Quantum mechanics of many-Fermion systems

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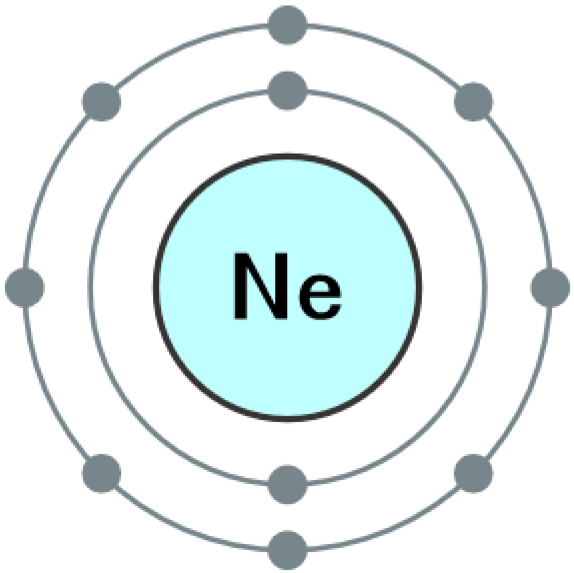
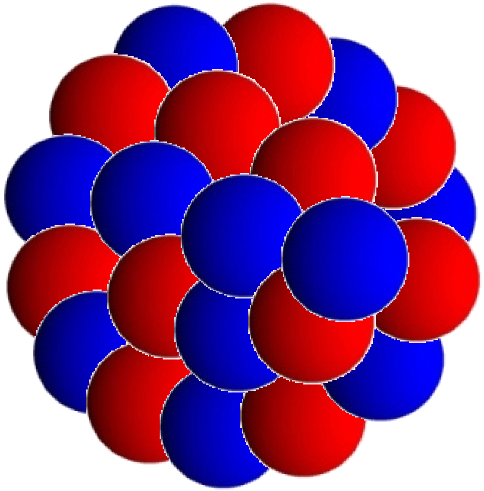
1. Identical particles: Fermions and Bosons
2. Simple examples: systems with two identical particles
3. Pauli principle and Slater determinants
4. Magic numbers
5. Fermi gas model and application to white dwarfs

Introduction





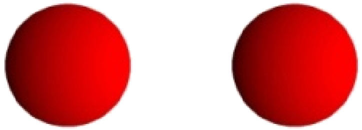
atom = nucleus
+ many electrons

nucleus = many protons
+ many neutrons

Quantum mechanics for those many Fermion systems?

Exchange operator: Fermions and Bosons

a two-particle system



1 2

$$H(1,2) = \frac{\boldsymbol{p}_1^2}{2m} + \frac{\boldsymbol{p}_2^2}{2m} + V(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

two particles are identical: particle 1 and 2 cannot be distinguished

$$H(2,1) \equiv \frac{\boldsymbol{p}_2^2}{2m} + \frac{\boldsymbol{p}_1^2}{2m} + V(\boldsymbol{r}_2, \boldsymbol{r}_1) = H(1,2)$$

Exchange operator: Fermions and Bosons

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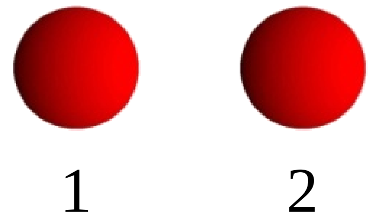

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mathematically, $[H, P_{12}] = 0$

where $P_{12}\Psi(1,2) = \Psi(2,1)$ exchange operator

“the Hamiltonian is invariant under the exchange of 1 $\longleftrightarrow$ 2”

Exchange operator: Fermions and Bosons

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➡ wave functions have to be simultaneous eigen-states of H and P_{12}

Exchange operator: Fermions and Bosons

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⇒ wave functions have to be simultaneous eigen-states of *H* and P_{12}

Eigen-values of P_{12}

$$P_{12}\Psi(1,2) = \Psi(2,1)$$

⇒ $$(P_{12})^2\Psi(1,2) = P_{12}\Psi(2,1) = \Psi(1,2)$$

⇒ $$(P_{12})^2 = 1$$

⇒ $$\boxed{P_{12} = \pm 1}$$

Exchange operator: Fermions and Bosons

$$P_{12} = \pm 1$$

Natural Laws: each particle has a definite value of P_{12}
(independent of e.g., experimental setup and temperature)

- particles with a half-integer spin: P_{12} = -1 ("Fermion")

  electrons, protons, neutrons,…..

$$\psi^{(-)}(1,2) = \frac{1}{\sqrt{2}}[\Psi(1,2) - \Psi(2,1)]$$

- particles with an integer spin: P_{12} = +1 ("Boson")

  photons, pi mesons,….

$$\psi^{(+)}(1,2) = \frac{1}{\sqrt{2}}[\Psi(1,2) + \Psi(2,1)]$$

Exchange operator: Fermions and Bosons

Extension to N-particle systems:

Wave functions have to be symmetric (anti-symmetric) for an exchange of *any* two particles

example: for N=3

$$\Psi^{(\pm)}(1,2,3) = \frac{1}{\sqrt{6}}[\Psi(1,2,3) \pm \Psi(2,1,3) + \Psi(2,3,1) + \Psi(3,2,1) + \Psi(3,1,2) \pm \Psi(1,3,2)]$$

Simple examples: systems with two identical particles

Assume a spin-independent Hamiltonian for a two-particle system:

$$H = \frac{\boldsymbol{p}_1^2}{2m} + \frac{\boldsymbol{p}_2^2}{2m} + V(\boldsymbol{r}_1, \boldsymbol{r}_2)$$

→ separable between the space and the spin

$$\Psi(x_1, x_2) = \Psi_{\mathsf{space}}(\boldsymbol{r}_1, \boldsymbol{r}_2) \cdot \Psi_{\mathsf{spin}}$$

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$$\Psi(x_1, x_2) = \Psi_{\text{space}}(\boldsymbol{r}_1, \boldsymbol{r}_2) \cdot \Psi_{\text{spin}}$$

◆spin-zero bosons

no spin → symmetrize the spatial part

$$\begin{aligned} \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) &= \Psi_{\text{space}}(\boldsymbol{r}_1, \boldsymbol{r}_2) \\ &= \frac{1}{\sqrt{2}}[\phi(\boldsymbol{r}_1, \boldsymbol{r}_2) + \phi(\boldsymbol{r}_2, \boldsymbol{r}_1)] \end{aligned}$$

Simple examples: systems with two identical particles

$$\Psi(x_1,x_2)=\Psi_{\text{space}}(\boldsymbol{r}_1,\boldsymbol{r}_2)\cdot\Psi_{\text{spin}}$$

◆spin-1/2 Fermions $\quad \Psi(x_1,x_2)=-\Psi(x_2,x_1)$

Spin part:

$$|S=1\rangle \;=\; |\uparrow\uparrow\rangle,\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle),\ |\downarrow\downarrow\rangle \qquad \text{symmetric}$$

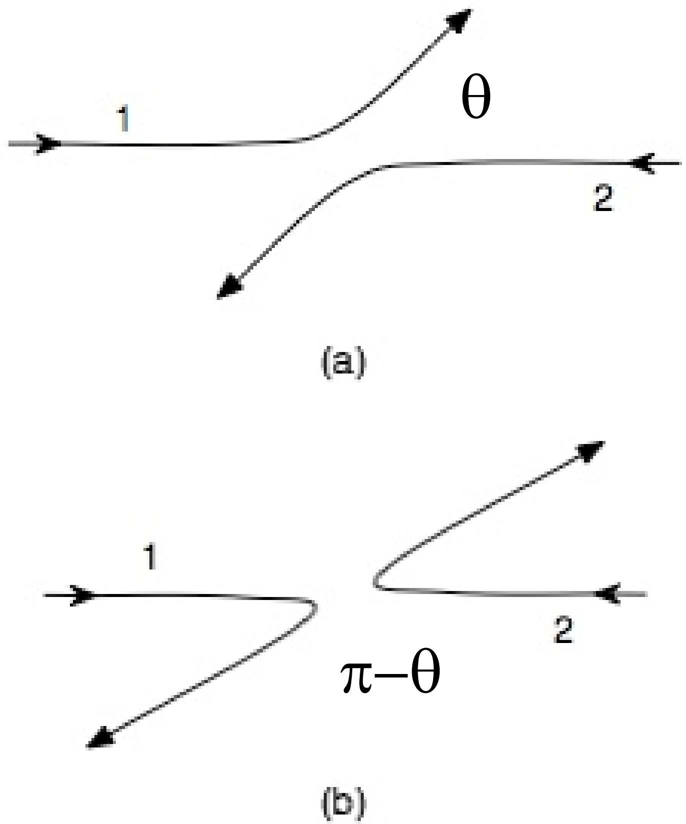
$$|S=0\rangle \;=\; \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle) \qquad \text{anti-symmetric}$$

⟶ spatial part: anti-symmetric for S=1
symmetric for S=0

$$\Psi_{S=0}(x_1,x_2) \;=\; \frac{1}{\sqrt{2}}[\phi(\boldsymbol{r}_1,\boldsymbol{r}_2)+\phi(\boldsymbol{r}_2,\boldsymbol{r}_1)]|S=0\rangle$$

$$\Psi_{S=1}(x_1,x_2) \;=\; \frac{1}{\sqrt{2}}[\phi(\boldsymbol{r}_1,\boldsymbol{r}_2)-\phi(\boldsymbol{r}_2,\boldsymbol{r}_1)]|S=1\rangle$$

Scattering of identical particles



these two processes cannot be distinguished

↓

add two amplitudes and then take square

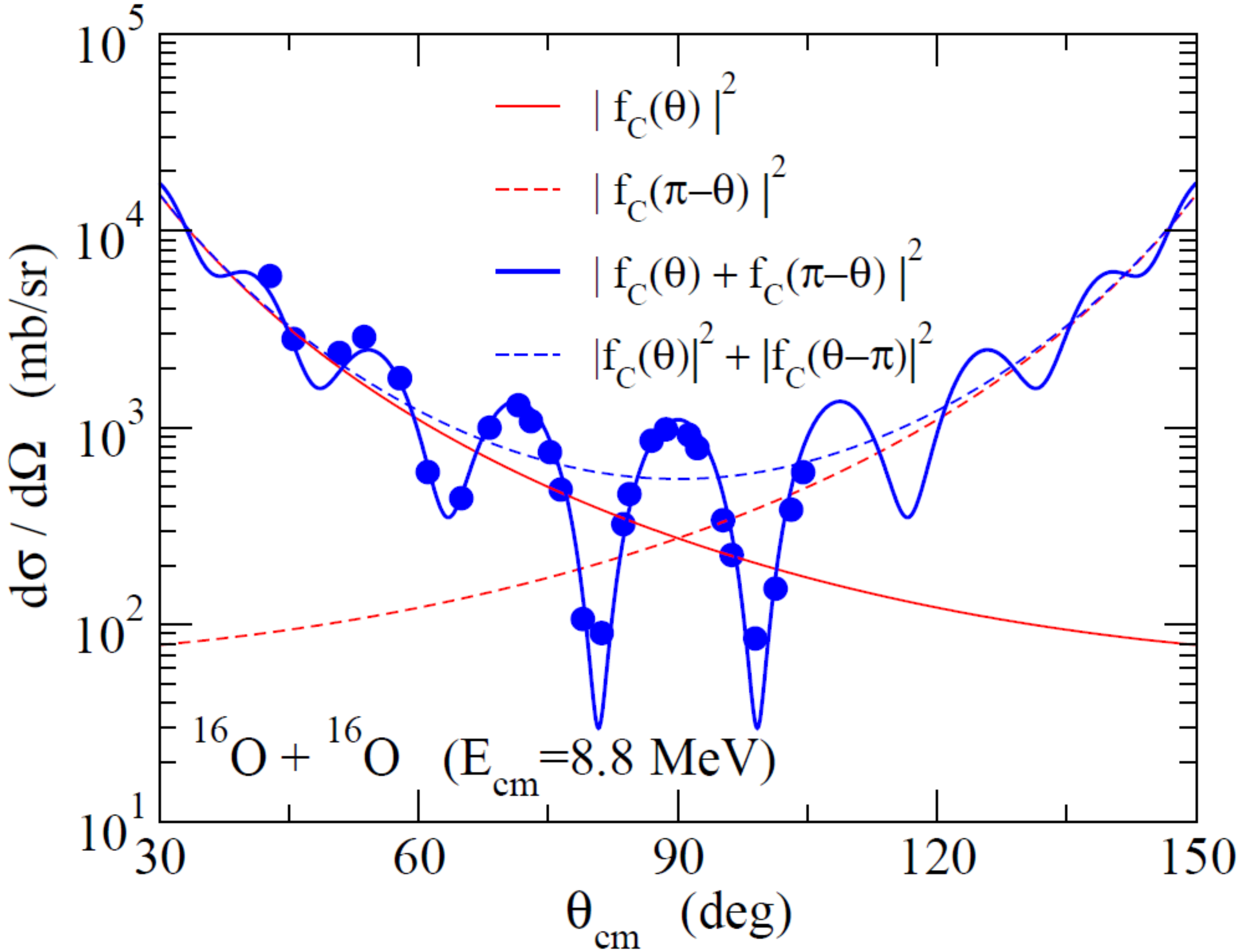
⟶ interference

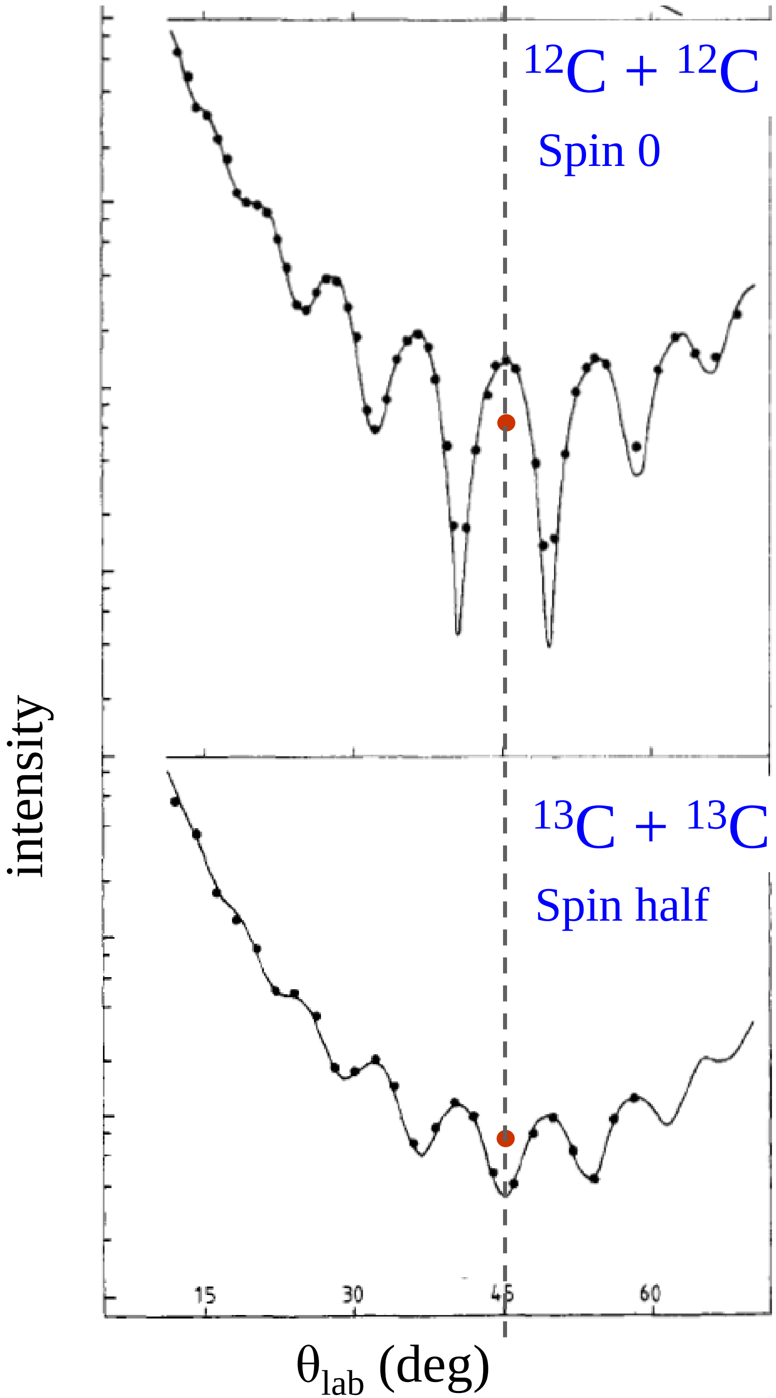
$$\frac{d\sigma}{d\Omega} = |f(\theta) \pm f(\pi-\theta)|^2$$
$$= |f(\theta)|^2 + |f(\pi-\theta)|^2 \pm f^*(\theta)f(\pi-\theta) \pm f(\theta)f^*(\pi-\theta)$$

+: for spatially symmetric, and – : for spatially anti-symmetric

$^{16}O + ^{16}O$ elastic scattering

^{16}O: spin-zero Boson → $\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2$





identical Bosons

→ constructive interference

$$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2$$

identical Fermions

→ destructive interference

$$\frac{d\sigma}{d\Omega} = \frac{3}{4}|f(\theta) - f(\pi - \theta)|^2 + \frac{1}{4}|f(\theta) + f(\pi - \theta)|^2$$

S=1

S=0

Pauli exclusion principle and Slater determinants

Pauli exclusion principle: two identical Fermion cannot take the same state

Let us assume:

$$H(1,2) = \underbrace{\frac{\boldsymbol{p}_1^2}{2m} + V(\boldsymbol{r}_1)}_{\equiv h_1} + \underbrace{\frac{\boldsymbol{p}_2^2}{2m} + V(\boldsymbol{r}_2)}_{\equiv h_2}$$

(no interaction between 1 and 2)

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(no interaction between 1 and 2)

separation of variables → a product form of wave function

$$\left(\frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})\right)\phi_n(x) = \epsilon_n \phi_n(x); \quad x \equiv (\boldsymbol{r}, \sigma)$$

$$\longrightarrow \Psi^{(-)}(x_1, x_2) = \frac{1}{\sqrt{2}}[\phi_n(x_1)\phi_{n'}(x_2) - \phi_n(x_2)\phi_{n'}(x_1)]$$

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$$\Psi^{(-)}(x_1,x_2) = 0 \quad \text{if} \ \ n = n'$$

(Pauli principle)

Pauli exclusion principle and Slater determinants

Pauli exclusion principle: two identical Fermion cannot take the same state

$$\Psi^{(-)}(x_1, x_2) = \frac{1}{\sqrt{2}}[\phi_n(x_1)\phi_{n'}(x_2) - \phi_n(x_2)\phi_{n'}(x_1)]$$

(note)

$$\Psi^{(-)}(x_1, x_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_n(x_1) & \phi_n(x_2) \\ \phi_{n'}(x_1) & \phi_{n'}(x_2) \end{vmatrix}$$

the determinant of a matrix

Pauli exclusion principle and Slater determinants

non-interacting N-Fermion systems

$$H = \sum_{i=1}^{N} \left(\frac{\boldsymbol{p}_i^2}{2m} + V(x_i) \right)$$

$$\longrightarrow \quad \Psi(x_1, \cdots, x_N) = \mathcal{A}[\phi_{n_1}(x_1) \cdots \phi_{n_N}(x_N)]$$

(separation of variables)

anti-symmetrizer

Pauli exclusion principle and Slater determinants

N=2: $$\Psi^{(-)}(x_1, x_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) \\ \phi_2(x_1) & \phi_2(x_2) \end{vmatrix}$$

N=3:

$$\begin{aligned} \Psi^{(\pm)}(1,2,3) &= \frac{1}{\sqrt{6}}[\Psi(1,2,3) \pm \Psi(2,1,3) + \Psi(2,3,1) \\ &\quad + \Psi(3,2,1) + \Psi(3,1,2) \pm \Psi(1,3,2)] \\ &= \frac{1}{\sqrt{6}}[\phi_1(1)\phi_2(2)\phi_3(3) - \phi_1(2)\phi_2(1)\phi_3(3) \\ &\quad + \phi_1(2)\phi_2(3)\phi_3(1) - \phi_1(3)\phi_2(2)\phi_3(1) \\ &\quad + \phi_1(3)\phi_2(1)\phi_3(2) - \phi_1(1)\phi_2(3)\phi_3(2)] \\ &= \frac{1}{\sqrt{6}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(x_3) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(x_3) \\ \phi_3(x_1) & \phi_3(x_2) & \phi_3(x_3) \end{vmatrix} \end{aligned}$$

Pauli exclusion principle and Slater determinants

N=2:
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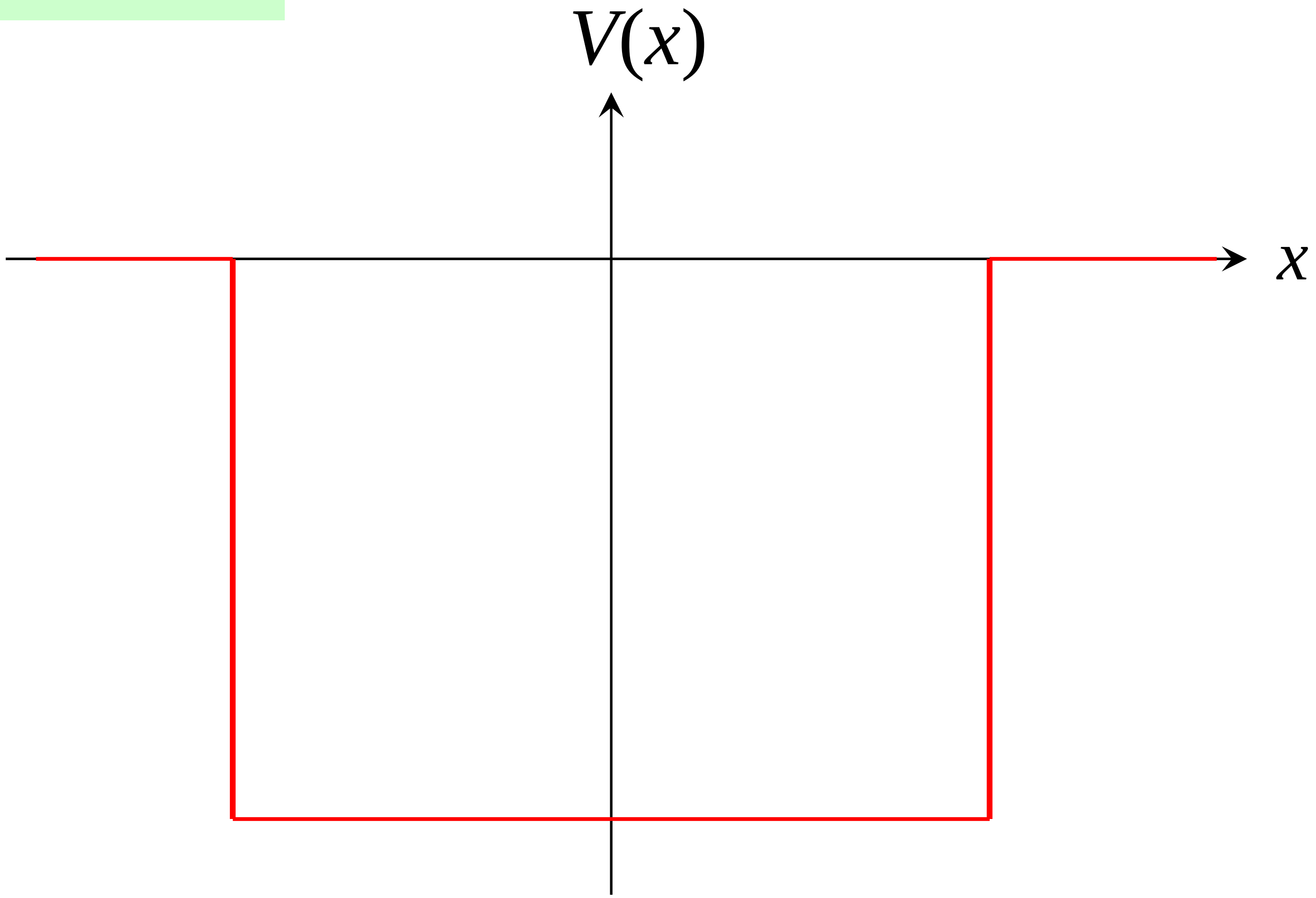
in general:
$$\Psi^{(\pm)}(x_1, \cdots x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \cdots & \phi_1(x_N) \\ \vdots & & \vdots \\ \phi_N(x_1) & \cdots & \phi_N(x_N) \end{vmatrix}$$

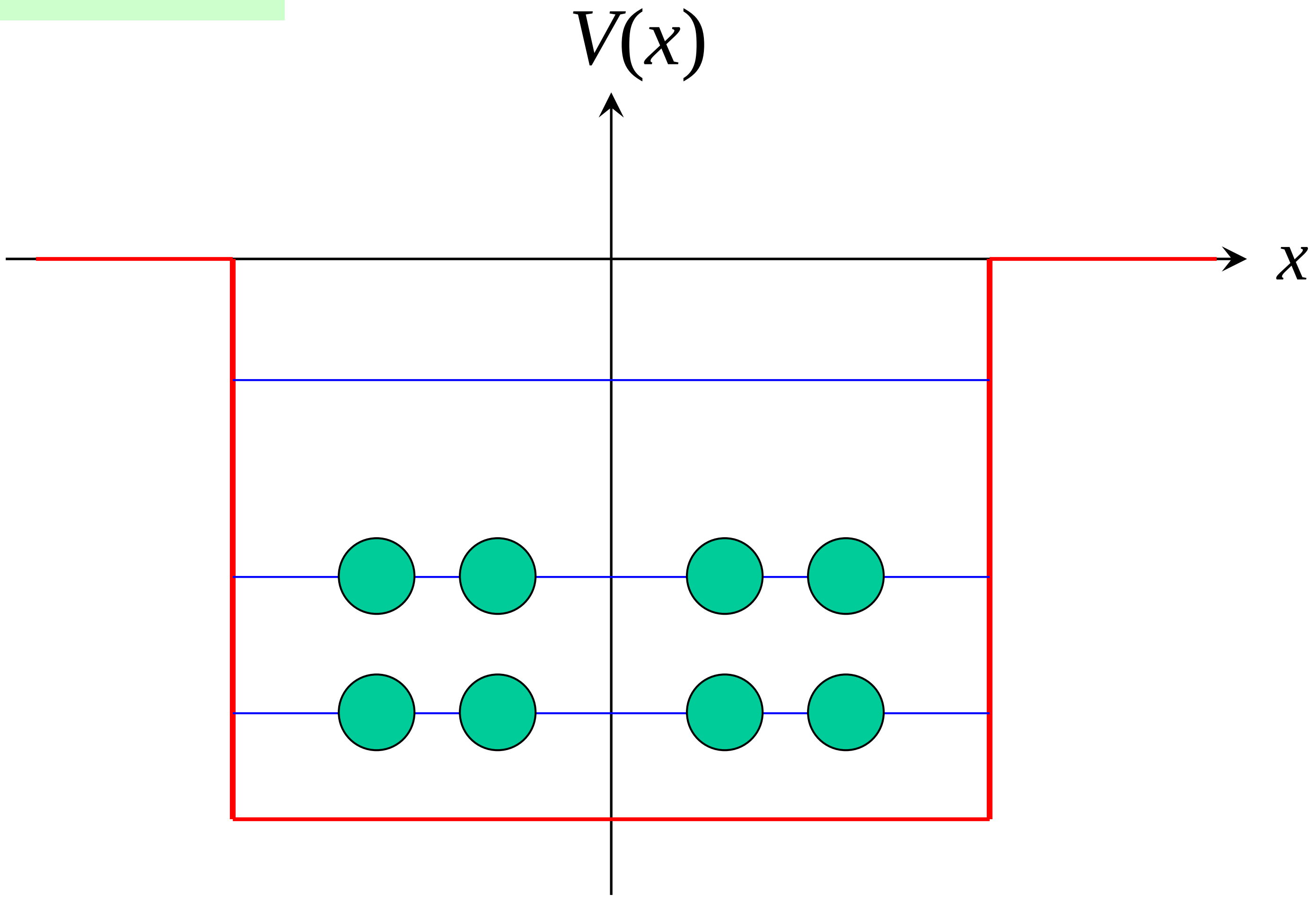
Slater determinant

Magic numbers



$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x)$$

Magic numbers



discrete bound states

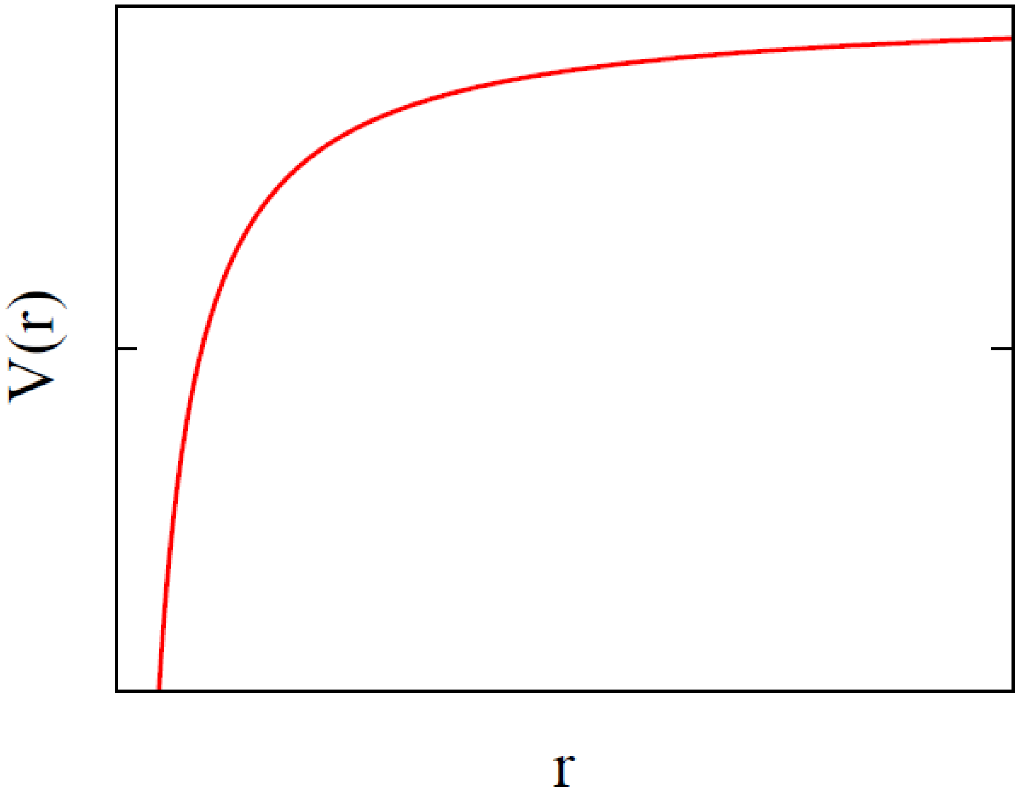
The lowest state of many-Fermion systems

= put particles from the bottom of the potential well (Pauli principle)

Magic numbers

Hydrogen-like potential:

$$V(r) = -\frac{Ze^2}{r}$$



$$E_n = -\frac{(Z\alpha)^2}{2n^2} mc^2$$

$$\alpha = \frac{e^2}{\hbar c} \sim \frac{1}{137}$$

$$n = n_r + l + 1$$

Magic numbers

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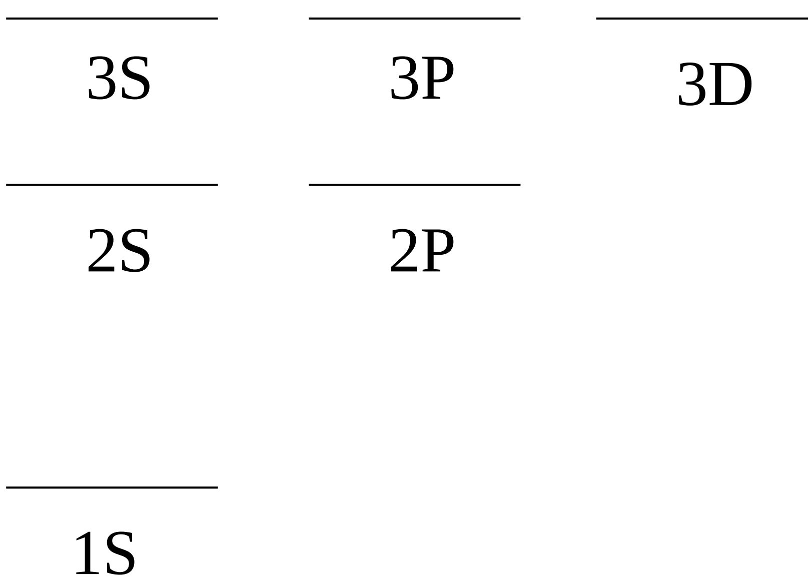

Magic numbers

Hydrogen-like potential: $$V(r) = -\frac{Ze^2}{r}$$

degeneracy = 2 * (2 *l* +1)

(spin x l_z)

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3S [2] 3P [6] 3D [10]

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1S [2]

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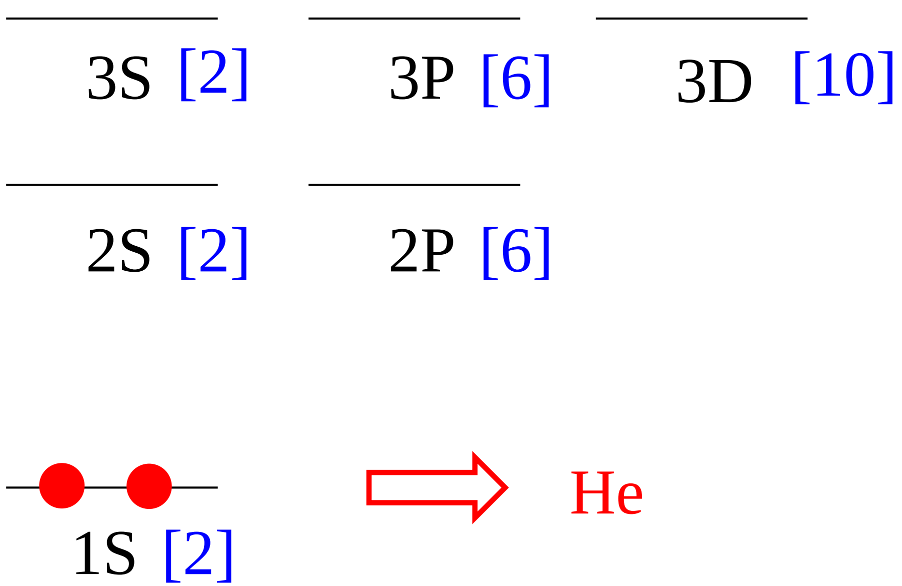

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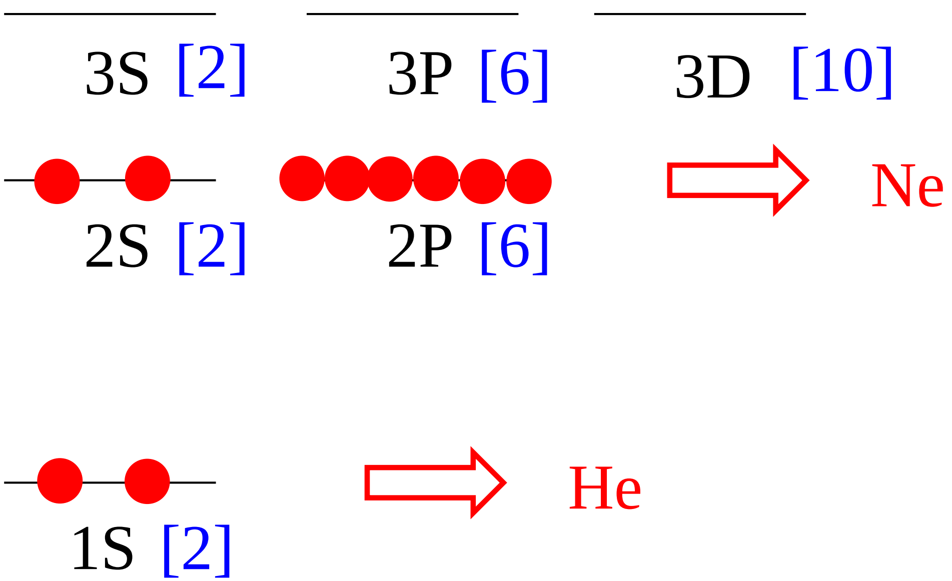

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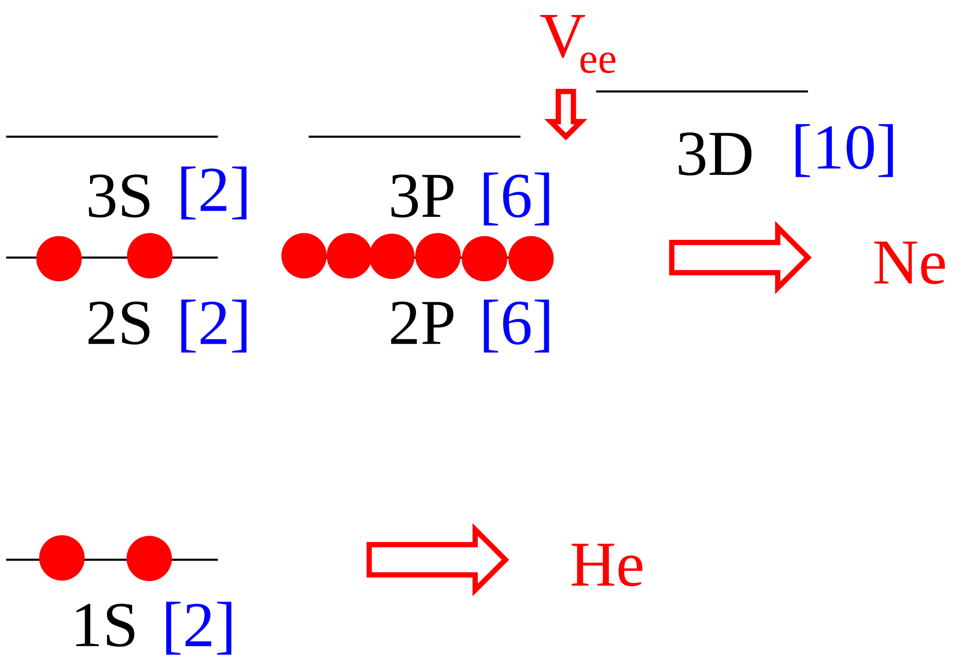

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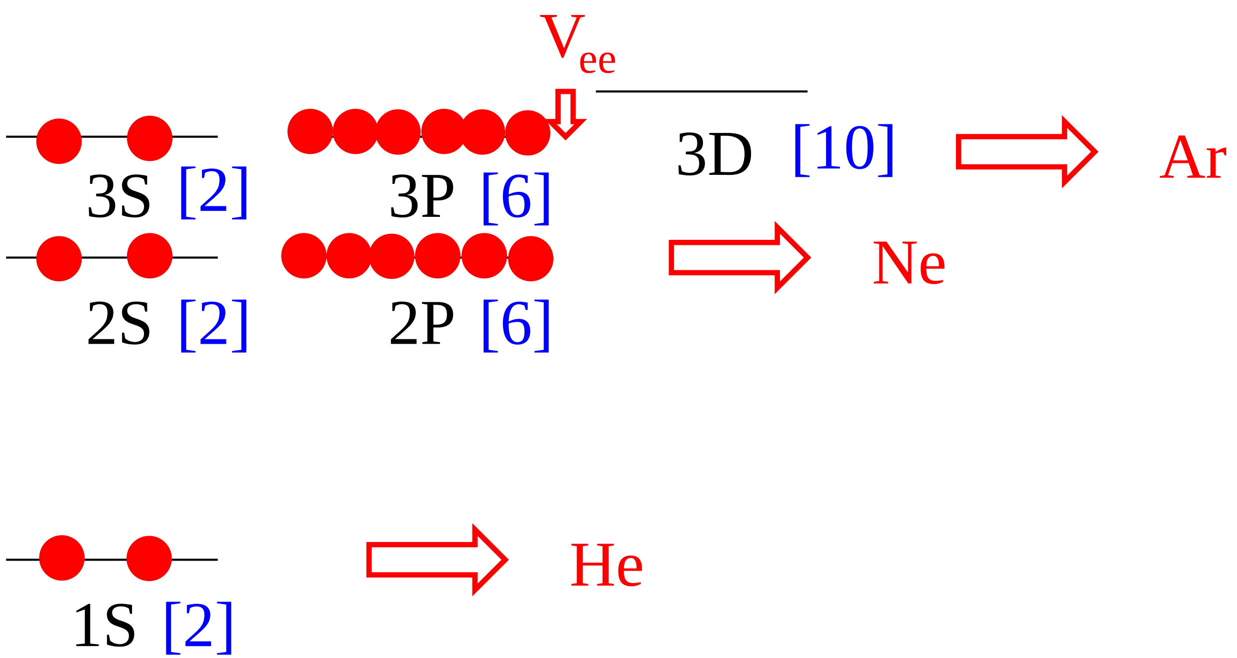

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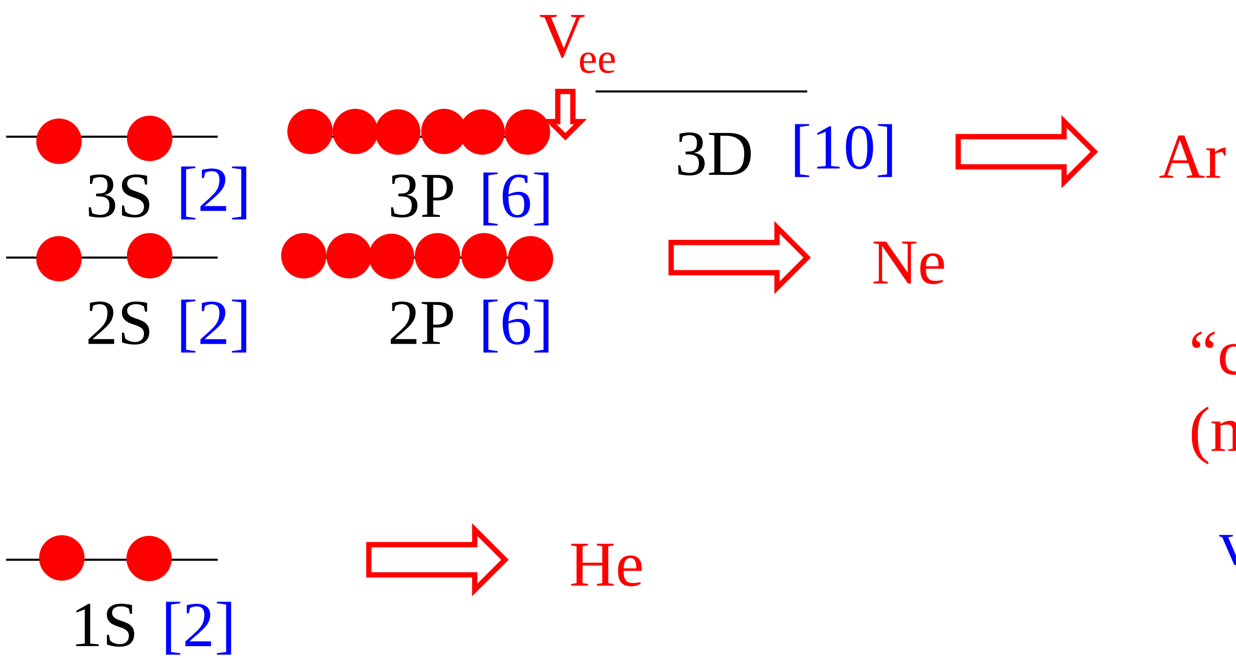


"closed shell"
(magic numbers)

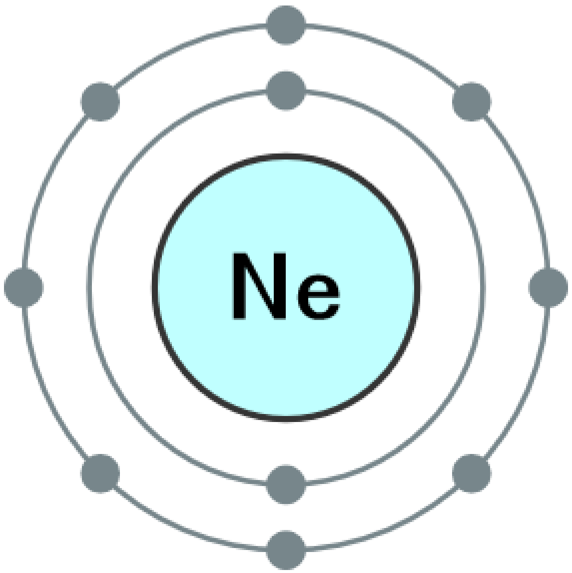
very stable

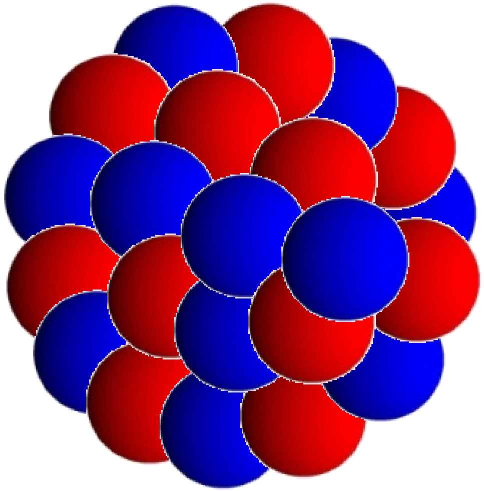
Periodic Table of elements

noble gas

Group → / Period ↓	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La *	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac **	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
			*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
			**	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

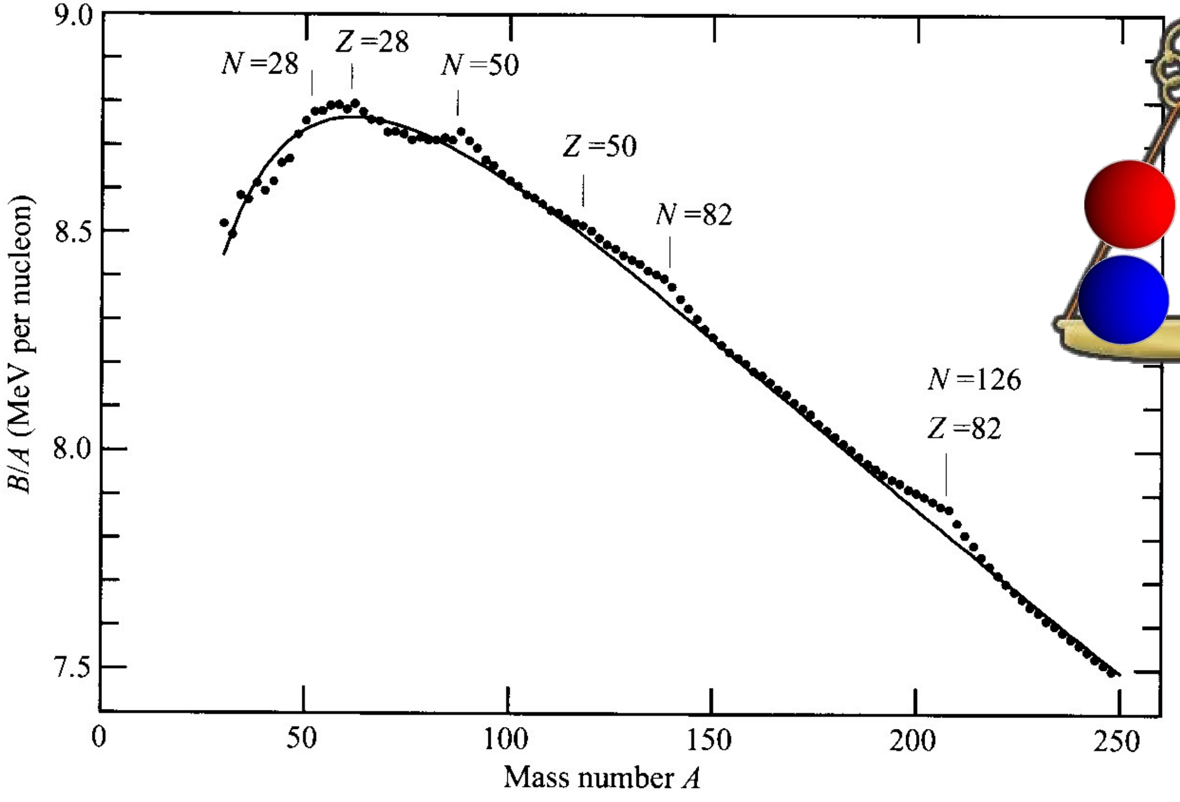
Magic numbers

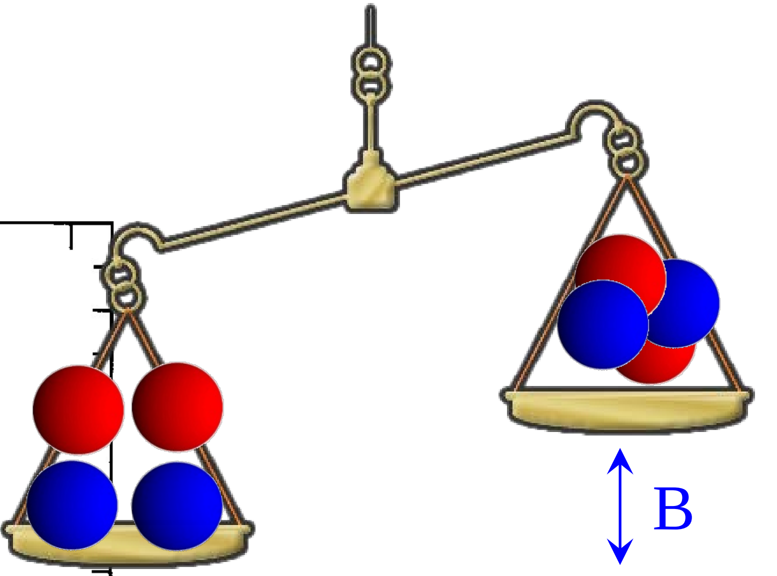




similar magic numbers also in atomic nuclei

Magic numbers





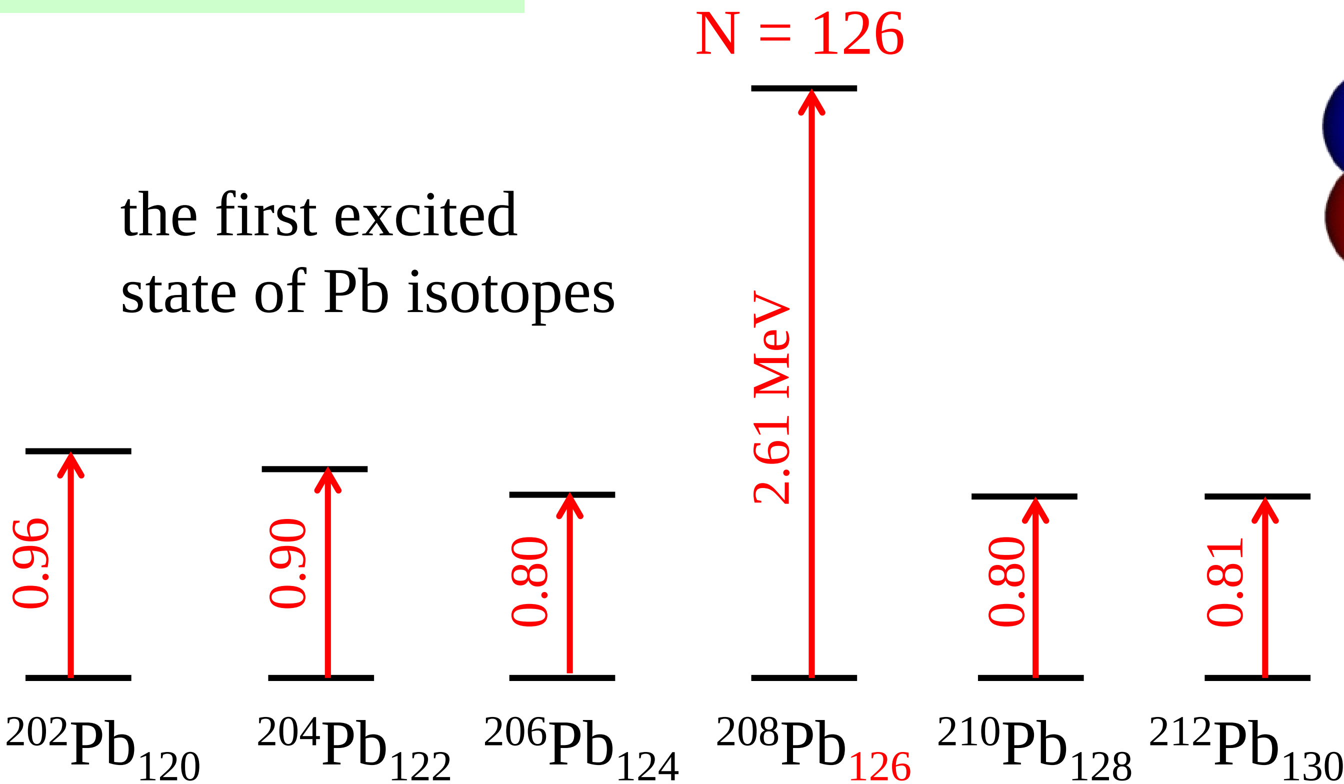
Extra binding for N or Z = 2, 8, 20, 28, 50, 82, 126 (magic numbers)

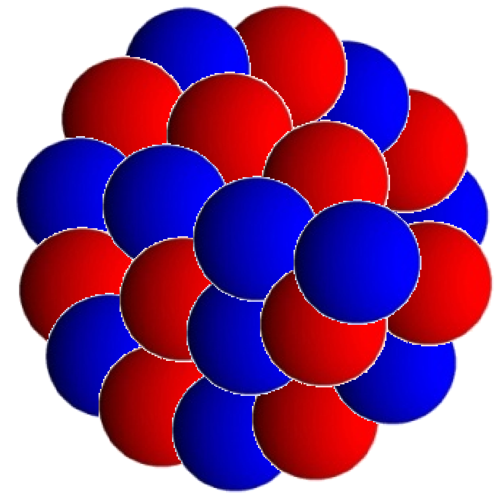
⇨ Very stable

${}^{4}_{2}He_{2}$, ${}^{16}_{8}O_{8}$, ${}^{40}_{20}Ca_{20}$, ${}^{48}_{20}Ca_{28}$, ${}^{208}_{82}Pb_{126}$

Magic numbers

the first excited
state of Pb isotopes





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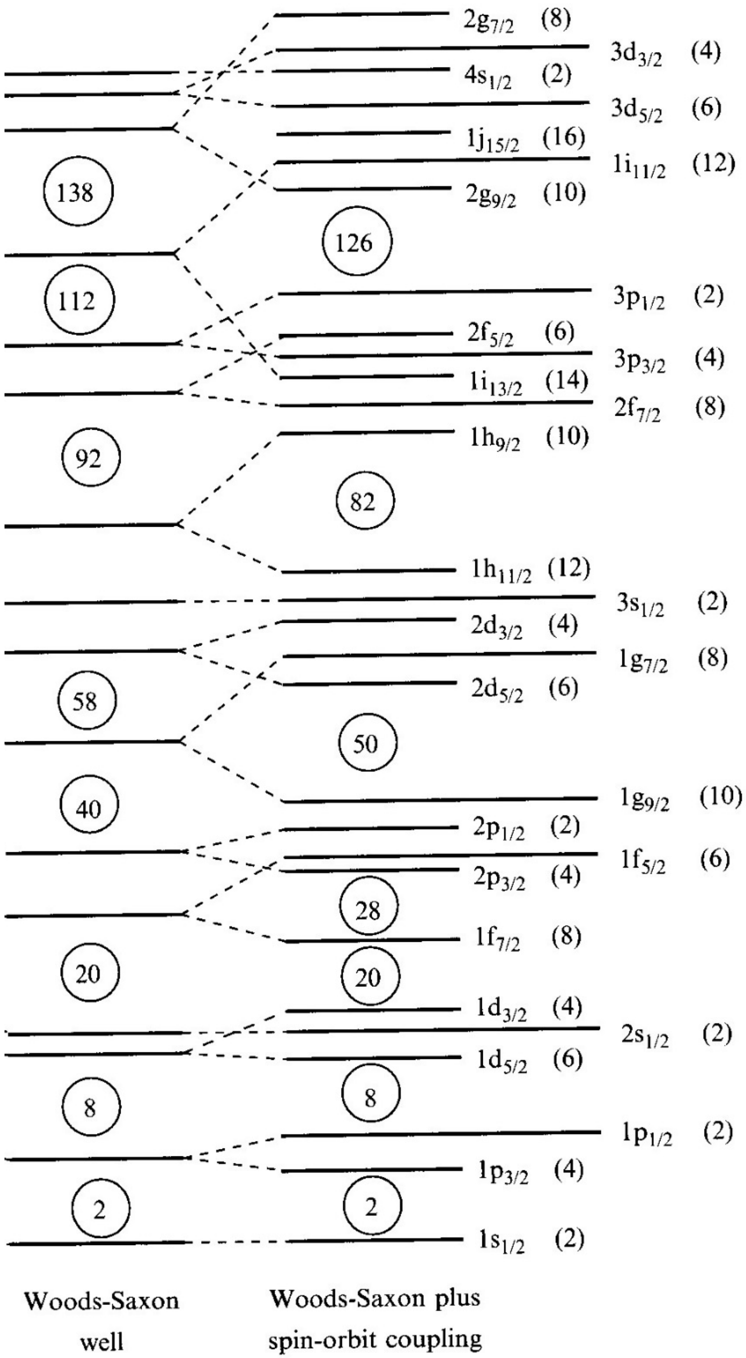
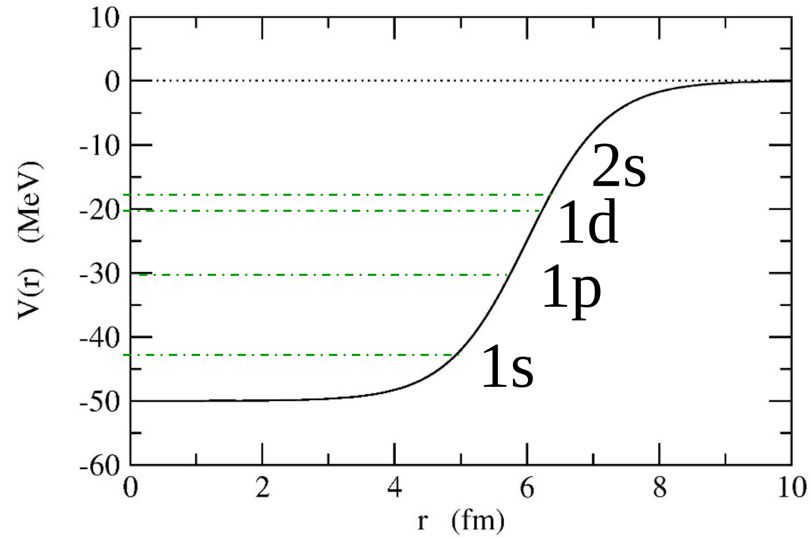


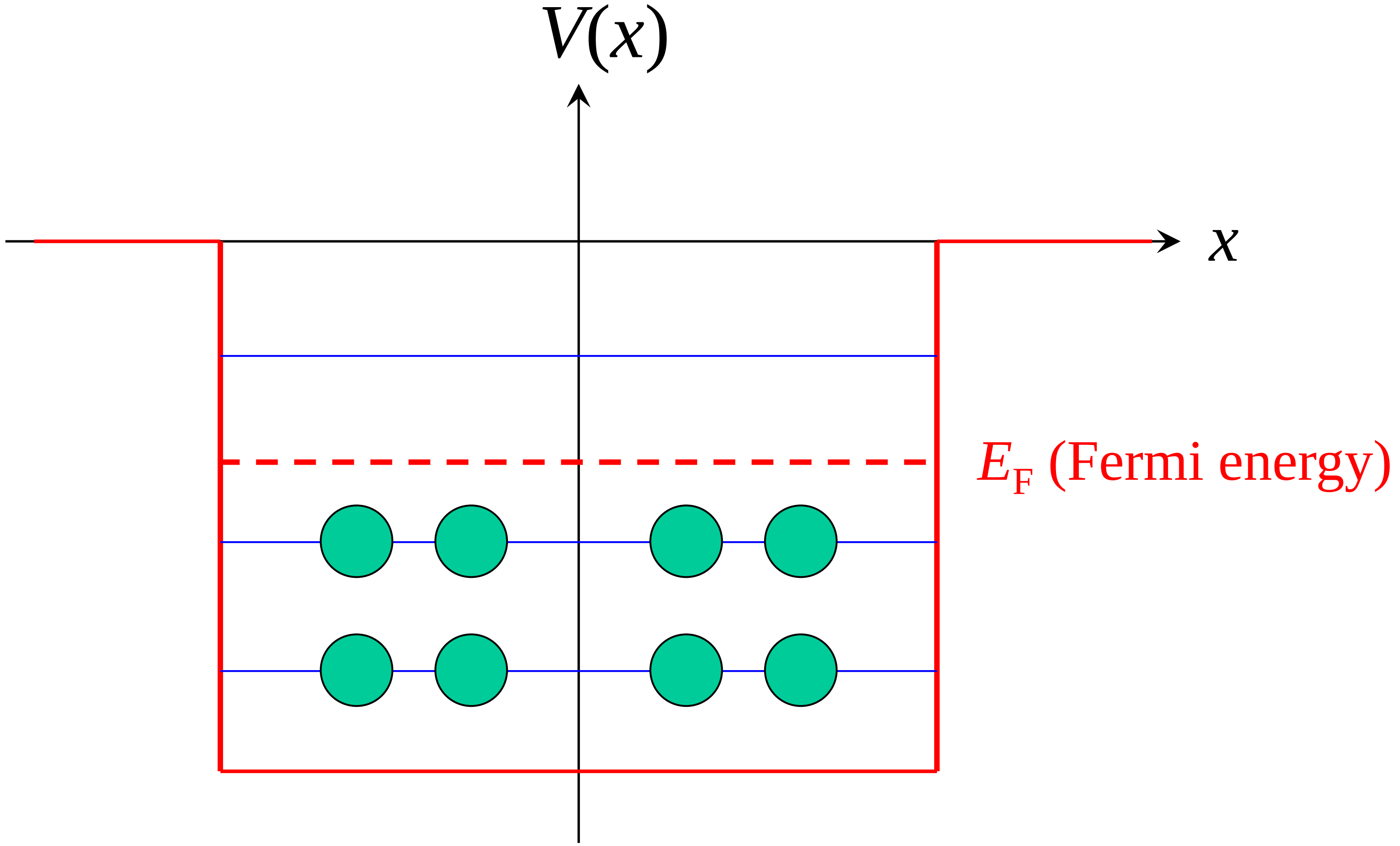
$$V(r) = \frac{-V_0}{1 + \exp((r - R_0)/a)}$$



+ spin-orbit potential

$$V_{ls}(r)\boldsymbol{l} \cdot \boldsymbol{s}$$

Fermi gas model

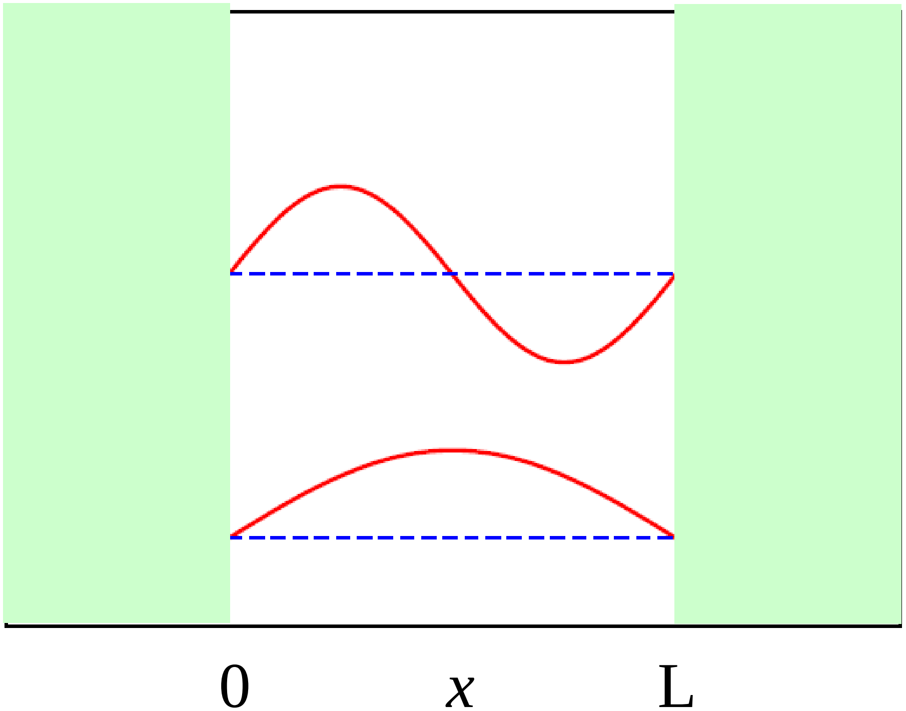


What is the relation between E_F and the particle number?

→ Fermi gas model

Fermi gas model

non-interaction many Fermion system (with no external potential)



put infinite walls at $x = 0$ and $x = L$:

$$\longrightarrow \quad \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

$$(n = 1, 2, \cdots)$$

three-dimensional case:

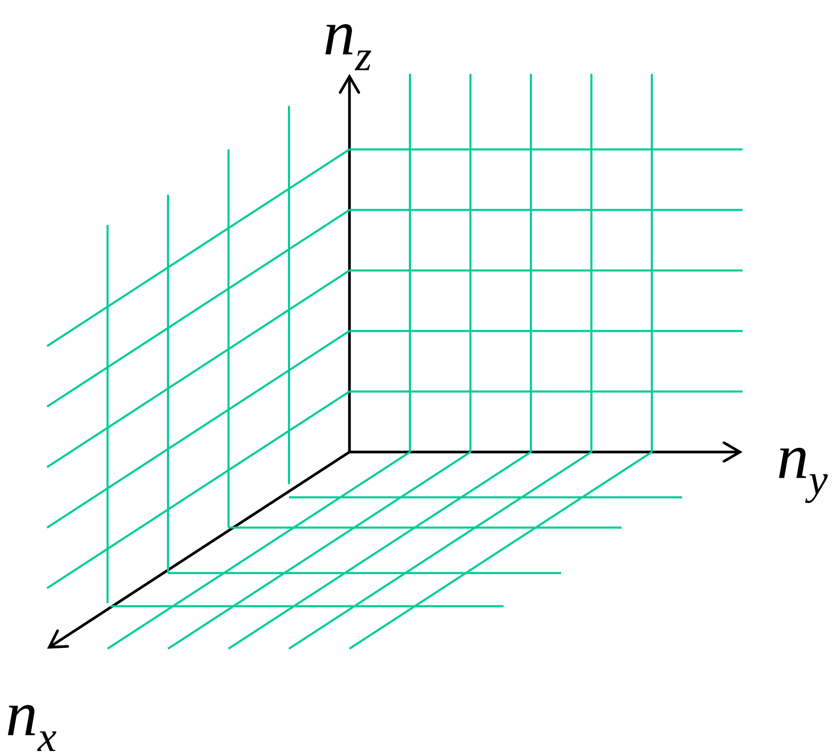
$$\psi_{n_x n_y n_z}(x) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x\pi}{L}x\right) \sin\left(\frac{n_y\pi}{L}y\right) \sin\left(\frac{n_z\pi}{L}z\right)$$

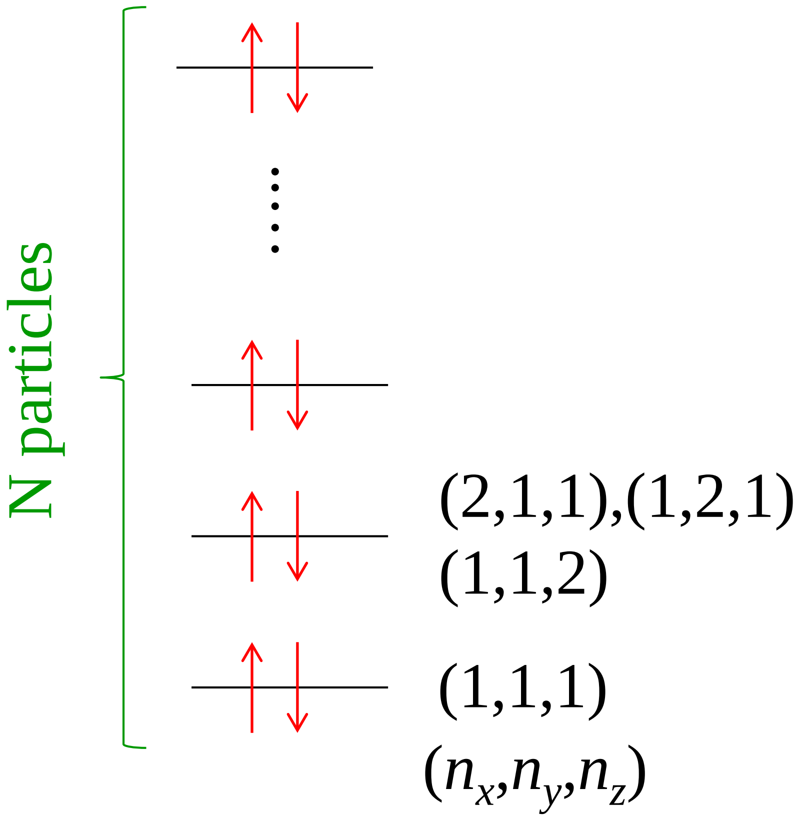
$$E_{n_x n_y n_z} = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

Fermi gas model

$$\psi_{n_x n_y n_z}(x) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{n_x\pi}{L}x\right) \sin\left(\frac{n_y\pi}{L}y\right) \sin\left(\frac{n_z\pi}{L}z\right)$$

$$E_{n_x n_y n_z} = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

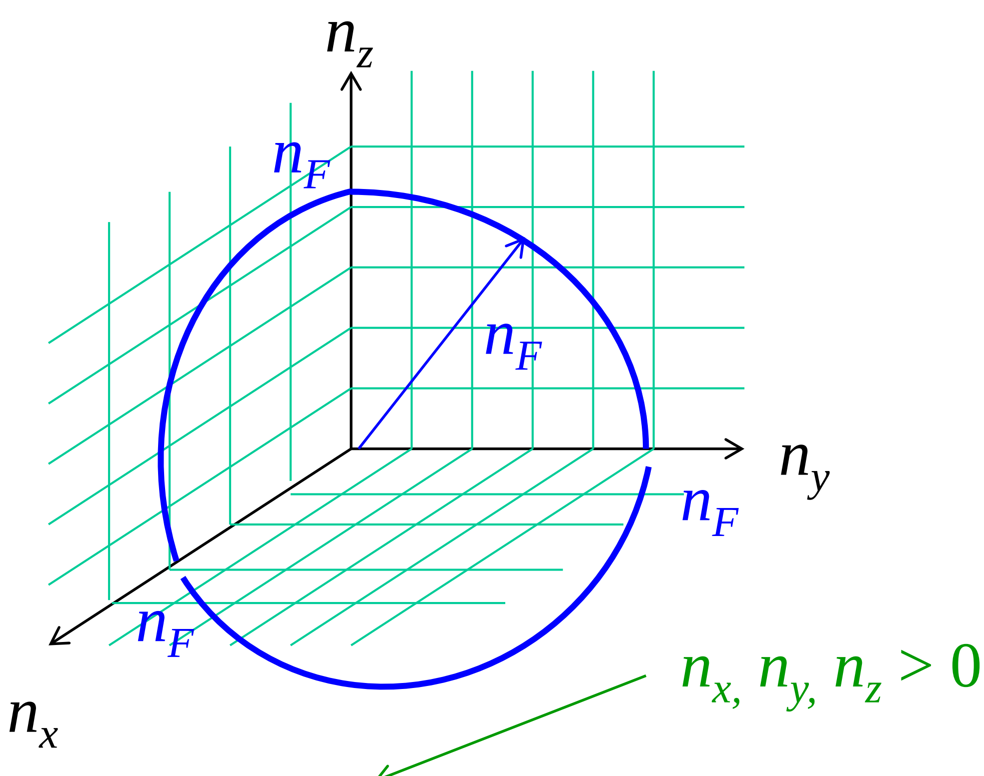


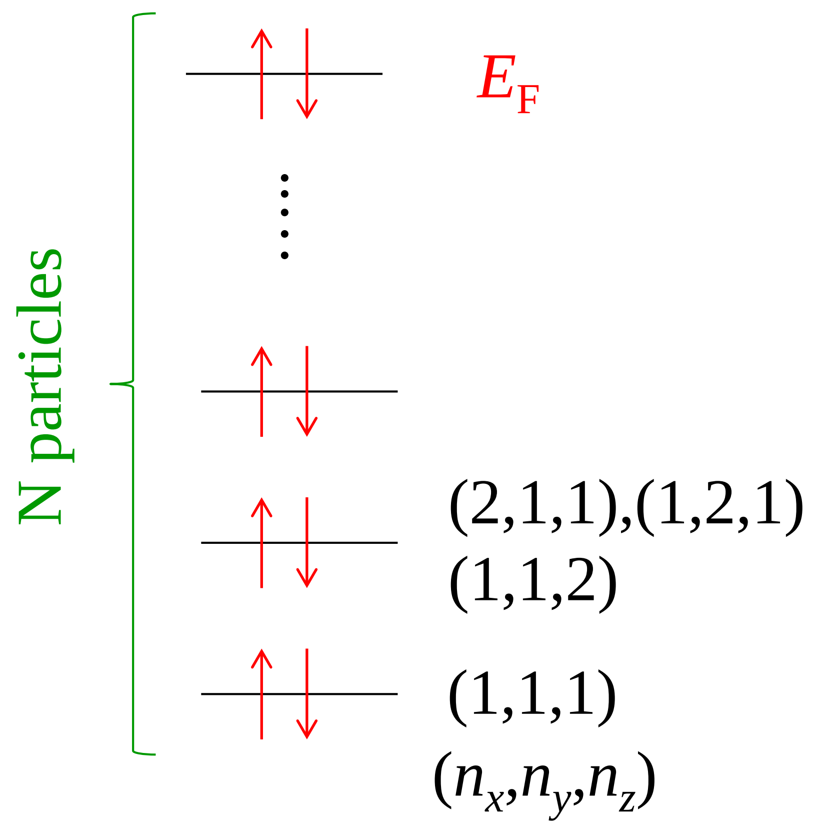


Fermi gas model

the highest energy: $$E_F = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) \equiv \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n_F^2$$

$$\longrightarrow \quad n_F^2 = \frac{2mE_F}{\hbar^2\pi^2}L^2$$



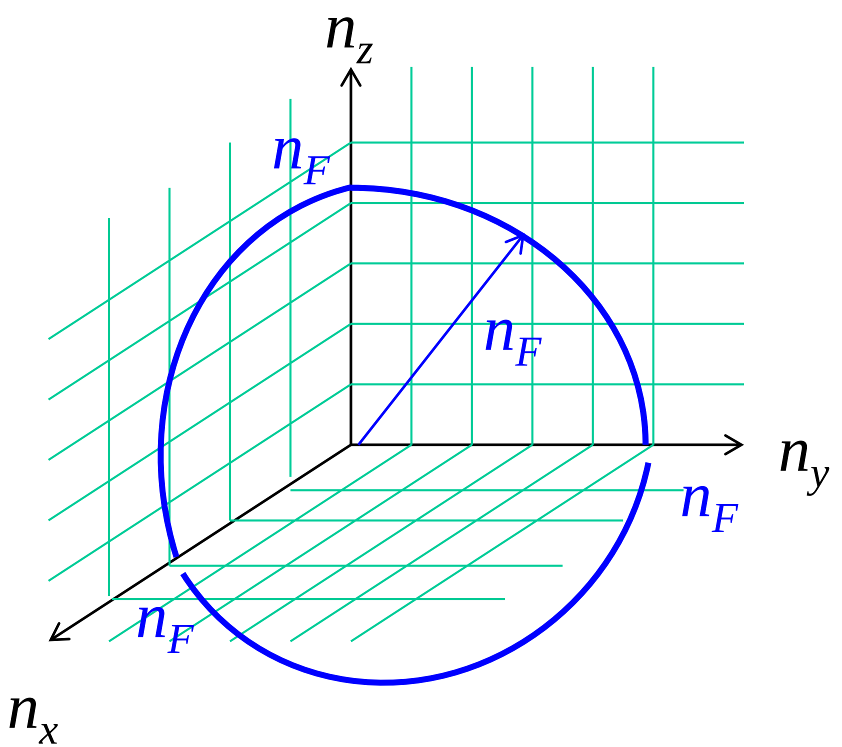


$$N = 2 \times \frac{1}{8} \times \frac{4}{3}\pi n_F^3$$

Fermi gas model

the highest energy: $$E_F = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2) \equiv \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n_F^2$$

$$\longrightarrow \quad n_F^2 = \frac{2mE_F}{\hbar^2\pi^2} L^2$$



$$N = 2 \times \frac{1}{8} \times \frac{4}{3}\pi n_F^3 = \frac{\pi}{3}\left(\frac{2mE_F}{\hbar^2\pi^2} L^2\right)^{3/2} = \frac{\pi}{3}\left(\frac{2mE_F}{\hbar^2\pi^2}\right)^{3/2} L^3$$

Fermi gas model

$$N = 2 \times \frac{1}{8} \times \frac{4}{3}\pi n_F^3 = \frac{\pi}{3}\left(\frac{2mE_F}{\hbar^2\pi^2}L^2\right)^{3/2} = \frac{\pi}{3}\left(\frac{2mE_F}{\hbar^2\pi^2}\right)^{3/2} L^3$$

$$\longrightarrow \quad \rho = \frac{N}{V} = \frac{N}{L^3} = \frac{\pi}{3}\left(\frac{2mE_F}{\hbar^2\pi^2}\right)^{3/2}$$

or

$$E_F = \frac{\pi^2\hbar^2}{2m}\left(\frac{3}{\pi}\rho\right)^{2/3}$$

Fermi gas model

total energy

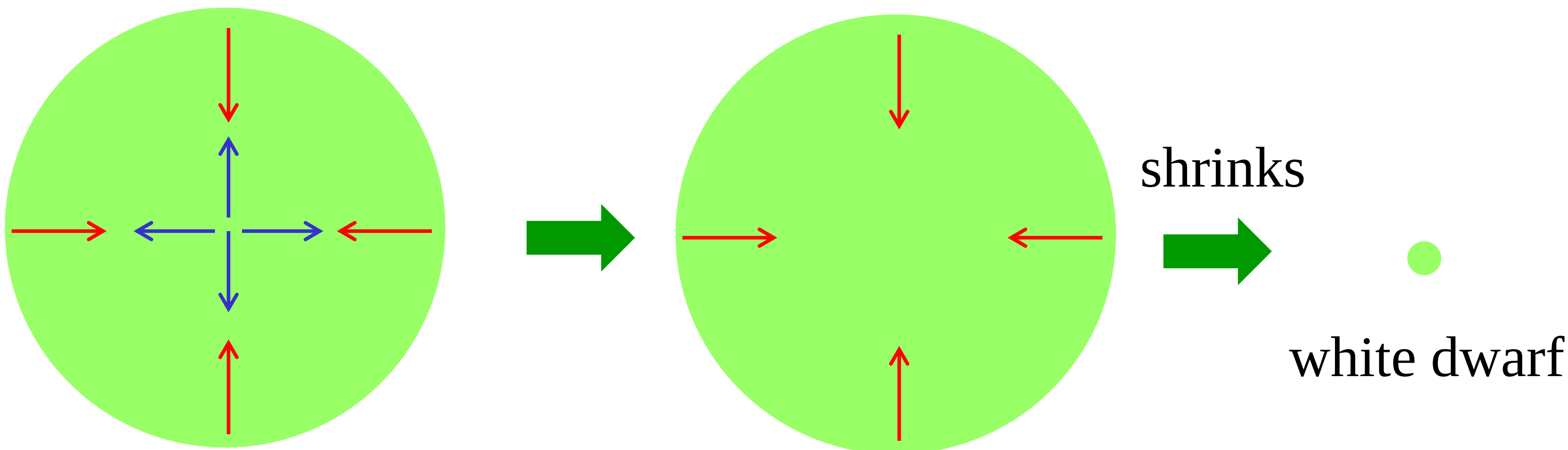
$$\begin{aligned} E_{\rm tot} &= 2\times\frac{1}{8}\int_{|\boldsymbol{n}|\le n_F} E_{n_x n_y n_z}\, d^3n \\ &= 2\times\frac{1}{8}\int_{|\boldsymbol{n}|\le n_F}\frac{\pi^2\hbar^2}{2mL^2}(n_x^2+n_y^2+n_z^2)\, d^3n \\ &= 2\cdot\frac{1}{8}\cdot\frac{\pi^2\hbar^2}{2mL^2}\int_0^{n_F} 4\pi n^2 dn\, n^2 \\ &= 2\cdot\frac{1}{8}\cdot\frac{\pi^2\hbar^2}{2mL^2}\cdot 4\pi\frac{n_F^5}{5} = \frac{\hbar^2\pi^3}{10mL^2}n_F^5 \end{aligned}$$

$$N = 2\times\frac{1}{8}\times\frac{4}{3}\pi n_F^3$$

$$\longrightarrow \quad \boxed{E_{\rm tot} = \frac{3}{5}N\cdot\frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{V}\right)^{2/3} = \frac{3}{5}NE_F}$$

Application to white dwarfs

light stars ($M < 1.4\, M_\odot$)



gravitational effects

$\longleftrightarrow$ outgoing pressure
due to nuclear fusion

equilibrium

electron energy:

$$E_e = \frac{3}{5} N \cdot \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V} \right)^{2/3}$$

$V \downarrow \rightarrow E_e \uparrow$

$\longrightarrow$ the shrinkage stopps
at some volume

Application to white dwarfs

the total energy of a star with the mass *M* and the radius *r*:

$$E = E_G + E_{\text{kin}}$$

the gravitational energy: $E_G = -\frac{3}{5} G \frac{M^2}{r}$

the kinetic energy:

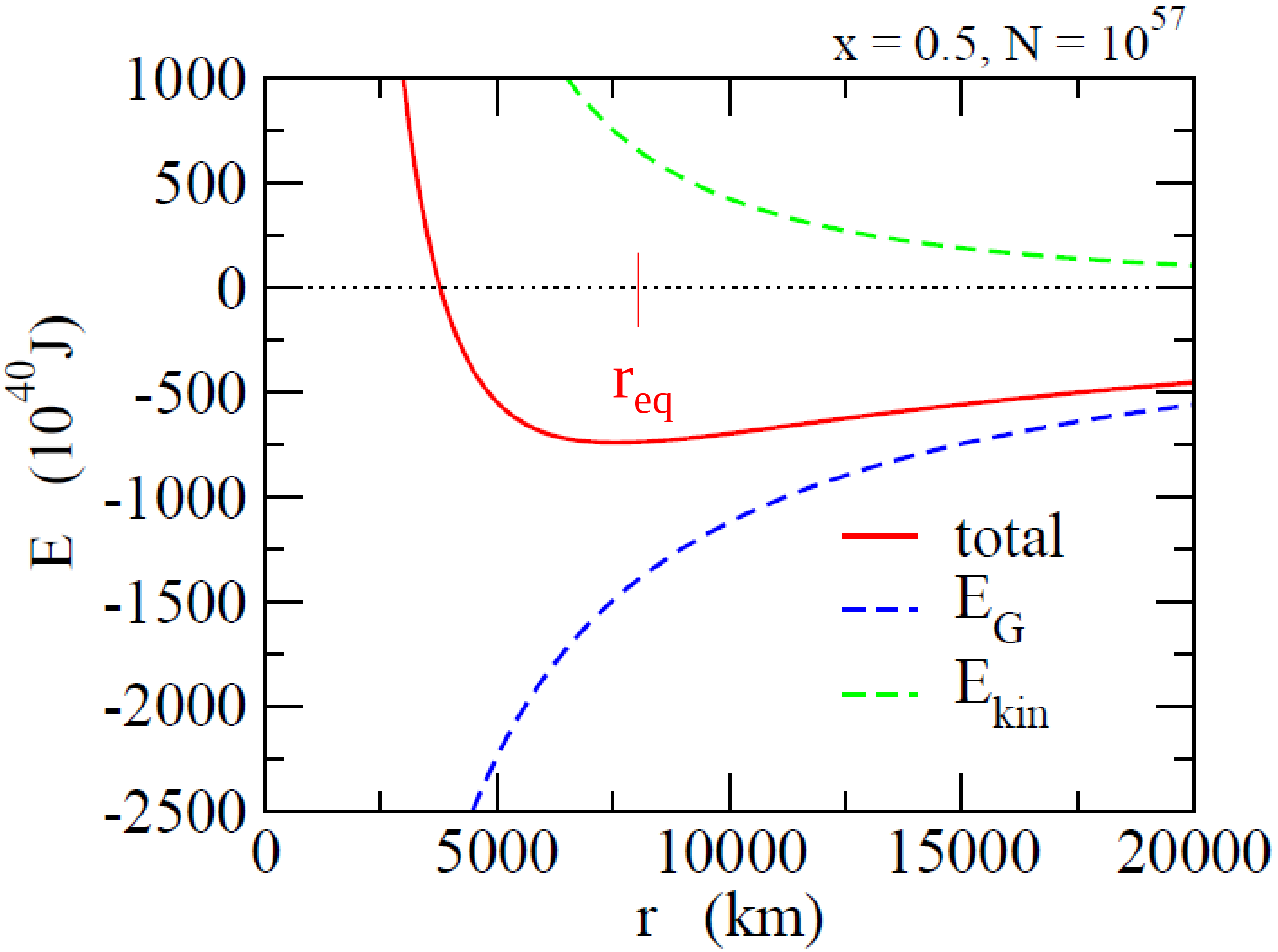
a star with
- xN protons
- $(1\text{-}x)*N$ neutrons
- xN electrons

$$\begin{aligned} E_{\text{kin}} &= E_e + E_p + E_n \sim E_e \\ &= \frac{3}{5} xN \cdot \frac{\hbar^2}{2m_e} \left(3\pi^2 \frac{xN}{V}\right)^{2/3} \\ &= \frac{3}{5} \frac{xN}{r^2} \cdot \frac{\hbar^2}{2m_e} \left(\frac{9\pi}{4} xN\right)^{2/3} \end{aligned}$$

⟵ $V = \frac{4}{3}\pi r^3$

Application to white dwarfs

$$E = E_G + E_{\text{kin}} = -\frac{3}{5} G \frac{M^2}{r} + \frac{3}{5} \frac{xN}{r^2} \cdot \frac{\hbar^2}{2m_e} \left(\frac{9\pi}{4} xN \right)^{2/3}$$



Application to white dwarfs

$$E = E_G + E_{\mathrm{kin}} = -\frac{3}{5}G\frac{M^2}{r} + \frac{3}{5}\frac{xN}{r^2}\cdot\frac{\hbar^2}{2m_e}\left(\frac{9\pi}{4}xN\right)^{2/3}$$

$$\left.\frac{d}{dr}E\right|_{r=r_{\mathrm{eq}}} = 0$$

$$\longrightarrow \quad r_{\mathrm{eq}} = \frac{2x}{GNm_N^2}\cdot\frac{\hbar^2}{2m_e}\left(\frac{9\pi}{4}xN\right)^{2/3}$$

$$(M = Nm_N)$$

$$M = M_\odot, N = M_\odot/m_N = 10^{57}, x = 1/2$$

$$\longrightarrow \quad r_{\mathrm{eq}} = 7716\ \mathrm{km} = 0.011R_\odot$$

cf. $r_{\mathrm{earth}} = 6371$ km