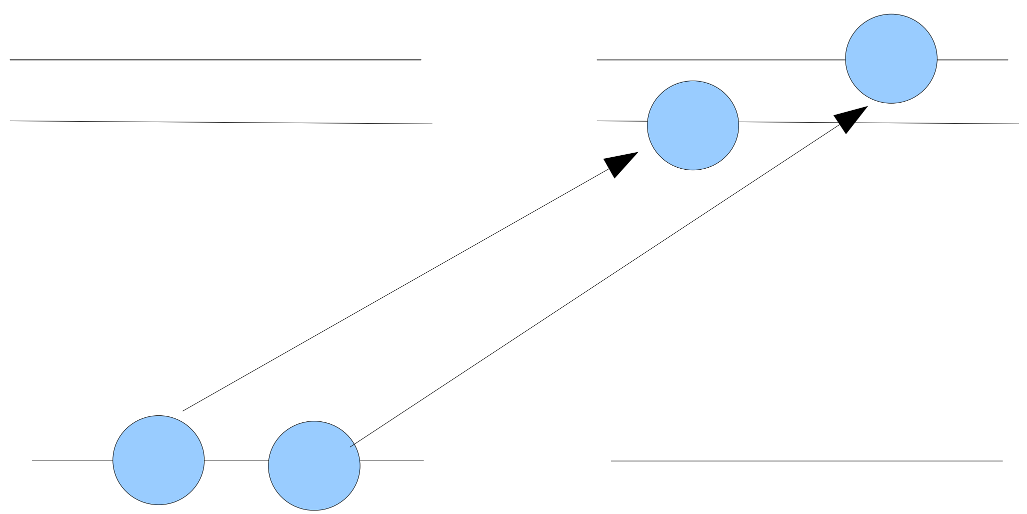
18 digits agreement with


E(eV)
0
-10
-20
-30
-40
-50
-60
-70
He⁺⁺ + e⁻ + e⁻
He⁺ (n = 3) + e⁻
He⁺ (n = 2) + e⁻
Doubly excited
(autoionising) levels of helium
He⁺ (n = 1) + e⁻
He (2¹S)
He (2³S)
Discrete helium levels
He (1¹S)



Autoionization
Autoionizing states

Auger Effect (autoionization from already ionized atom)



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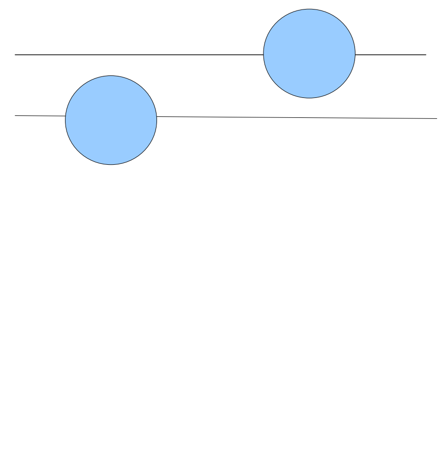

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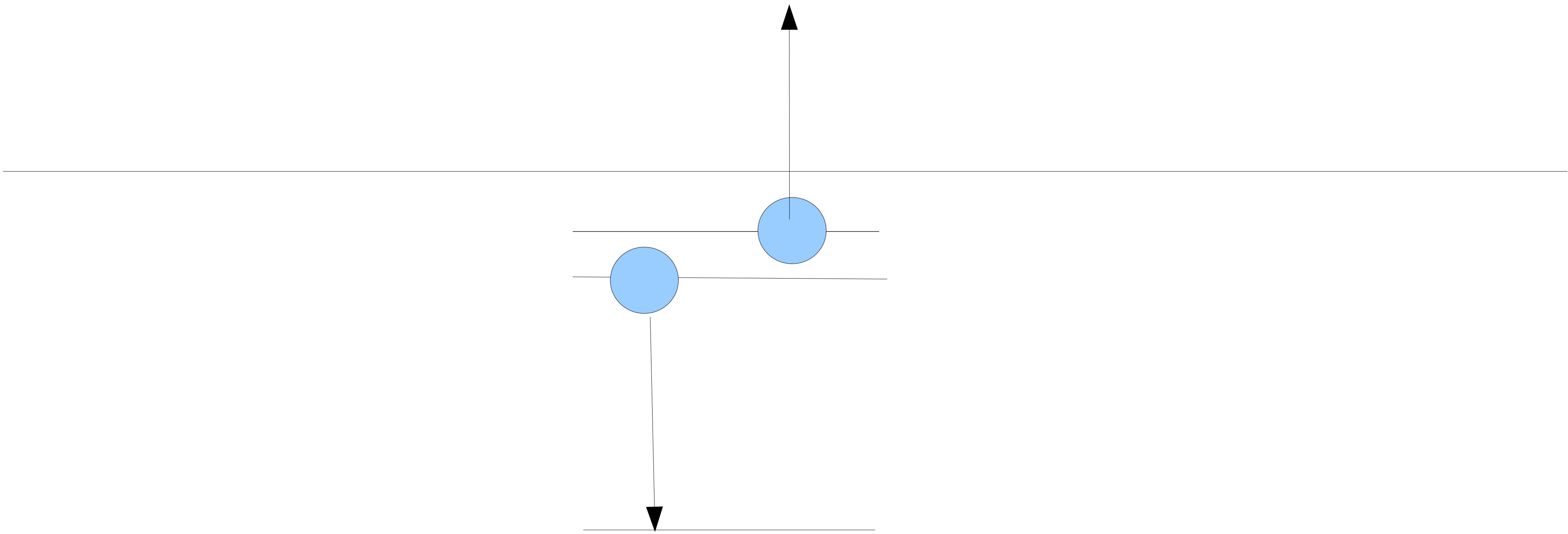

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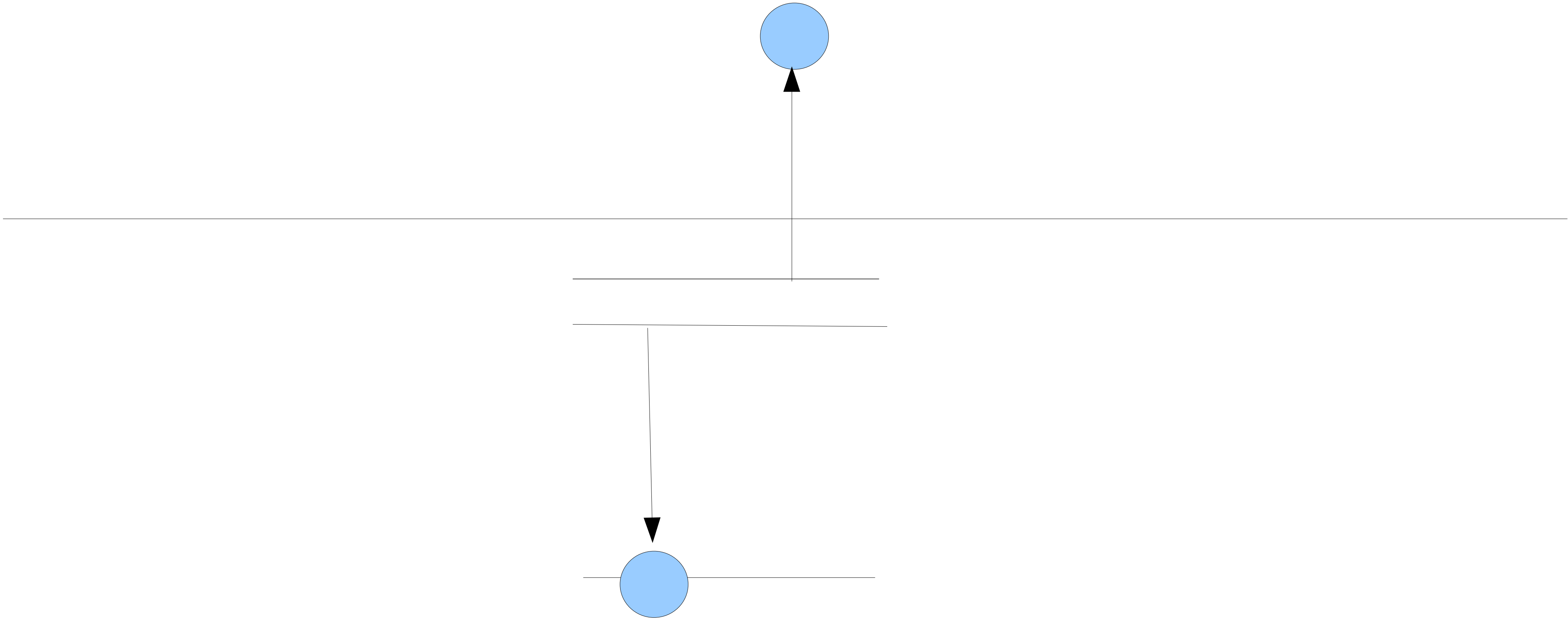

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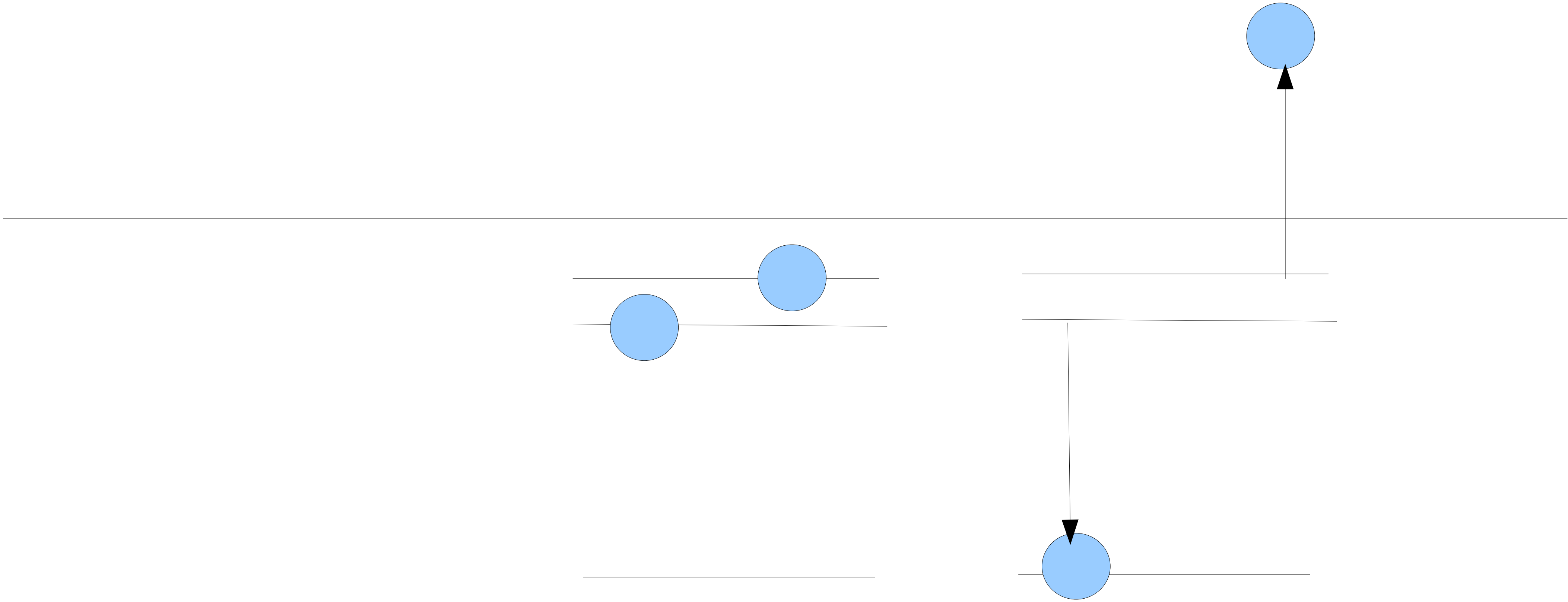

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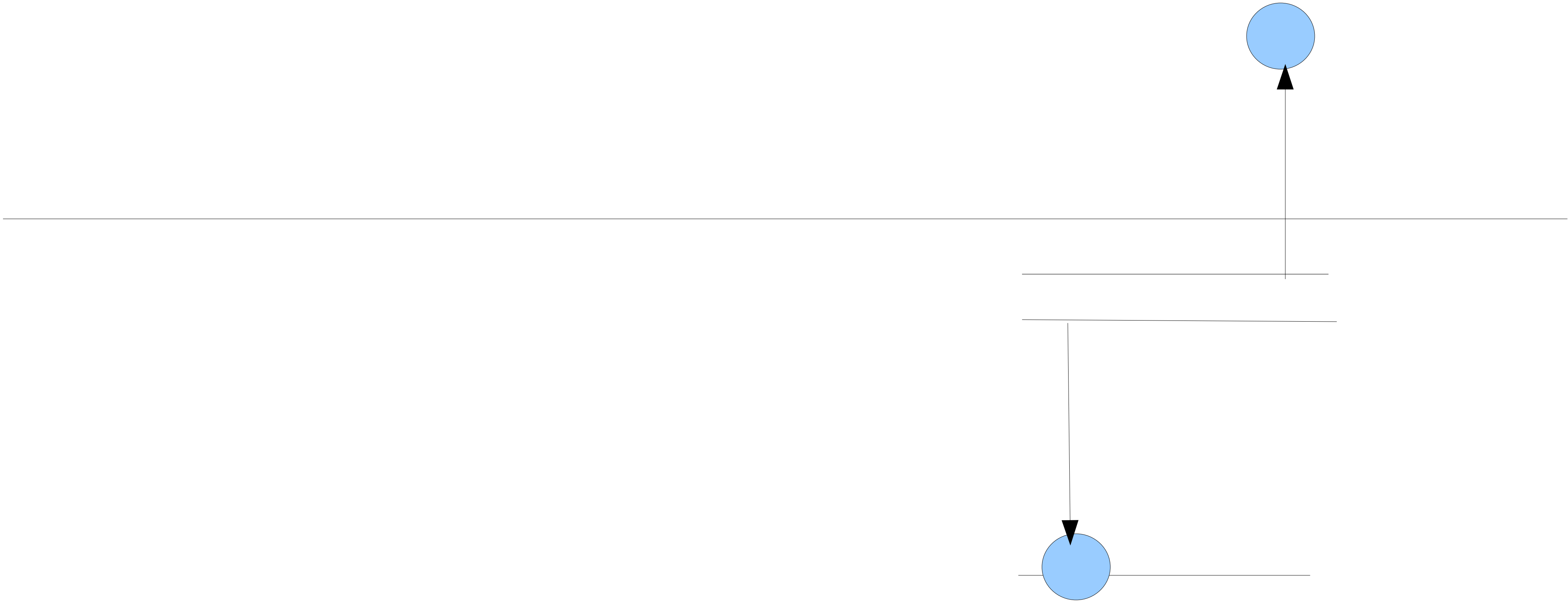

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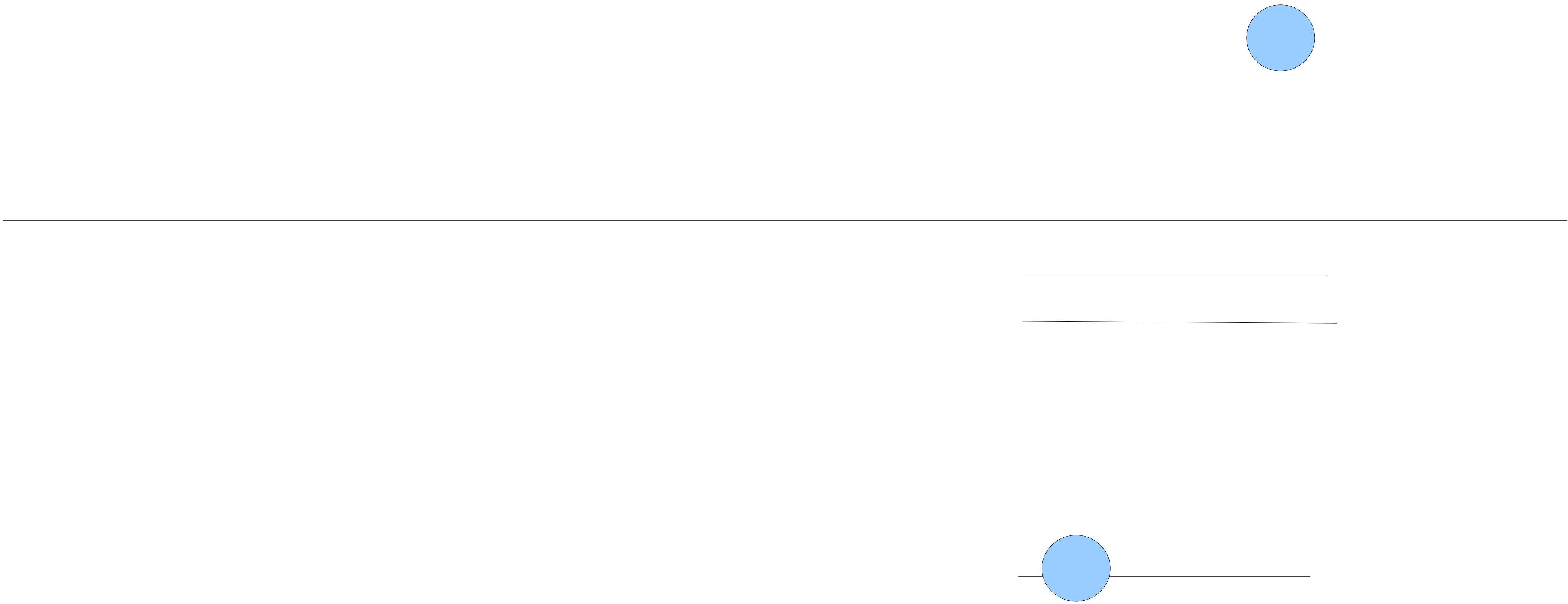

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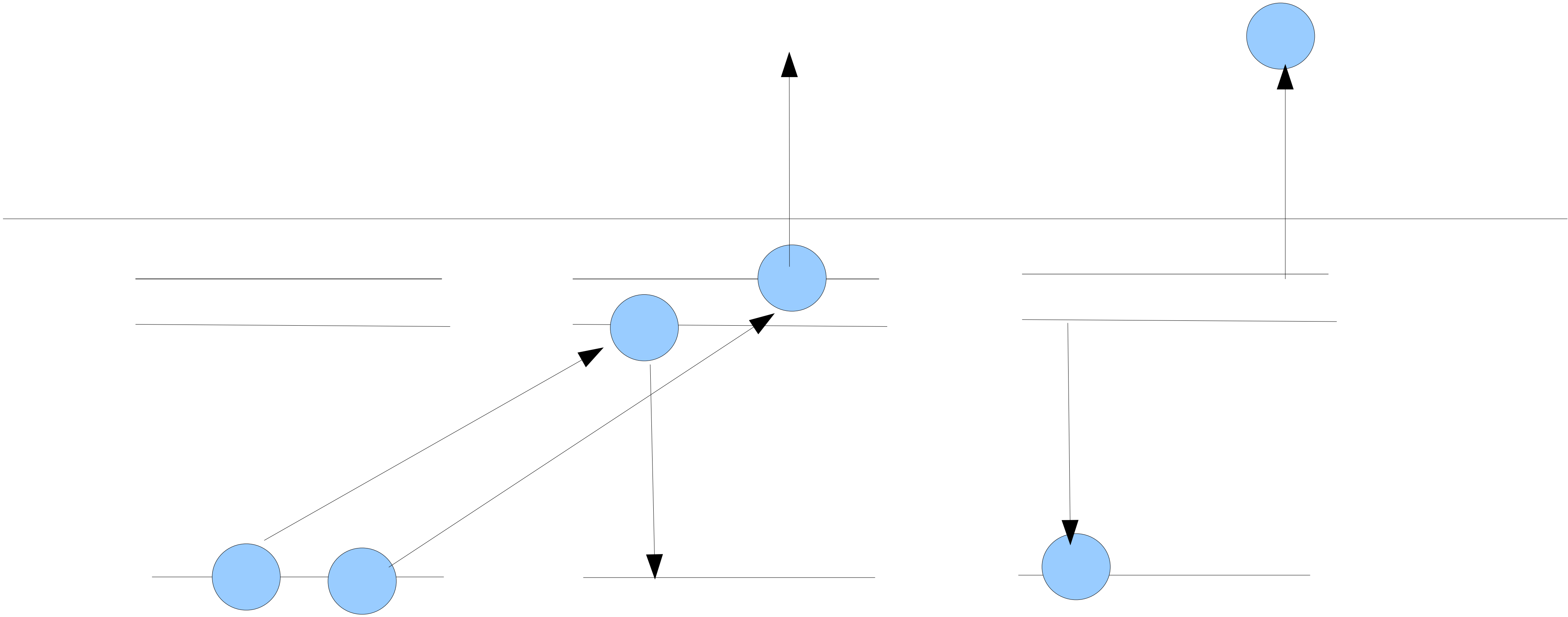

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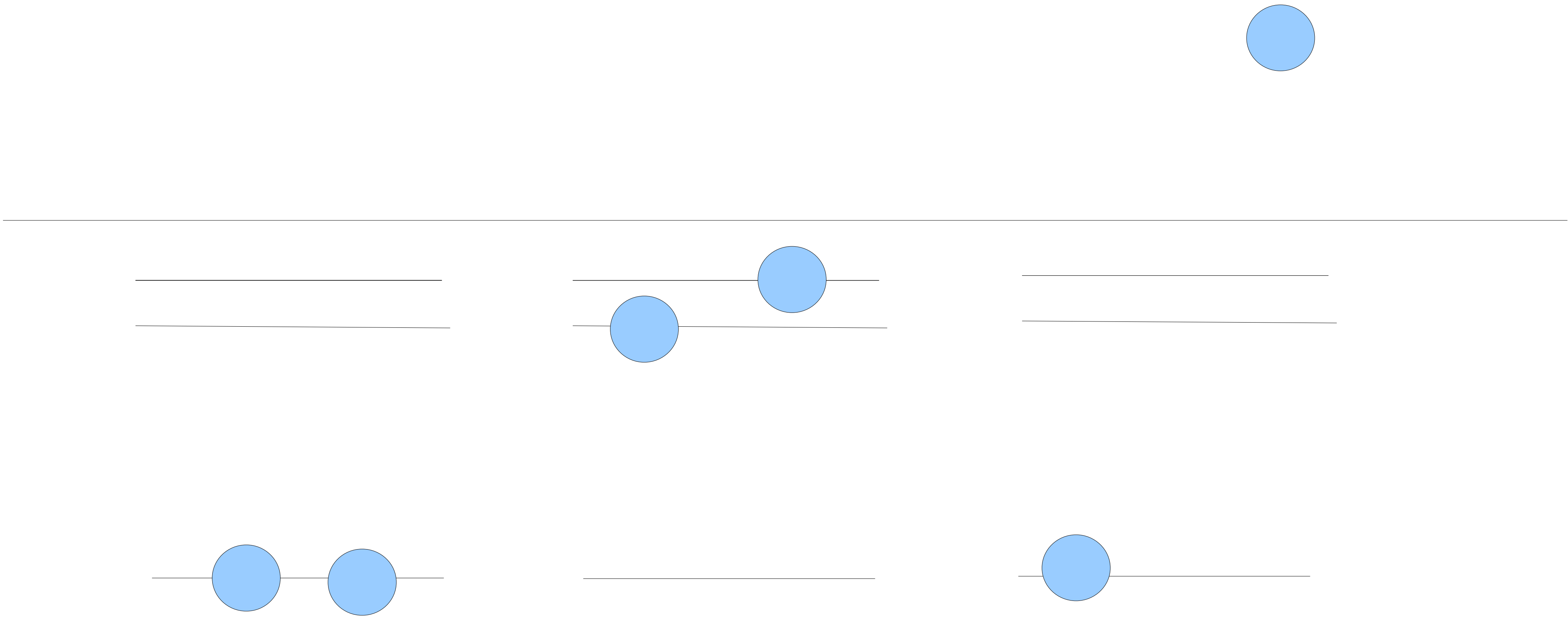

Autoionization
Autoionizing states

Auger Effect (autoionization from already ionized atom)

Helium

Triplet × Singlet (Spin)

Symmetric – Antisymmetric

→ Ferromagnetism

Perturbation → effective Z

→ variation

~~Independent electrons~~

Correlation → Hylleraas

Singly-excited

Doubly-excited → Autoion

Many electron-atoms