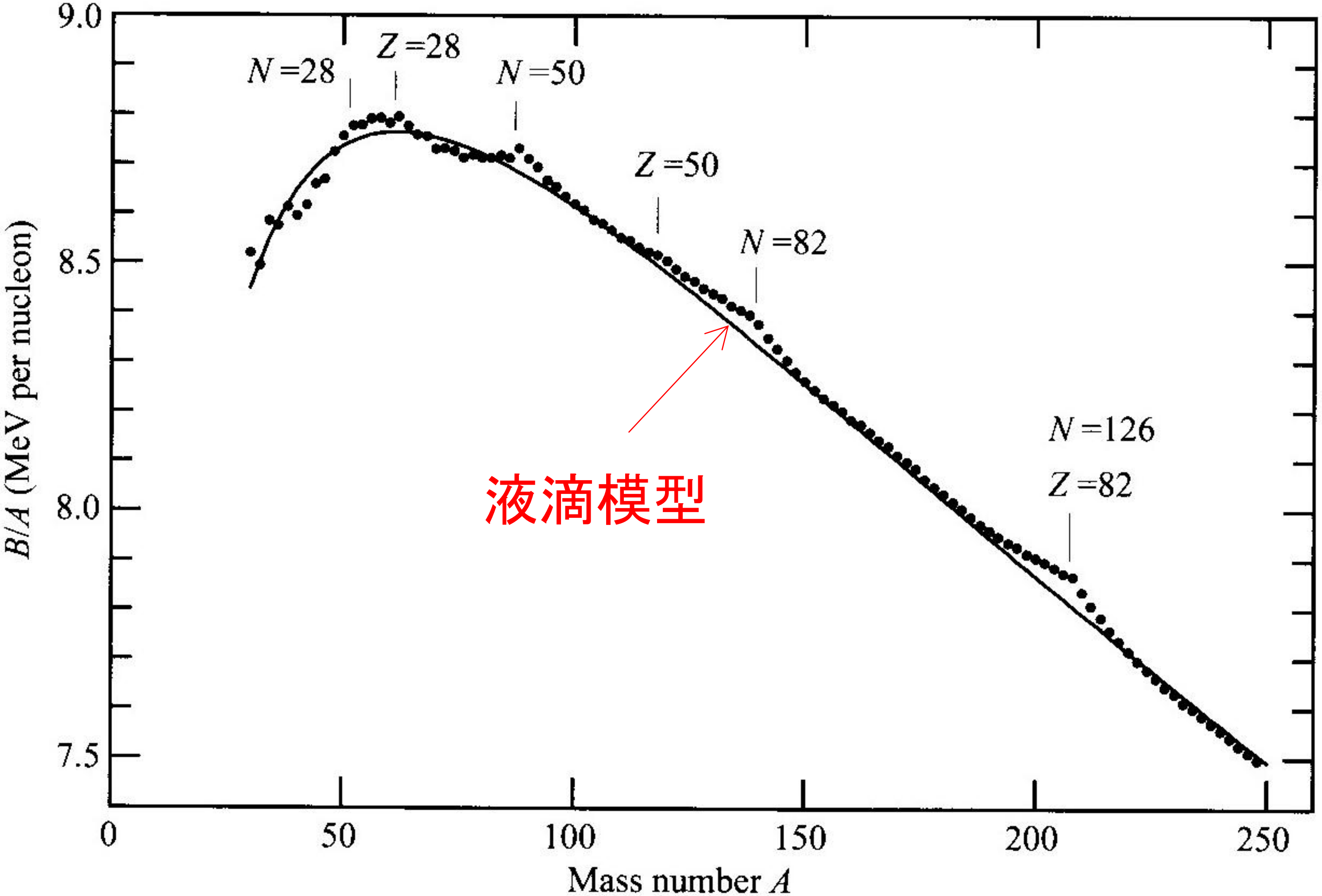


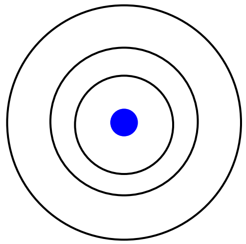
✓ 大体OK、だけど所々にずれ

✓ N,Z = 2, 8, 20, 28, 50, 82, 126 (魔法数)に対して束縛エネルギー大

→ 「殻構造」

(note) 原子の魔法数（貴ガス･希ガス）

He (Z=2), Ne (Z=10), Ar (Z=18), Kr (Z=36), Xe (Z=54), Rn (Z=86)



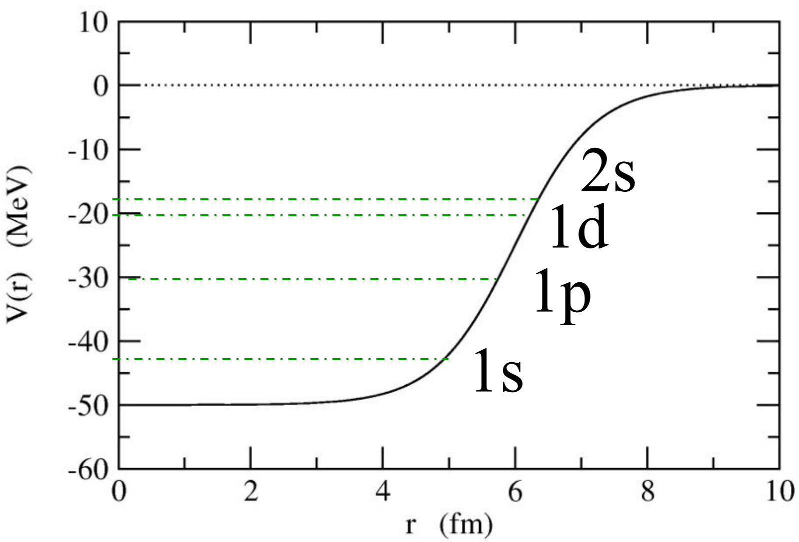
殻構造

原子核の周りを回る電子の軌道が埋まると安定になる

原子核物理における似た試み: ポテンシャル中の独立粒子運動

Woods-Saxon ポテンシャル

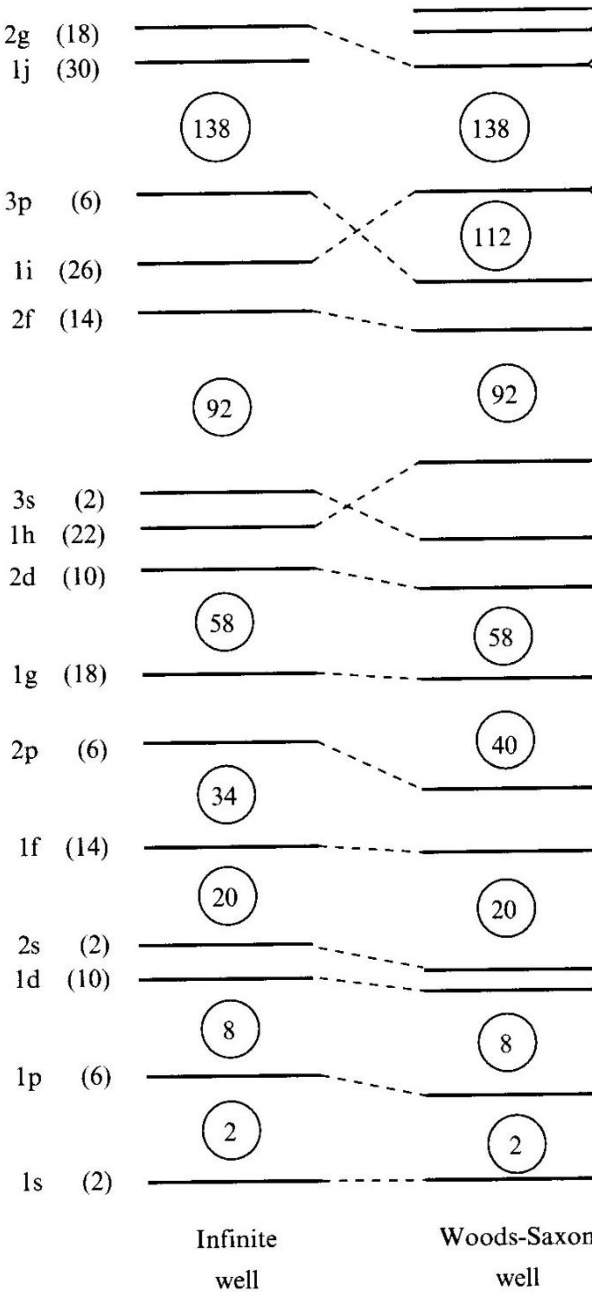
$$V(r) = -V_0/[1 + \exp((r - R_0)/a)]$$



$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - \epsilon\right]\psi(\boldsymbol{r}) = 0$$

$$\psi(\boldsymbol{r}) = \frac{u_l(r)}{r}Y_{lm}(\hat{\boldsymbol{r}})\cdot\chi_{m_s}$$

縮退度に応じて下のレベルから核子を順々につめていく



Woods-Saxon itself does not provide the correct magic numbers (2,8,20,28, 50,82,126).

Mayer and Jensen (1949):
Strong spin-orbit interaction

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) + V_{ls}(r)\boldsymbol{l}\cdot\boldsymbol{s} - \epsilon\right]\psi(\boldsymbol{r}) = 0$$

$$V_{ls}(r) \sim -\lambda \frac{1}{r}\frac{dV}{dr} \qquad (\lambda > 0)$$

jj 結合殻模型

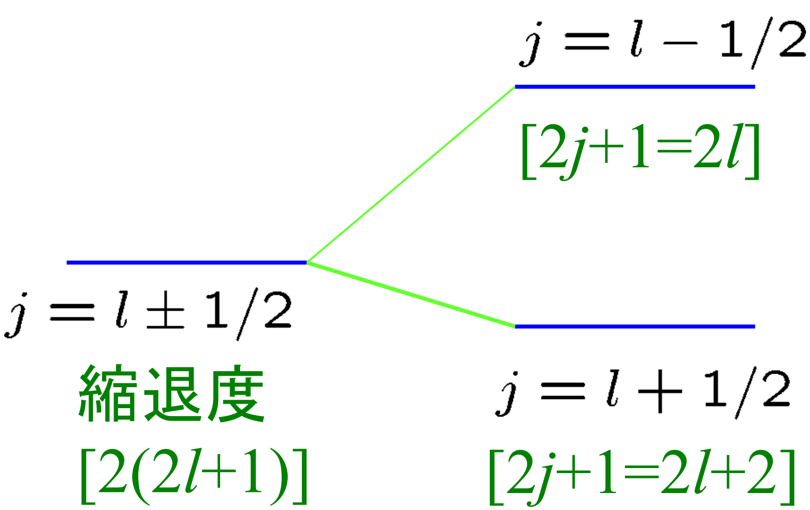
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) + V_{ls}(r)\boldsymbol{l}\cdot\boldsymbol{s} - \epsilon\right]\psi(\boldsymbol{r}) = 0$$

$$\boldsymbol{l}\cdot\boldsymbol{s}\,|\mathcal{Y}_{jlm}\rangle = \frac{l}{2}|\mathcal{Y}_{jlm}\rangle \quad (j = l + 1/2)$$

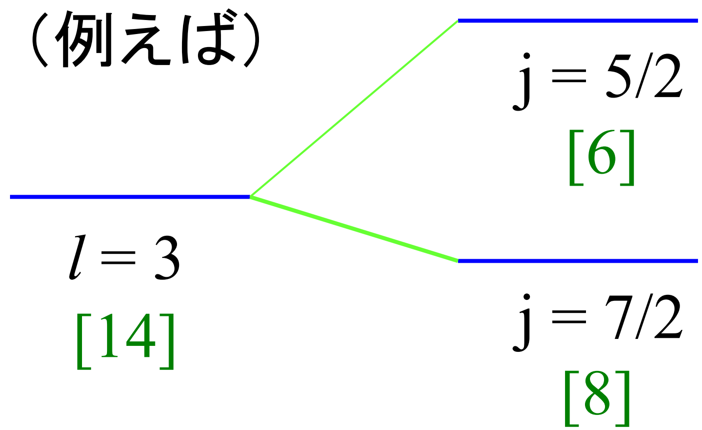
$$\boldsymbol{l}\cdot\boldsymbol{s}\,|\mathcal{Y}_{jlm}\rangle = -\frac{l+1}{2}|\mathcal{Y}_{jlm}\rangle \quad (j = l - 1/2)$$

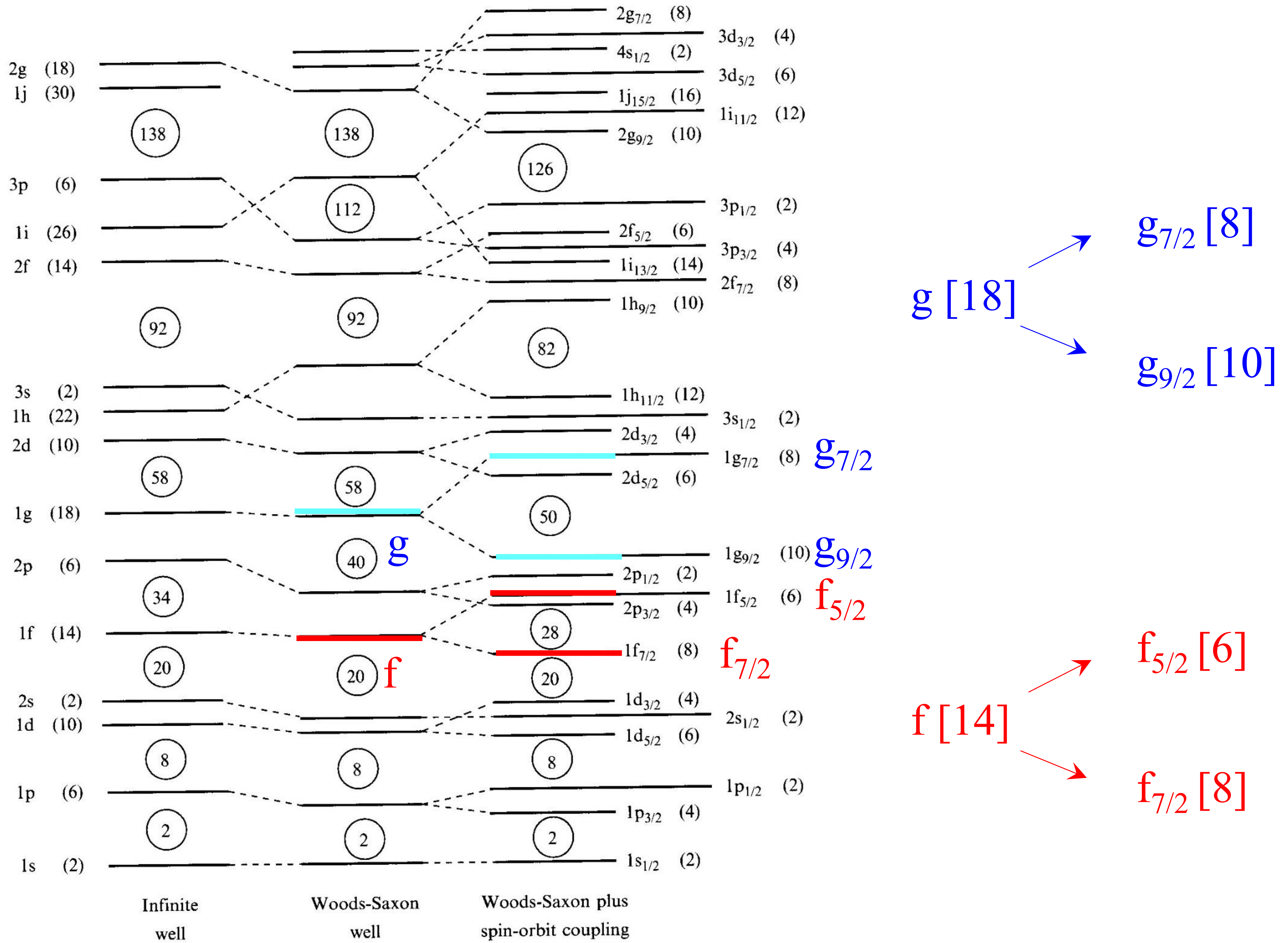
符号が逆！

$j = l \pm 1/2$ で準位が分離



（例えば）

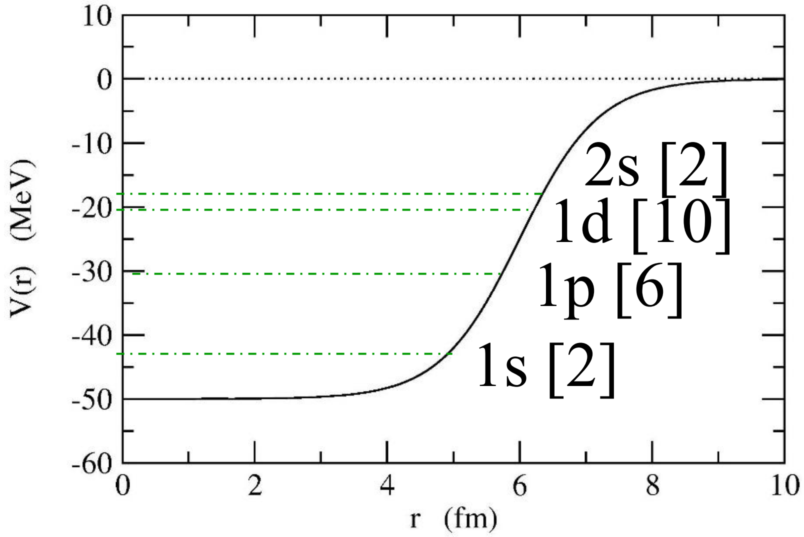




2g (18)
1j (30)
3p (6)
1i (26)
2f (14)
3s (2)
1h (22)
2d (10)
1g (18)
2p (6)
1f (14)
2s (2)
1d (10)
1p (6)
1s (2)
138
112
126
92
82
58
50
40
34
28
20
8
2
g
f
2g$_{7/2}$ (8)
3d$_{3/2}$ (4)
4s$_{1/2}$ (2)
3d$_{5/2}$ (6)
1j$_{15/2}$ (16)
1i$_{11/2}$ (12)
2g$_{9/2}$ (10)
3p$_{1/2}$ (2)
2f$_{5/2}$ (6)
3p$_{3/2}$ (4)
1i$_{13/2}$ (14)
2f$_{7/2}$ (8)
1h$_{9/2}$ (10)
1h$_{11/2}$ (12)
3s$_{1/2}$ (2)
2d$_{3/2}$ (4)
1g$_{7/2}$ (8)
2d$_{5/2}$ (6)
1g$_{9/2}$ (10)
2p$_{1/2}$ (2)
1f$_{5/2}$ (6)
2p$_{3/2}$ (4)
1f$_{7/2}$ (8)
1d$_{3/2}$ (4)
2s$_{1/2}$ (2)
1d$_{5/2}$ (6)
1p$_{1/2}$ (2)
1p$_{3/2}$ (4)
1s$_{1/2}$ (2)
g$_{7/2}$
g$_{9/2}$
f$_{5/2}$
f$_{7/2}$
Infinite well
Woods-Saxon well
Woods-Saxon plus spin-orbit coupling
g [18]
g$_{7/2}$ [8]
g$_{9/2}$ [10]
f [14]
f$_{5/2}$ [6]
f$_{7/2}$ [8]

原子核の殻模型

Shell Model: independent particle motion in a potential well



+ spin-orbit interaction

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - \epsilon\right]\psi(\boldsymbol{r}) = 0$$

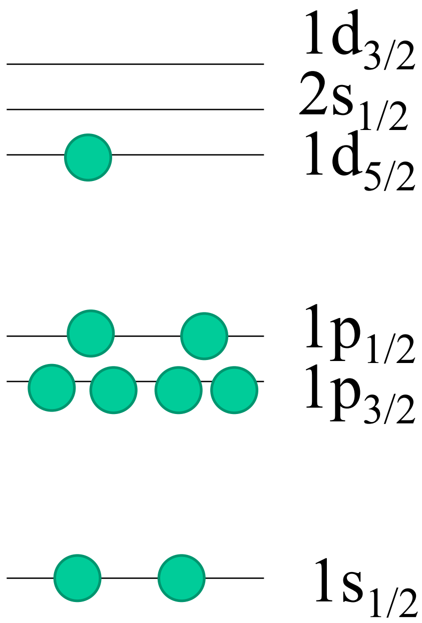
$$\psi(\boldsymbol{r}) = \frac{u_l(r)}{r}\mathcal{Y}_{jlm}(\hat{\boldsymbol{r}})$$

$$\mathcal{Y}_{jlm}(\hat{\boldsymbol{r}}) = \sum_{m_l,m_s}\langle l\ m_l\ 1/2\ m_s|j\ m\rangle Y_{lm_l}(\hat{\boldsymbol{r}})\chi_{m_s}$$

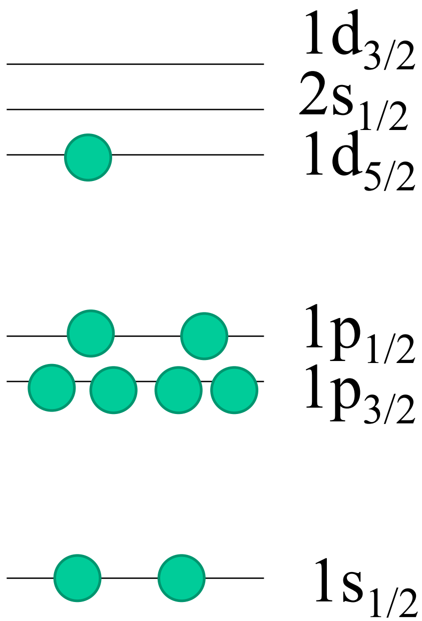
$$H = \sum_k \epsilon_k a_k^\dagger a_k$$

shell model

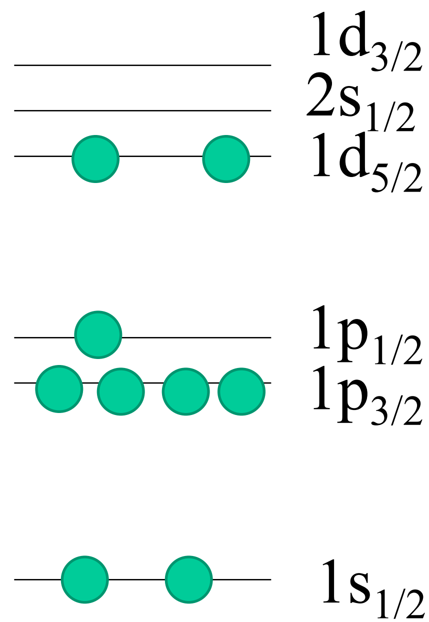
$$H = \sum_k \epsilon_k a_k^\dagger a_k$$



shell model $H = \sum_k \epsilon_k a_k^\dagger a_k$



configuration 1

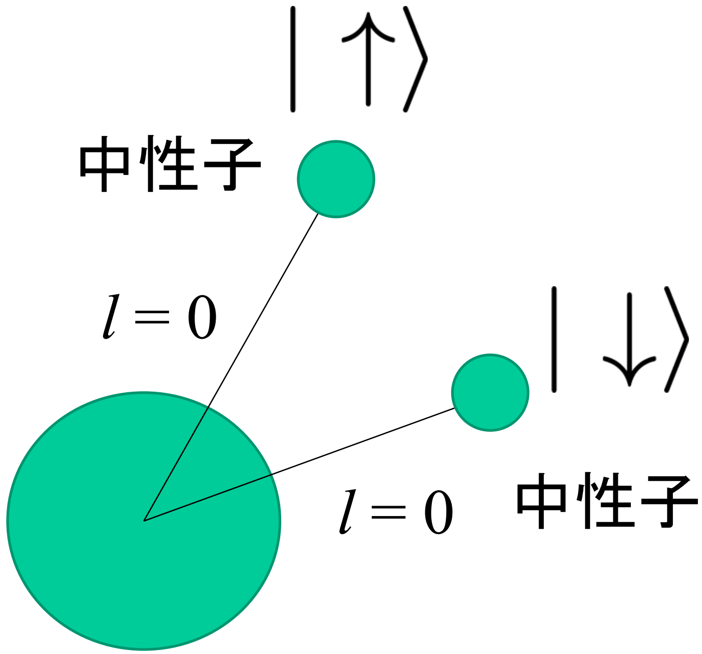


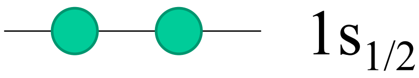
configuration 2

...... several others

angular momentum (spin) and parity for each configuration?

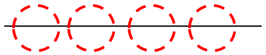
→ let us first investigate a single-j case the first example: $j = s_{1/2}$





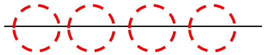
この系の全スピンは何か？

the next example: $j = p_{3/2}$



$p_{3/2}$ can accommodate 4 nucleons

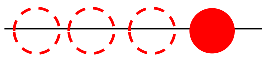
(j_z= +3/2, +1/2, -1/2, -3/2)

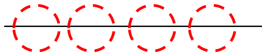
 $p_{3/2}$

can accommodate 4 nucleons

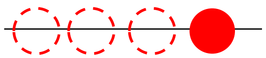
(j_z= +3/2, +1/2, -1/2, -3/2)

i) 1 nucleon

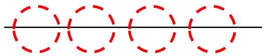
 $p_{3/2}$

 $p_{3/2}$ can accommodate 4 nucleons (j_z= +3/2, +1/2, -1/2, -3/2)

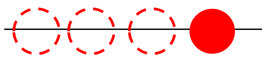
i) 1 nucleon

 $p_{3/2}$ → $I^{\pi} = 3/2^{-}$

(there are 4 ways to occupy this level)

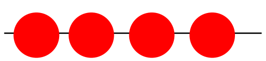
 $p_{3/2}$ can accommodate 4 nucleons
(j_z= +3/2, +1/2, -1/2, -3/2)

i) 1 nucleon

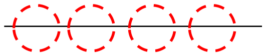
 $p_{3/2}$ → $I^\pi = 3/2^-$

(there are 4 ways to occupy this level)

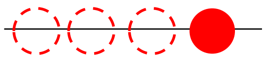
ii) 4 nucleons

 $p_{3/2}$

$$\boldsymbol{I} = \boldsymbol{j}_1 + \boldsymbol{j}_2 + \boldsymbol{j}_3 + \boldsymbol{j}_4$$

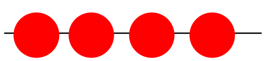
 $p_{3/2}$ can accommodate 4 nucleons (j_z= +3/2, +1/2, -1/2, -3/2)

i) 1 nucleon

 $p_{3/2}$ ⇒ $I^{\pi} = 3/2^{-}$

(there are 4 ways to occupy this level)

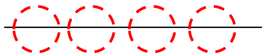
ii) 4 nucleons

 $p_{3/2}$ ⇒ $I^{\pi} = 0^{+}$

(there is only 1 way to occupy this level)

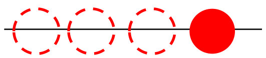
$$I = j_1 + j_2 + j_3 + j_4$$

parity: (-1) x (-1) x (-1) x (-1) = +1

 $p_{3/2}$ can accommodate 4 nucleons

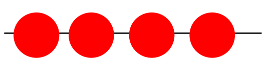
(j_z= +3/2, +1/2, -1/2, -3/2)

i) 1 nucleon

 $p_{3/2}$ → $I^{\pi} = 3/2^{-}$

(there are 4 ways to occupy this level)

ii) 4 nucleons

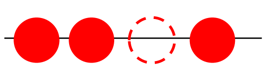
 $p_{3/2}$ → $I^{\pi} = 0^{+}$

$$\boldsymbol{I} = \boldsymbol{j}_1 + \boldsymbol{j}_2 + \boldsymbol{j}_3 + \boldsymbol{j}_4$$

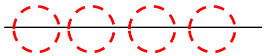
(there is only 1 way to occupy this level)

parity: (-1) x (-1) x (-1) x (-1) = +1

iii) 3 nucleons

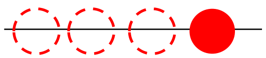
 $p_{3/2}$

$$\boldsymbol{I} = \boldsymbol{j}_1 + \boldsymbol{j}_2 + \boldsymbol{j}_3$$



$p_{3/2}$ can accommodate 4 nucleons (j_z= +3/2, +1/2, -1/2, -3/2)

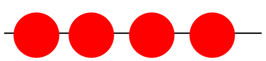
i) 1 nucleon



$p_{3/2}$ → $I^\pi = 3/2^-$

(there are 4 ways to occupy this level)

ii) 4 nucleons



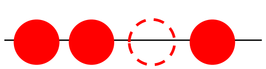
$p_{3/2}$ → $I^\pi = 0^+$

$$I = j_1 + j_2 + j_3 + j_4$$

(there is only 1 way to occupy this level)

parity: (-1) x (-1) x (-1) x (-1) = +1

iii) 3 nucleons



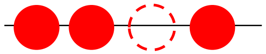
$p_{3/2}$ → $I^\pi = 3/2^-$

$$I = j_1 + j_2 + j_3$$

(there are 4 ways to make a hole)

parity: (-1) x (-1) x (-1) = -1

iii) 3 nucleons



$p_{3/2}$

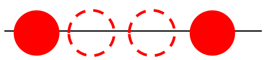
$I^{\pi} = 3/2^{-}$

(there are 4 ways to make a hole)

$$\boldsymbol{I} = \boldsymbol{j}_1 + \boldsymbol{j}_2 + \boldsymbol{j}_3$$

parity: (-1) x (-1) x (-1) = -1

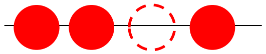
iv) 2 nucleons



$p_{3/2}$

$$\boldsymbol{I} = \boldsymbol{j}_1 + \boldsymbol{j}_2$$

iii) 3 nucleons



$p_{3/2}$

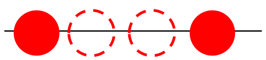
$\boldsymbol{I} = \boldsymbol{j}_1 + \boldsymbol{j}_2 + \boldsymbol{j}_3$

$I^{\pi} = 3/2^{-}$

(there are 4 ways to make a hole)

parity: (-1) x (-1) x (-1) = -1

iv) 2 nucleons



$p_{3/2}$

$\boldsymbol{I} = \boldsymbol{j}_1 + \boldsymbol{j}_2$

there are 4 x 3/2=6 ways to occupy this level with 2 nucleons.

$I^{\pi} = 0^{+}$ or 2^{+} (= 1+5)

3/2 + 3/2 → I = 0, ~~1~~, 2, ~~3~~

anti-symmetrization

レポート問題3：PandAから提出、提出〆切　7/27（日）23:59

角運動量 j を持つ軌道(j は半整数)にフェルミオン2つを生成する以下の演算子を考える。

$$[a_j^\dagger a_j^\dagger]^{(JM)} = \sum_{m,m'} \langle jmjm'|JM\rangle\, a_{jm}^\dagger a_{jm'}^\dagger$$

ここで、J は2粒子系の全角運動量、M はその z 成分である。

フェルミオン演算子の反交換関係

$$\{a_{jm}^\dagger, a_{jm'}^\dagger\} = 0$$

及び Clebsch-Gordan 係数の性質

$$\langle jmjm'|JM\rangle = (-1)^{j+j-J}\langle jm'jm|JM\rangle$$

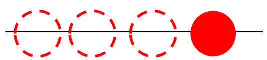
を用いて、角運動量 J は偶数の値しかとらないことを示せ。

レポート問題4: PandAから提出、提出〆切 7/27（日）23:59

前問で、角運動量 j が整数のボゾンの場合、全角運動量 J がどのような値を取るか議論せよ。

$$[a_j^\dagger a_j^\dagger]^{(JM)} = \sum_{m,m'} \langle jmjm'|JM\rangle\, a_{jm}^\dagger a_{jm'}^\dagger$$

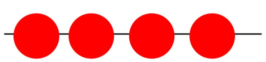
i) 1 nucleon



$p_{3/2}$ → $I^{\pi} = 3/2^{-}$

(there are 4 ways to occupy this level)

ii) 4 nucleons

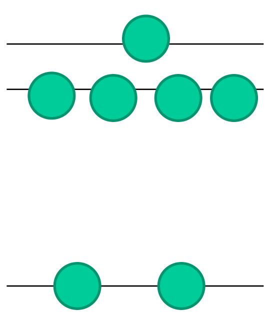


$p_{3/2}$ → $I^{\pi} = 0^{+}$

$$I = j_1 + j_2 + j_3 + j_4$$

(there is only 1 way to occupy this level)

parity: (-1) x (-1) x (-1) x (-1) = +1



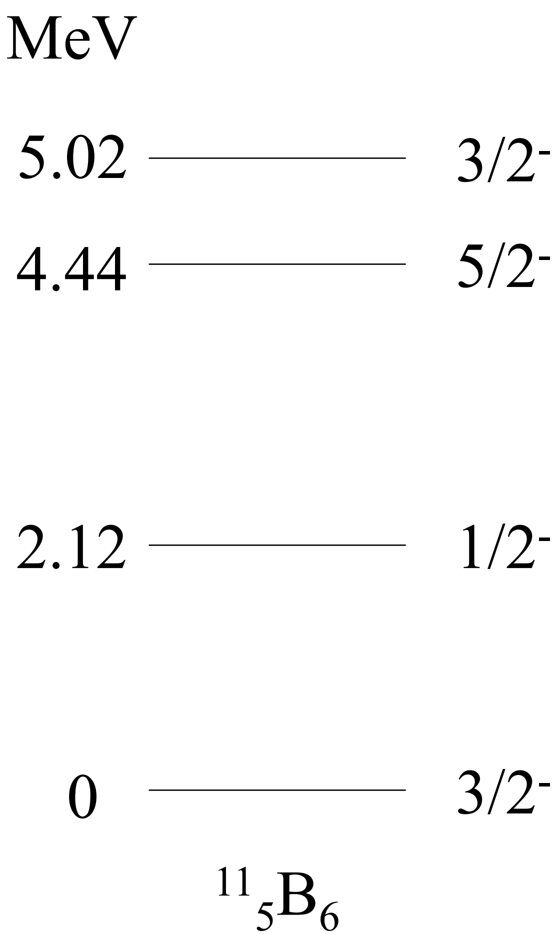
$1p_{1/2}$ → $I^{\pi} = 1/2^{-}$

$1p_{3/2}$ → $I^{\pi} = 0^{+}$

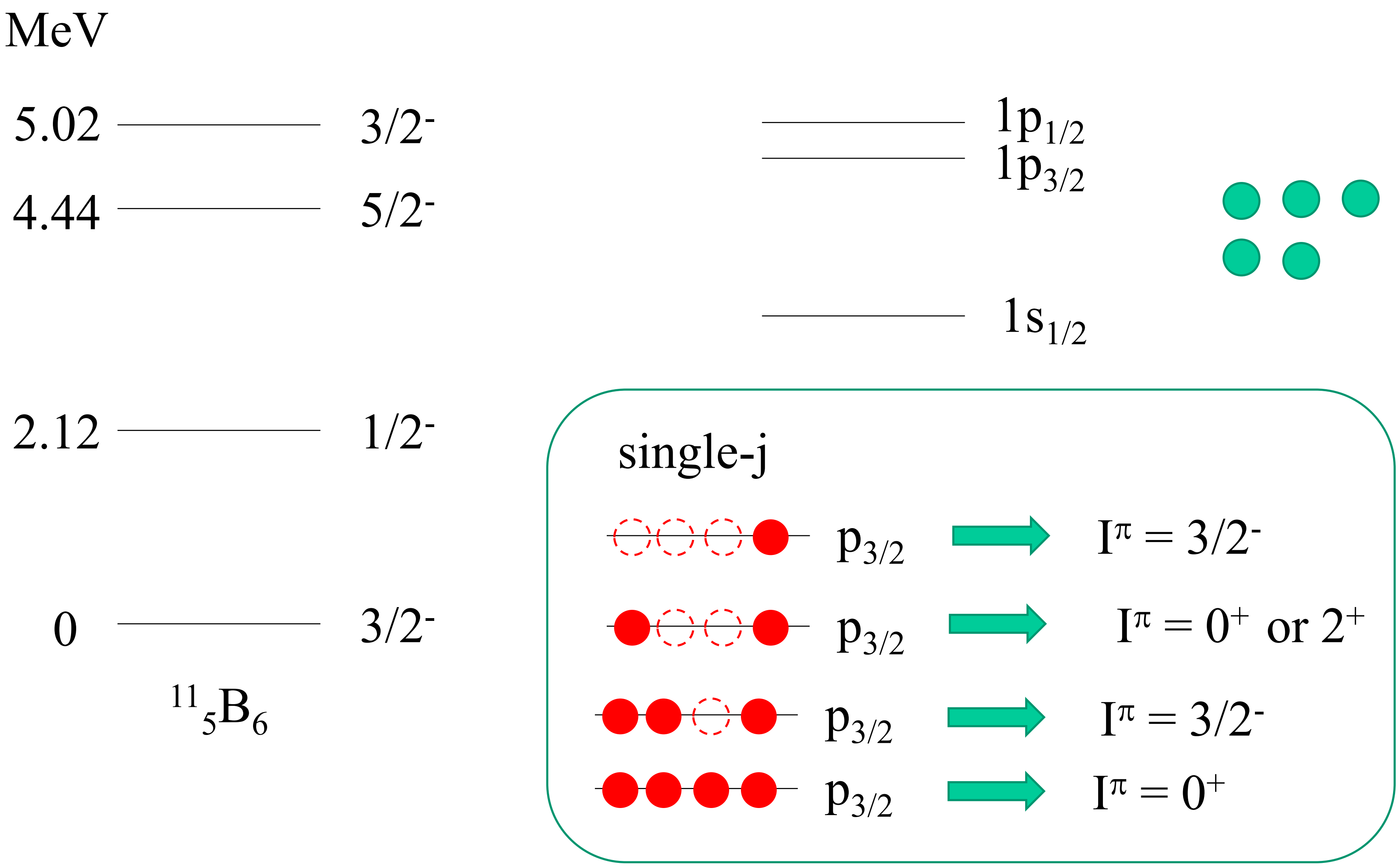
$1s_{1/2}$ → $I^{\pi} = 0^{+}$

in total,
$I^{\pi} = 1/2^{-}$

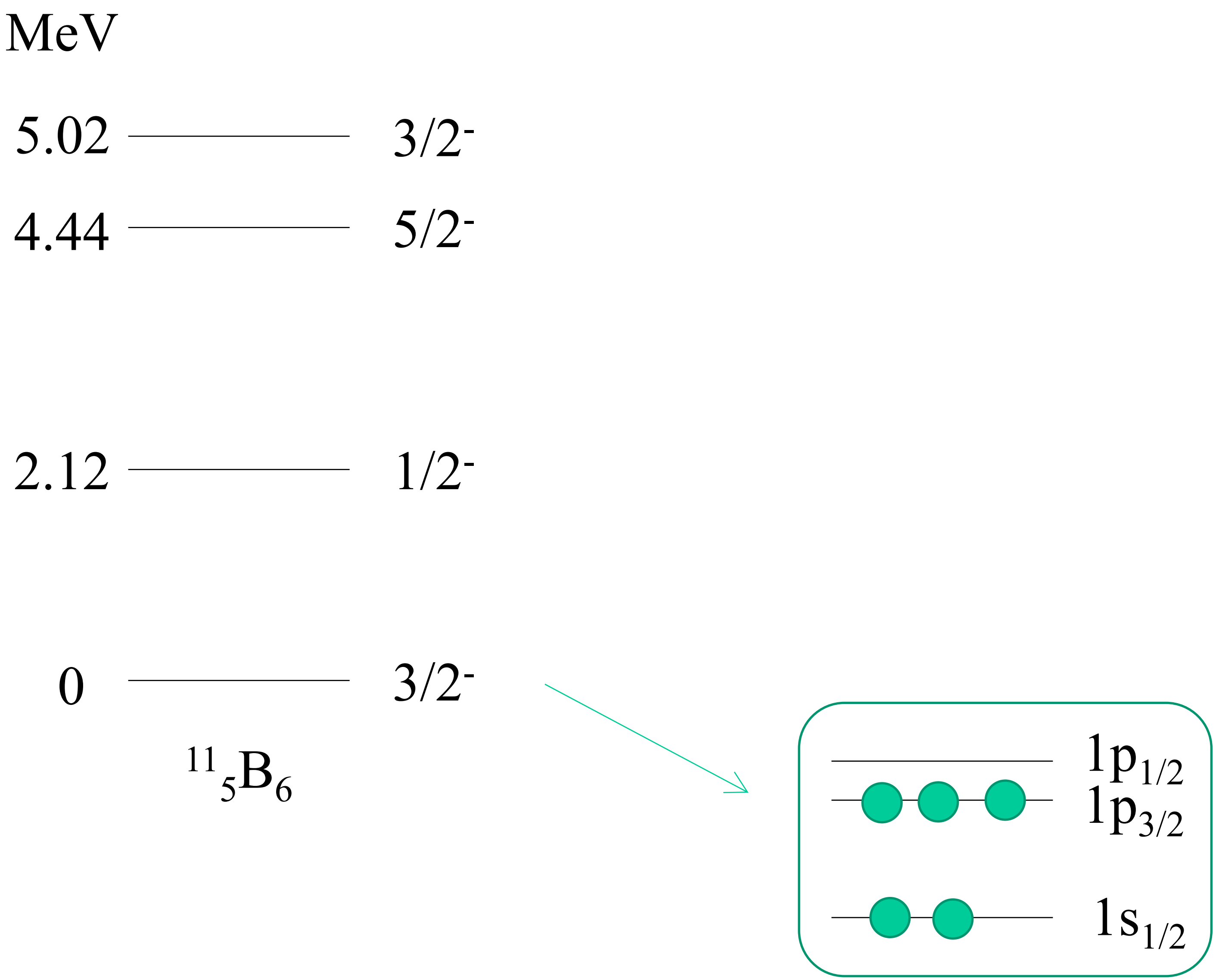
example: (main) shell model configurations for $^{11}_{5}B_6$



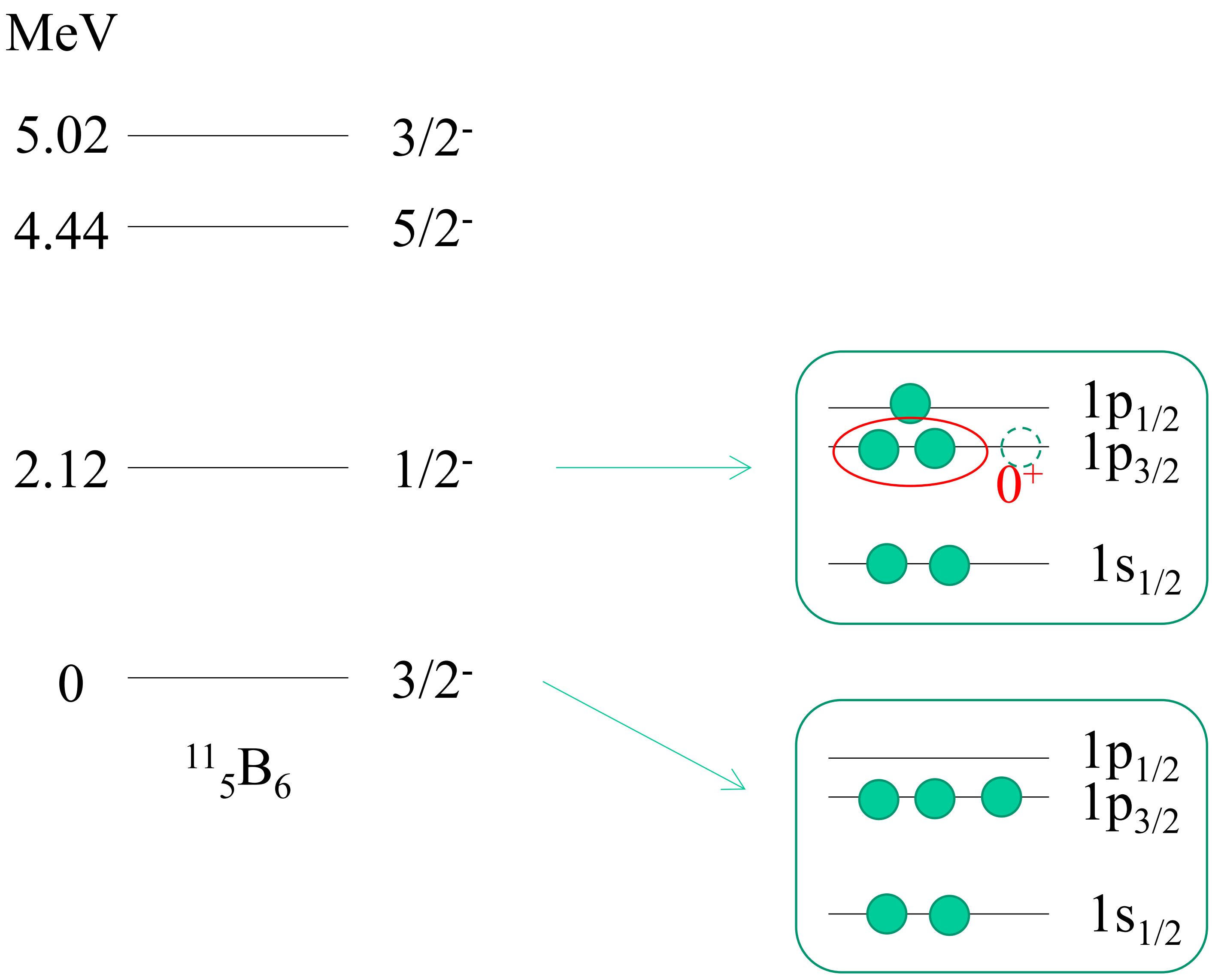
example: (main) shell model configurations for $^{11}_{5}B_6$



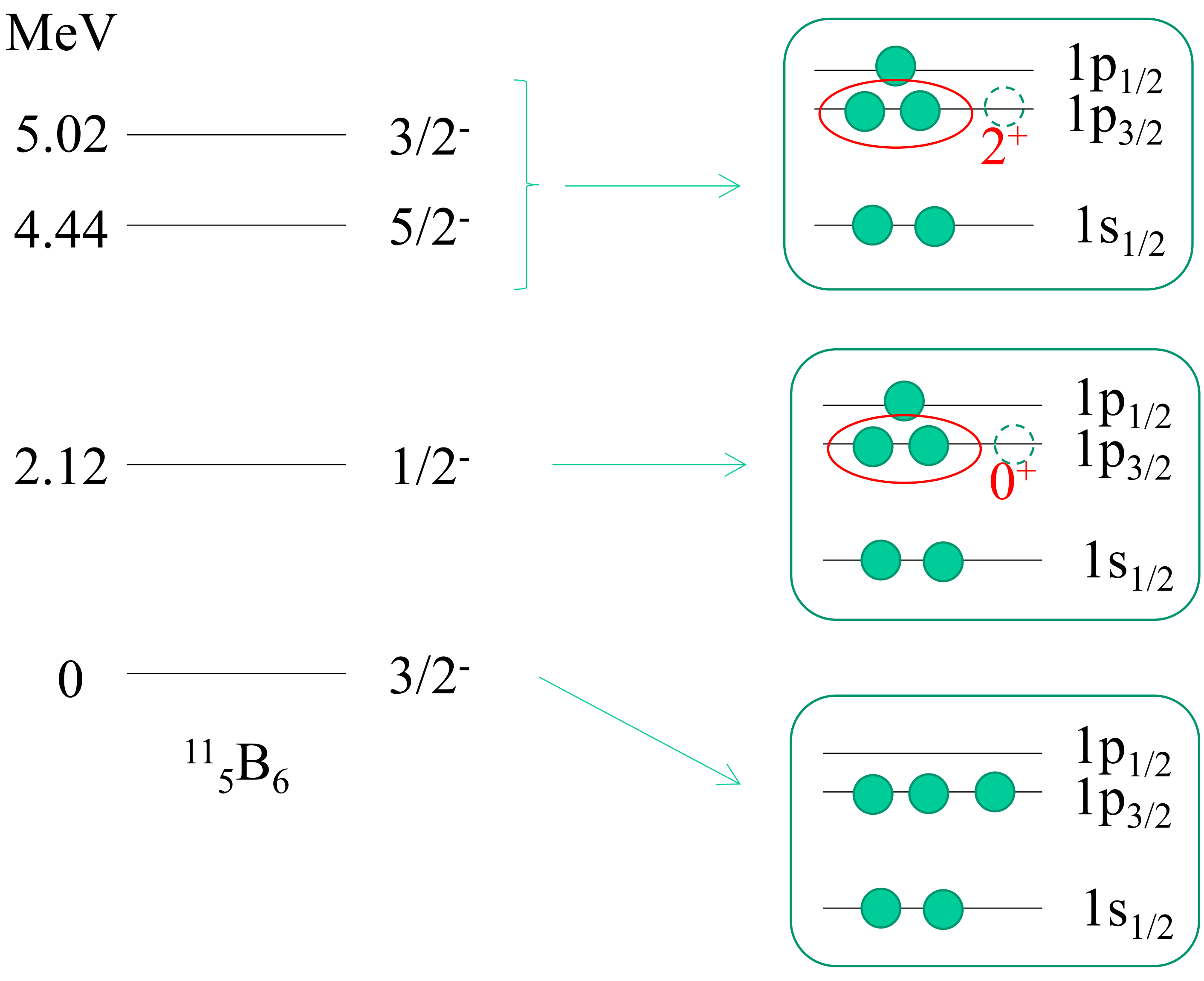
example: (main) shell model configurations for $^{11}_{5}B_6$



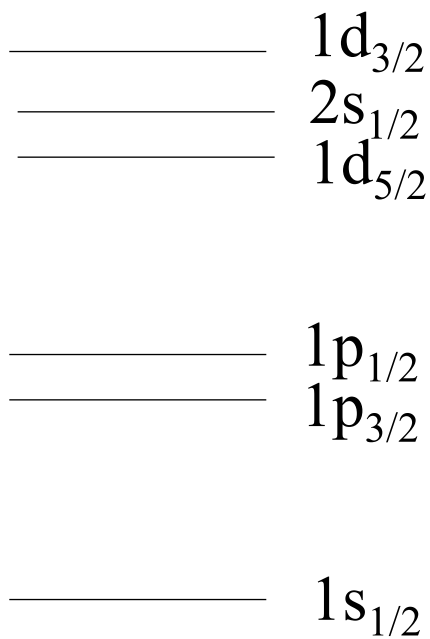
example: (main) shell model configurations for $^{11}{}_5B_6$



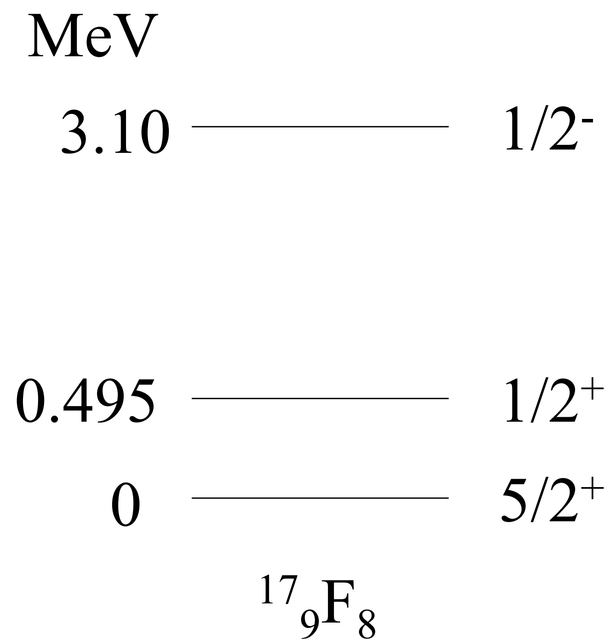
example: (main) shell model configurations for $^{11}{}_5B_6$



レポート問題５：$^{17}_{9}\mathrm{F}_{8}$の基底状態の陽子の配位を殻模型を使って説明せよ。第一励起状態、第二励起状態はどうなるか？



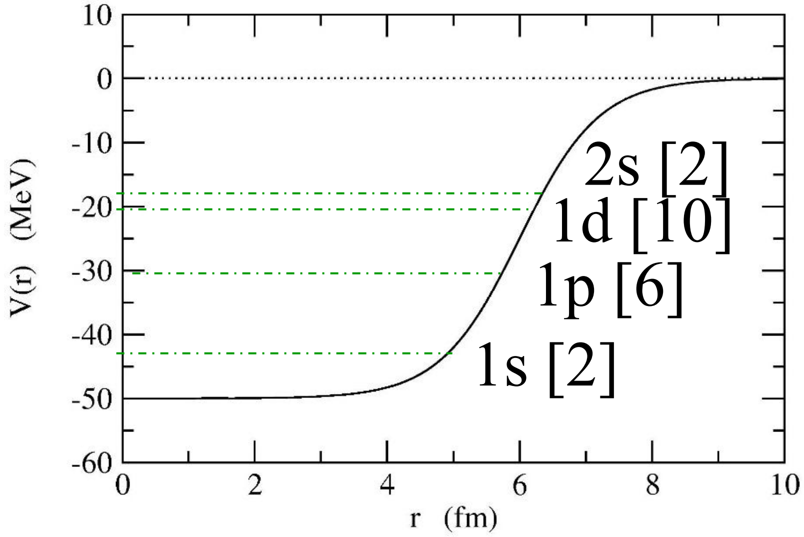
1粒子状態
ここに9つの陽子をつめる
（中性子は偶数なので考えなくてよい）



$^{17}_{9}\mathrm{F}_{8}$のスペクトル

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

An interpretation: independent particle motion *in a potential well*

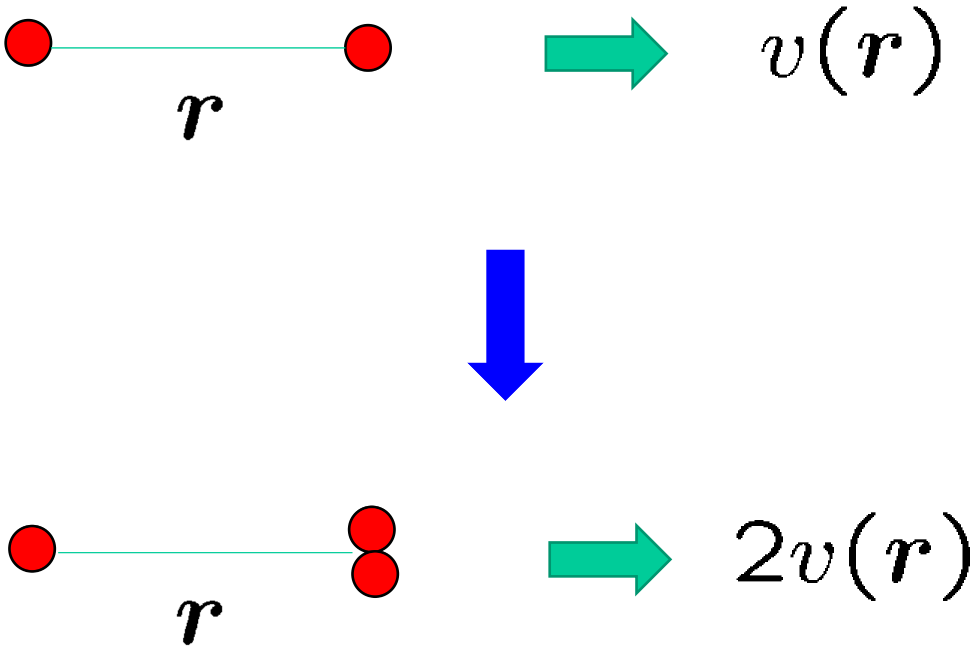


+ spin-orbit interaction

how to construct the potential well?

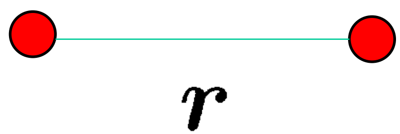
Mean-field (Hartree-Fock) Theory

nucleon-nucleon interaction



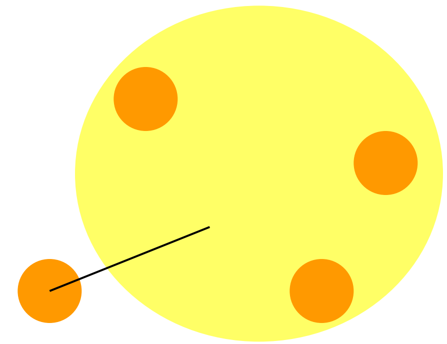
Mean-field (Hartree-Fock) Theory

nucleon-nucleon interaction



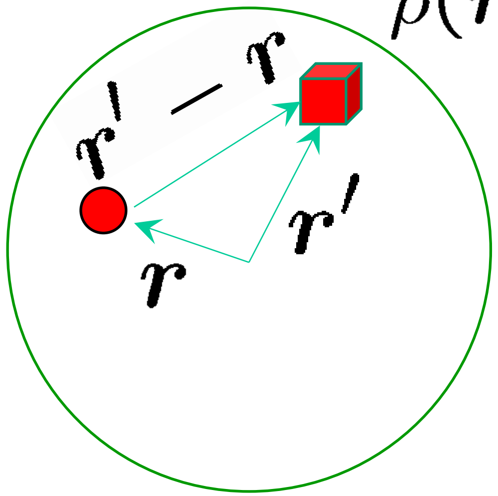
$\Rightarrow$ $v(\boldsymbol{r})$

平均場



interaction for a nucleon inside a nucleus:

$\rho(\boldsymbol{r}')d\boldsymbol{r}'$



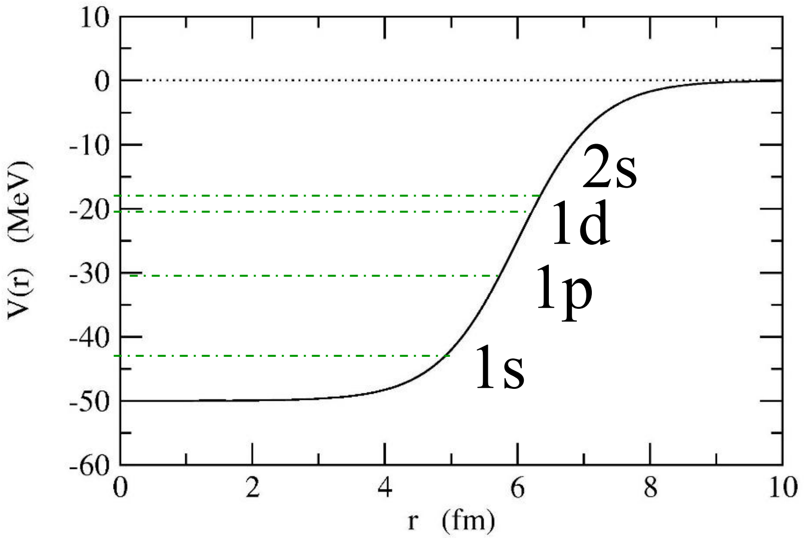
$$\Rightarrow \quad v(\boldsymbol{r}' - \boldsymbol{r}) \cdot \underline{\rho(\boldsymbol{r}')d\boldsymbol{r}'}$$

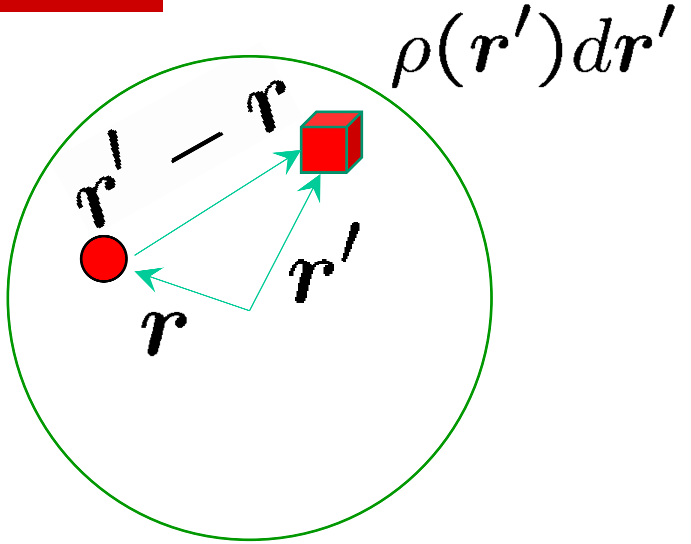
the number of nucleon at *r*'

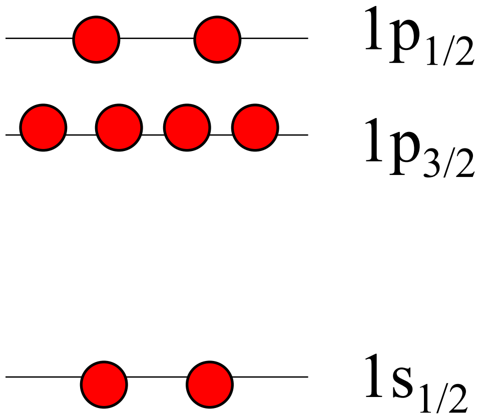
naively speaking,

$$\boxed{V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'}$$

Mean-field (Hartree-Fock) Theory





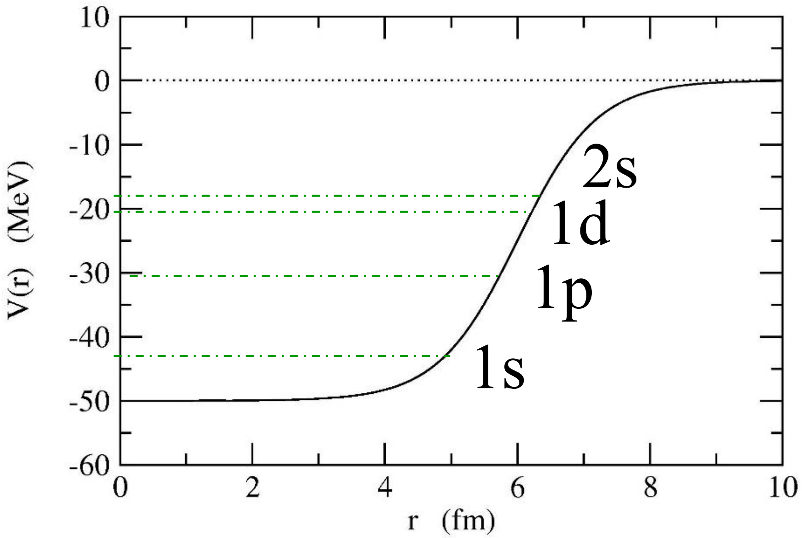


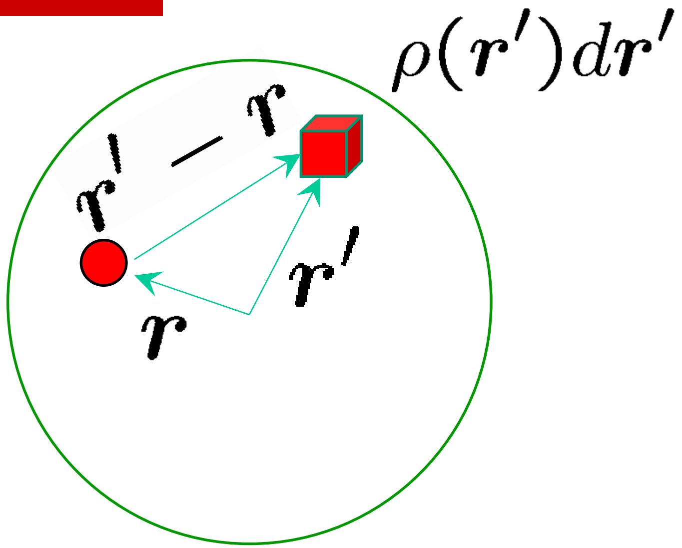
shell model

naively speaking,

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

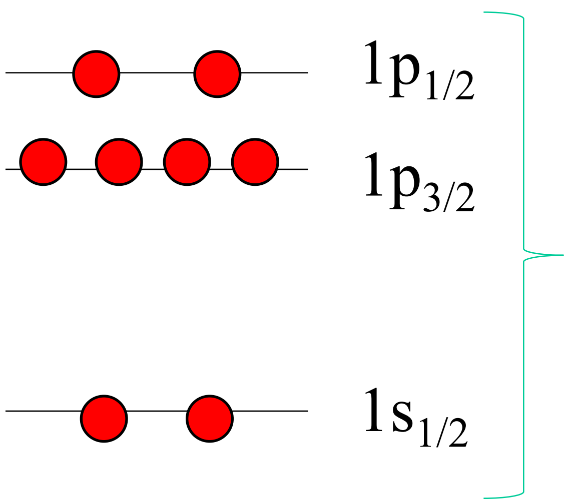
Mean-field (Hartree-Fock) Theory





naively speaking,

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

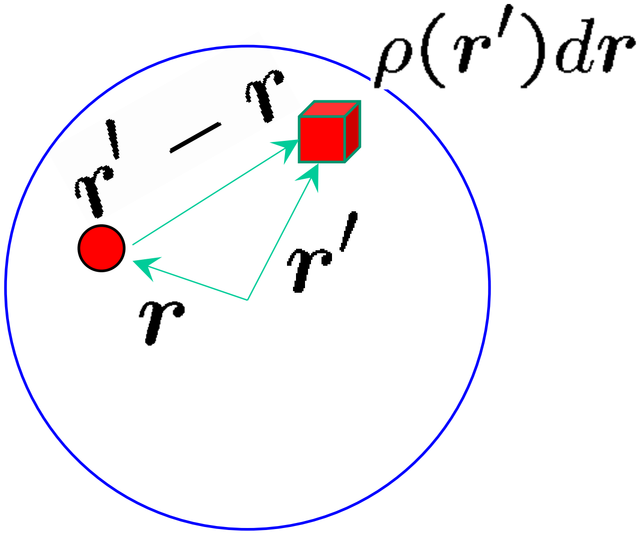


independent motion

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2$$

shell model

Mean-field (Hartree-Fock) Theory



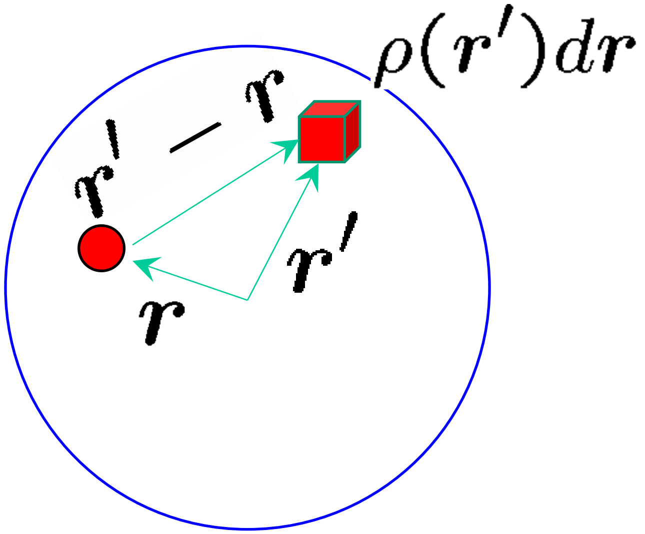
naively speaking,

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2$$

$$0 = \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r}) - \epsilon_i\right]\psi_i(\boldsymbol{r})$$

Mean-field (Hartree-Fock) Theory



naively speaking,

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2$$

$$\begin{aligned} 0 &= \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r}) - \epsilon_i\right]\psi_i(\boldsymbol{r}) \\ &= \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r} - \boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right)d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r}) \end{aligned}$$

the potential depends on the solutions

Mean-field (Hartree-Fock) Theory

$$0 = \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r}-\boldsymbol{r}') \left(\sum_j |\psi_j(\boldsymbol{r}')|^2 \right) d\boldsymbol{r}' - \epsilon_i \right] \psi_i(\boldsymbol{r})$$

the potential depends on the solutions

$\longrightarrow$ self-consistent solutions

Iteration: $\{\psi_i\} \rightarrow \rho \rightarrow V \rightarrow \{\psi_i\} \rightarrow \cdots$

Mean-field (Hartree-Fock) Theory

$$
\begin{aligned}
0 &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) - \epsilon_i\right]\psi_i(\boldsymbol{r}) \\
&= \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right)d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r})
\end{aligned}
$$

the potential depends on the solutions

→ self-consistent solutions

Iteration: $\{\psi_i\} \to \rho \to V \to \{\psi_i\} \to \cdots$

$$
\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2, \quad V(\boldsymbol{r}) \sim \int v(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'
$$

repeat until the first and the last wave functions are the same.

"self-consistent solutions"　　自己無撞着（むどうちゃく）解

Variational Principle (Rayleigh-Ritz method)

optimization $\longleftrightarrow$ variational principle

$$\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_{\mathsf{g.s.}}$$

Variational Principle (Rayleigh-Ritz method)

optimization $\longleftrightarrow$ variational principle

$$\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_{\mathrm{g.s.}}$$

$$|\Psi\rangle = \sum_n C_n |\phi_n\rangle$$

$$\longrightarrow \quad \mathrm{lhs} = \frac{\sum_n C_n^2 E_n}{\sum_n C_n^2} \geq E_0$$

H : many-body Hamiltonian

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots) = \psi_1(\boldsymbol{r}_1)\cdot\psi_2(\boldsymbol{r}_2)\cdot\psi_3(\boldsymbol{r}_3)\cdots$$

$\longleftarrow$ many-body wave function for independent particles

Variational Principle (Rayleigh-Ritz method)

optimization $\longleftrightarrow$ variational principle

$$\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_{\mathrm{g.s.}}$$

$$|\Psi\rangle = \sum_n C_n\,|\phi_n\rangle$$

$$\longrightarrow \quad \mathrm{lhs} = \frac{\sum_n C_n^2 E_n}{\sum_n C_n^2} \geq E_0$$

H : many-body Hamiltonian

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots) = \psi_1(\boldsymbol{r}_1)\cdot\psi_2(\boldsymbol{r}_2)\cdot\psi_3(\boldsymbol{r}_3)\cdots$$

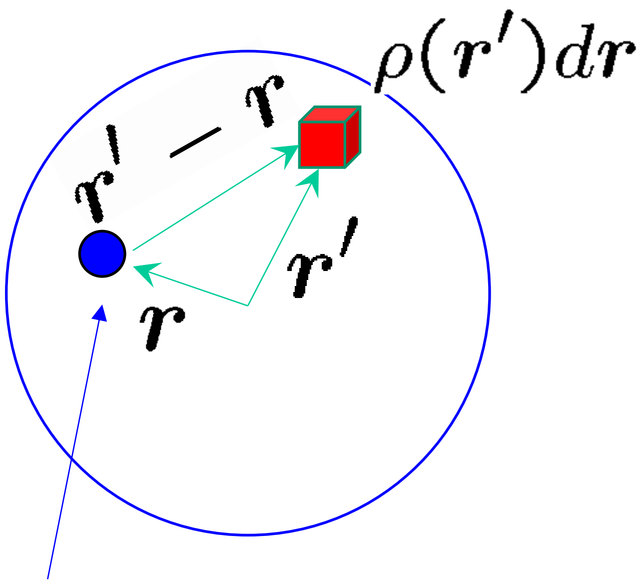
$\longleftarrow$ many-body wave function for independent particles

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r}) = 0$$

change gradually the single-particle potential so that the total energy becomes minimum

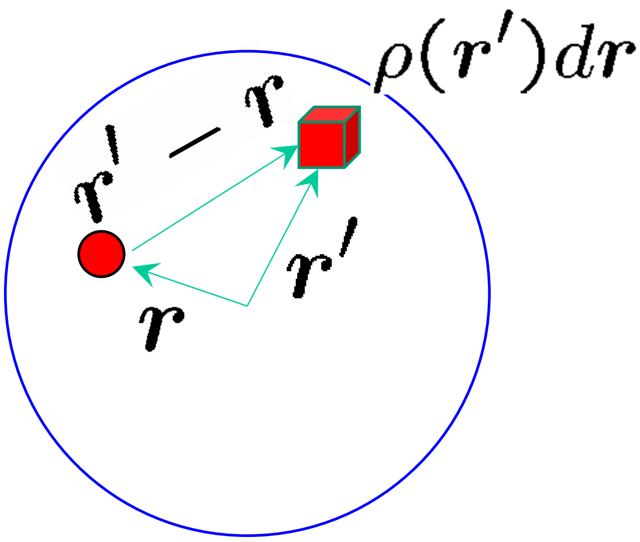
Mean-field (Hartree-Fock) Theory

electro-static potential



test charge

nucleus

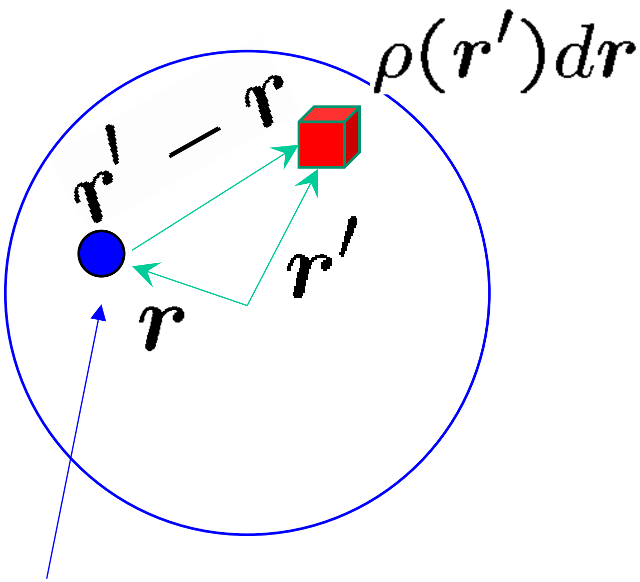


interaction between identical particles

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

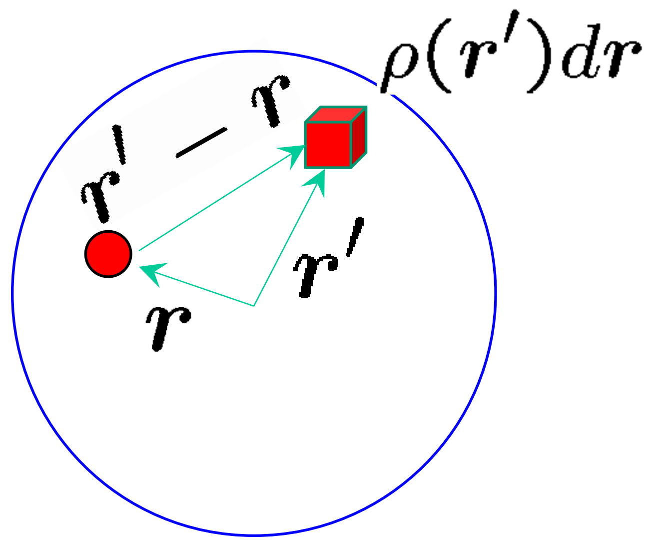
Mean-field (Hartree-Fock) Theory

electro-static potential



test charge

nucleus



interaction between identical particles
$\longrightarrow$ needs anti-symmetrization

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

anti-symmetrization

nucleon: fermion

$$\Psi(x_1, x_2, x_3 \cdots) = -\Psi(x_2, x_1, x_3 \cdots)$$

$$\psi_1(x_1)\psi_2(x_2) \to \frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)]$$

Slater determinat

$$0 = \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r})$$

$$\psi_j^*(\boldsymbol{r}')\psi_j(\boldsymbol{r}')\psi_i(\boldsymbol{r}) \to \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\psi_j(\boldsymbol{r})$$

anti-symmetrization

nucleon: fermion

$$\Psi(x_1, x_2, x_3 \cdots) = -\Psi(x_2, x_1, x_3 \cdots)$$

$$\psi_1(x_1)\psi_2(x_2) \to \frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)]$$

Slater determinat

$$0 = \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r} - \boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r})$$

$$\psi_j^*(\boldsymbol{r}')\psi_j(\boldsymbol{r}')\psi_i(\boldsymbol{r}) \to \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\psi_j(\boldsymbol{r})$$

$$\to \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r} - \boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r})$$

$$-\int v(\boldsymbol{r} - \boldsymbol{r}')\left(\sum_j \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\right) d\boldsymbol{r}'\psi_j(\boldsymbol{r})$$

exchange term

Hartree-Fock theory

anti-symmetrization

$$
\begin{aligned}
0 &= \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r}) \\
&\to \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r}) \\
&\quad - \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\right) d\boldsymbol{r}'\psi_j(\boldsymbol{r}) \\
&= \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r}) - \epsilon_i\right]\psi_i(\boldsymbol{r}) + \int d\boldsymbol{r}' V_{\mathrm{NL}}(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')
\end{aligned}
$$

non-local potential

Non-local potentials

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r}) - E\right]\psi(\boldsymbol{r}) + \int d\boldsymbol{r}' V_{\rm NL}(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r}') = 0$$

- Local equivalent potential

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r}) - E\right]\psi(\boldsymbol{r}) + \left[\frac{1}{\psi(\boldsymbol{r})}\int d\boldsymbol{r}' V_{\rm NL}(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r}')\right]\psi(\boldsymbol{r}) = 0$$

E-dep. potential

- Wigner 変換

$$V_W(\boldsymbol{r},\boldsymbol{p}) = \int V_{\rm NL}(\boldsymbol{r}-\boldsymbol{s}/2, \boldsymbol{r}+\boldsymbol{s}/2)\, e^{i\boldsymbol{p}\cdot\boldsymbol{s}/\hbar} d\boldsymbol{s}$$

✓ momentum expansion
✓ effective mass approximation

cf. Perrey-Buck 型 $\quad V_{\rm NL}(\boldsymbol{r},\boldsymbol{r}') = U\left(\frac{1}{2}|\boldsymbol{r}+\boldsymbol{r}'|\right)\exp\left[-\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{\beta}\right)^2\right]$