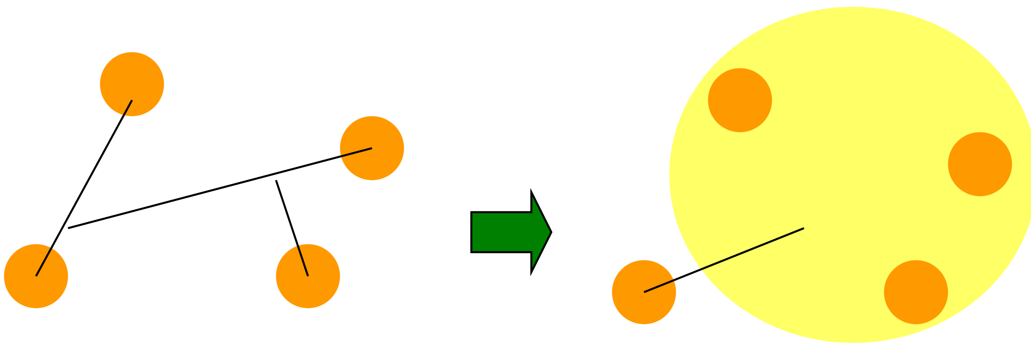
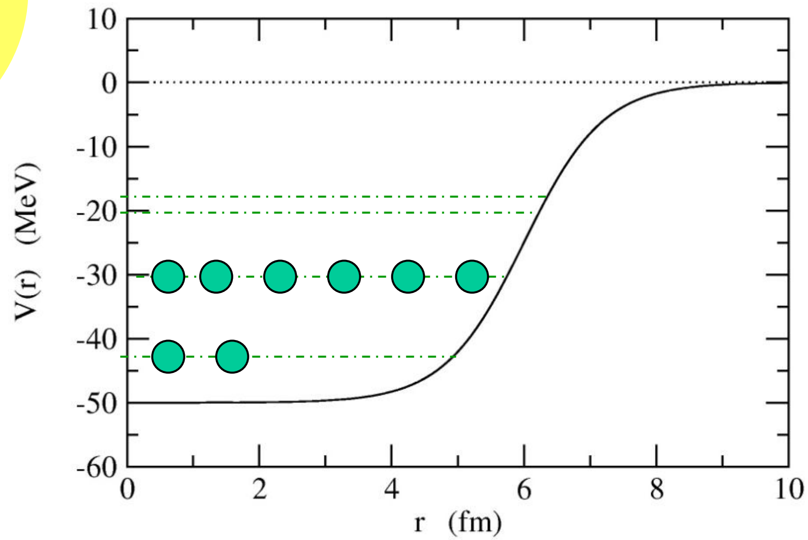
Hartree-Fock Method

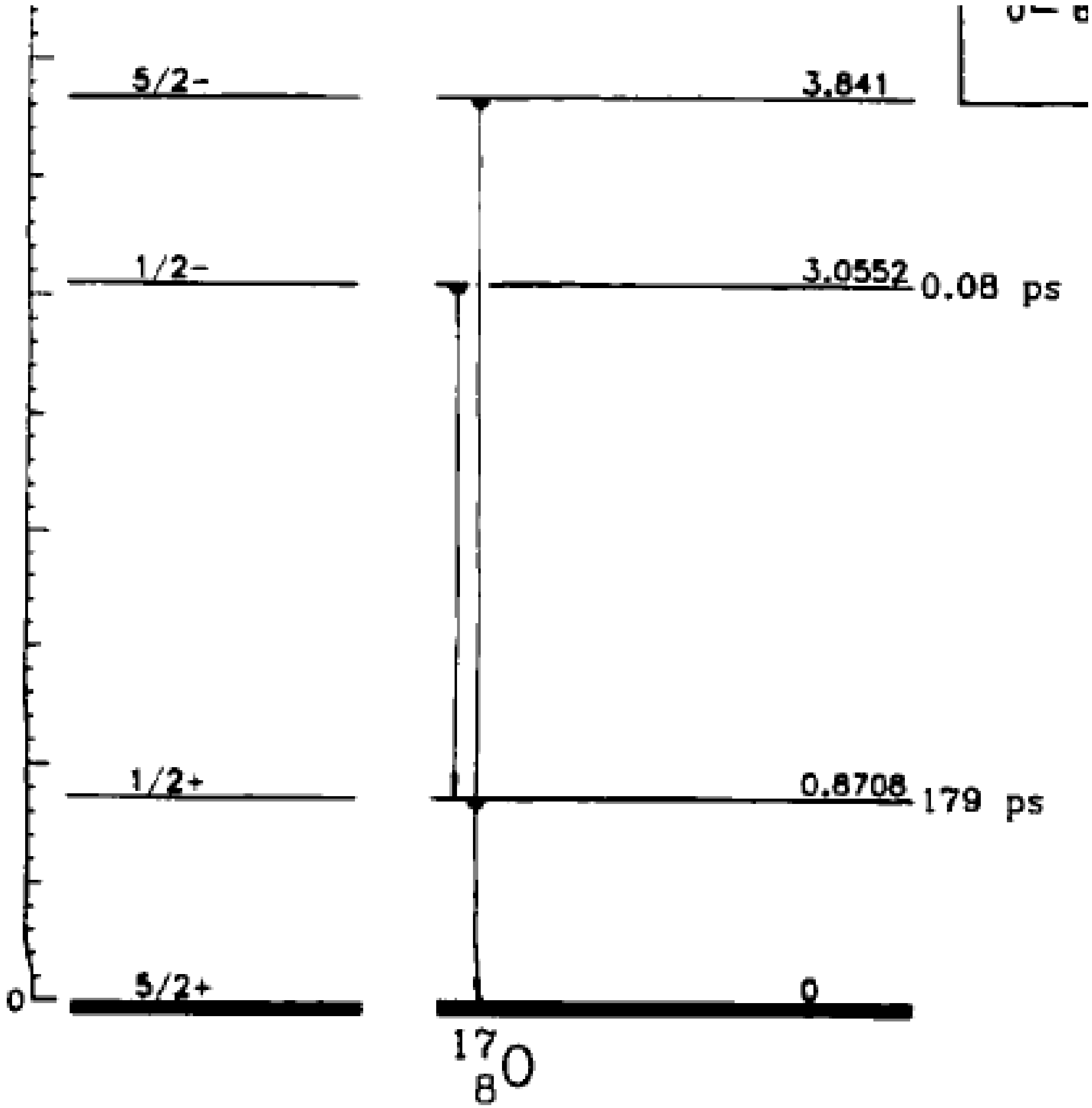




independent particle motion
in a potential well

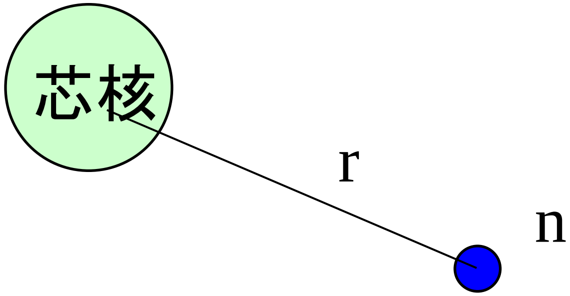
$$
\begin{aligned}
\Psi(1,2,\cdots,A) &= \mathcal{A}[\psi_1(1)\psi_2(2)\cdots\psi_A(A)] \\
&= \frac{1}{\sqrt{A!}}\begin{vmatrix} \psi_1(1) & \psi_2(1) & \cdots & \psi_A(1) \\ \psi_1(2) & \psi_2(2) & \cdots & \psi_A(2) \\ \vdots & & & \\ \psi_1(A) & \psi_2(A) & \cdots & \psi_A(A) \end{vmatrix}
\end{aligned}
$$

Slater determinant: antisymmetrization due to the Pauli principle

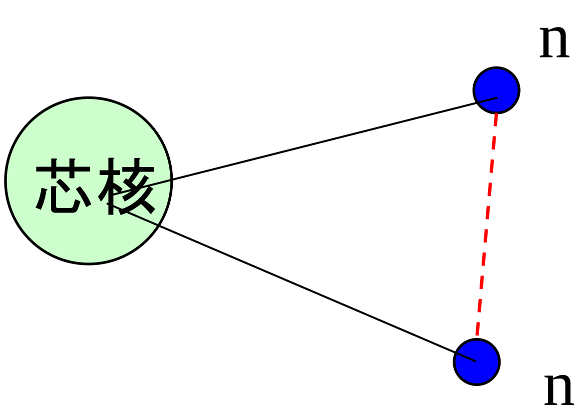


5/2-
3.841
1/2-
3.0552
0.08 ps
1/2+
0.8708
179 ps
5/2+
0
0
17 8 O

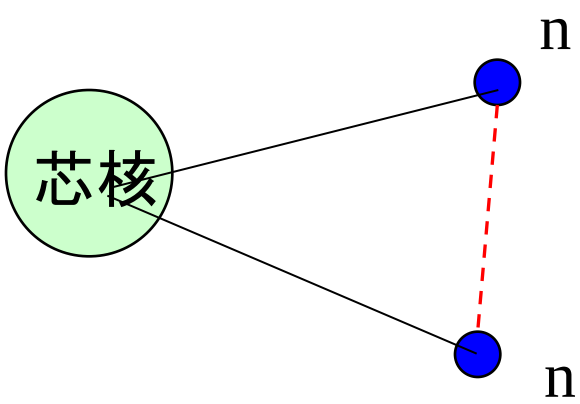
対相関



芯核のまわりに中性子が2個あるとどうなる?

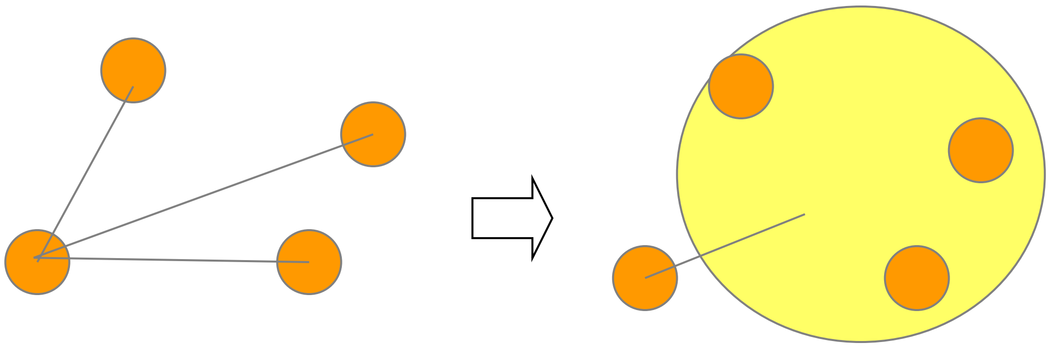


2中性子間に働く相互作用の影響は?



2中性子間に働く相互作用の影響は?

平均場理論



他の核子との相互作用を平均的に取り扱う

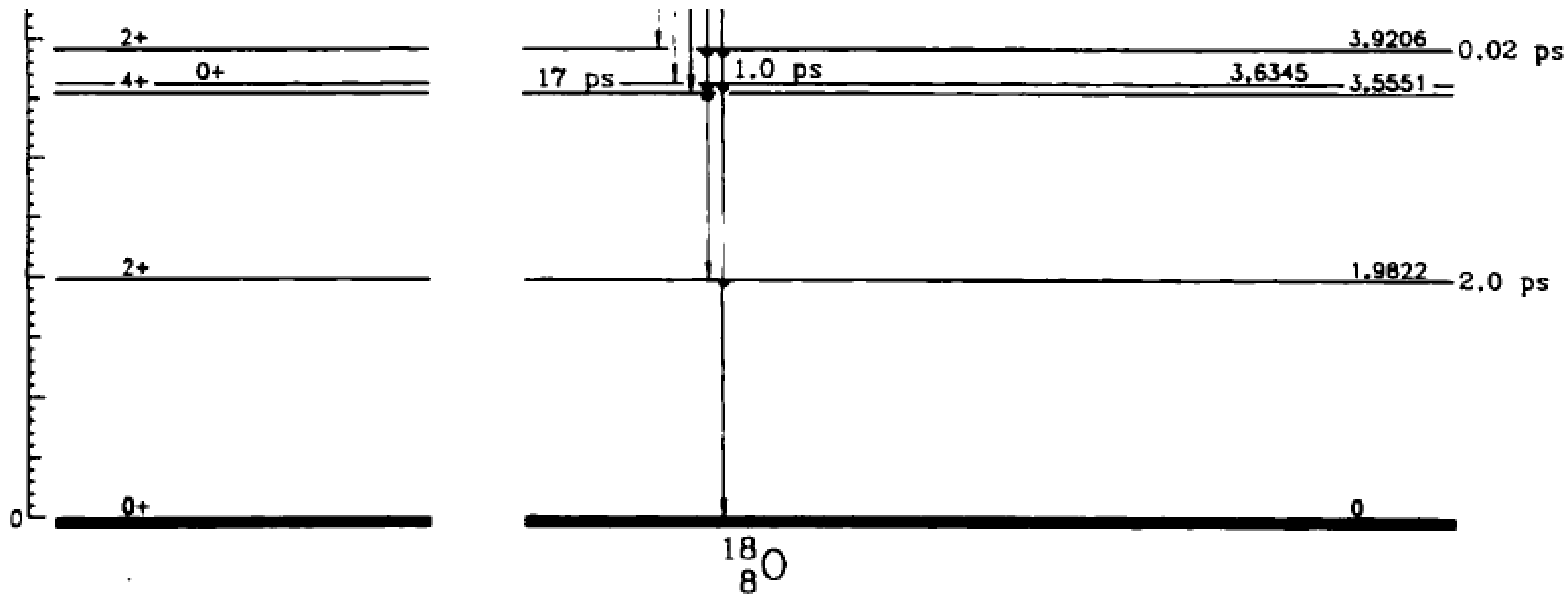
単純な平均場近似が完全に成り立っているとすると、2中性子間相互作用は平均場ポテンシャルを通じて考慮され、それ以上の相互作用を考える必要はない。(2中性子が独立に運動。)

$$H = \sum_i T_i + \sum_{i<j} v_{ij} \rightarrow H = \sum_i (T_i + V_i) + \sum_{i<j} v_{ij} - \sum_i V_i$$

平均からのずれ
（残留相互作用）

残留相互作用は完全に無視してもよいのか?

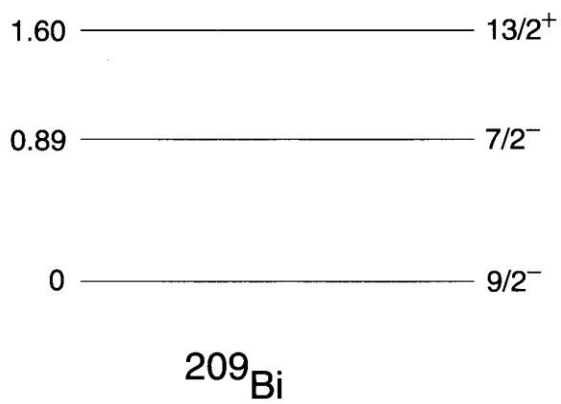
⟶ 開殻原子核では重要な役割を果たすことが知られている（ペアリング）

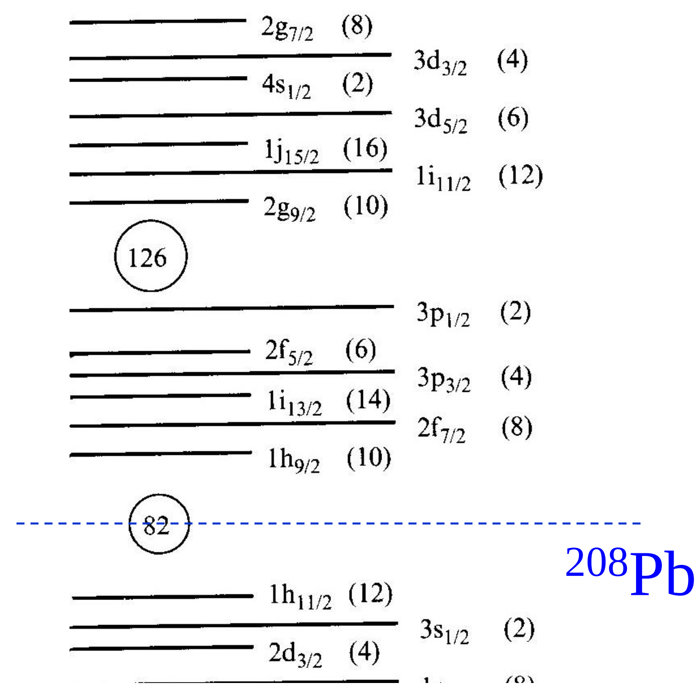


2+
4+
0+
2+
0+
0
17 ps
1.0 ps
3.9206
0.02 ps
3.6345
3.5551
1.9822
2.0 ps
0
$^{18}_{8}O$

対相関（ペアリング）

$^{209}_{83}Bi_{126} = {}^{208}_{82}Pb_{126} + p$





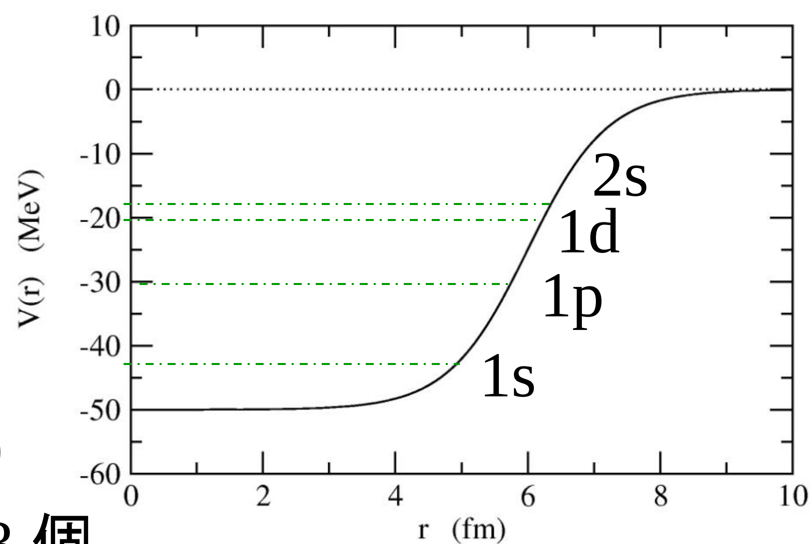
$^{210}_{84}Po_{126} = {}^{208}_{82}Pb_{126} + 2p$

もし独立粒子近似が成り立っていると:

E=0: $[h_{9/2} \otimes h_{9/2}]^I$ (I=0,2,4,6,8)

E=0.89 MeV: $[h_{9/2} \otimes f_{7/2}]^I$

(I=1,2,3,4,5,6,7,8)



⇨ 状態の数: 1 MeV以下に13 個

$^{210}_{84}Po_{126} = ^{208}_{82}Pb_{126} + 2p$

独立粒子近似が成り立っていると:

E=0: $[h_{9/2} \otimes h_{9/2}]^I$ (I=0,2,4,6,8)

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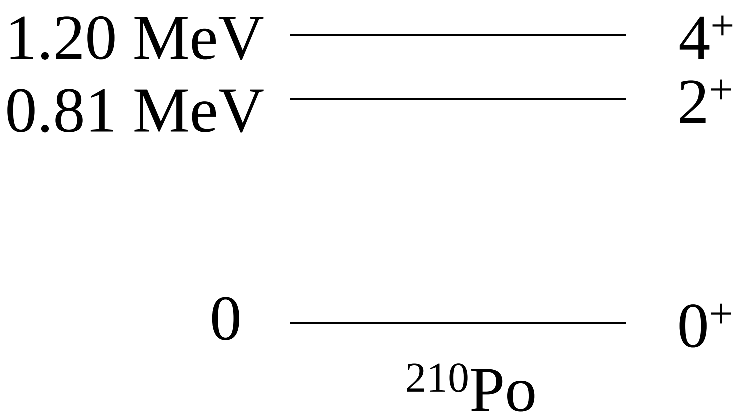
⇨ 状態の数: 1 MeV以下に13 個

実際のスペクトル:



⇔ 残留相互作用の効果

$$H = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\rm HF}(i)\right) + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j) - \sum_i V_{\rm HF}(i)$$

対相関(ペアリング)

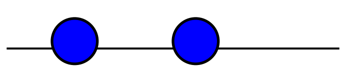
$$H=\sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2+V_{\rm HF}(i)\right)+\frac{1}{2}\sum_{i,j}^{A}v(\boldsymbol{r}_i,\boldsymbol{r}_j)-\sum_i V_{\rm HF}(i)$$

簡単のために、残留相互作用としてデルタ関数を仮定してみる
(超短距離力)

$$v_{\rm res}(\boldsymbol{r},\boldsymbol{r}')\sim -g\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$
$$=-g\frac{\delta(r-r')}{rr'}\sum_{\lambda\mu}Y^*_{\lambda\mu}(\hat{\boldsymbol{r}})Y_{\lambda\mu}(\hat{\boldsymbol{r}}')$$

摂動論で残留相互作用の効果を見積もってみる:

l



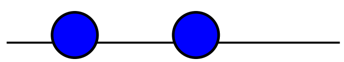
非摂動な波動関数:
角運動量 l の状態に中性子2個、それが
全角運動量 L を組んでいる

$$|(ll)LM\rangle=\sum_{m,m'}\langle lmlm'|LM\rangle\psi_{lm}(\boldsymbol{r})\psi_{lm'}(\boldsymbol{r}')$$

対相関(ペアリング)

$$v_{\mathrm{res}}(\boldsymbol{r},\boldsymbol{r}') \sim -g\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$
$$= -g\frac{\delta(r-r')}{rr'}\sum_{\lambda\mu} Y^*_{\lambda\mu}(\hat{\boldsymbol{r}})Y_{\lambda\mu}(\hat{\boldsymbol{r}}')$$

l



$$|(ll)LM\rangle = \sum_{m,m'}\langle lmlm'|LM\rangle\psi_{lm}(\boldsymbol{r})\psi_{lm'}(\boldsymbol{r}')$$

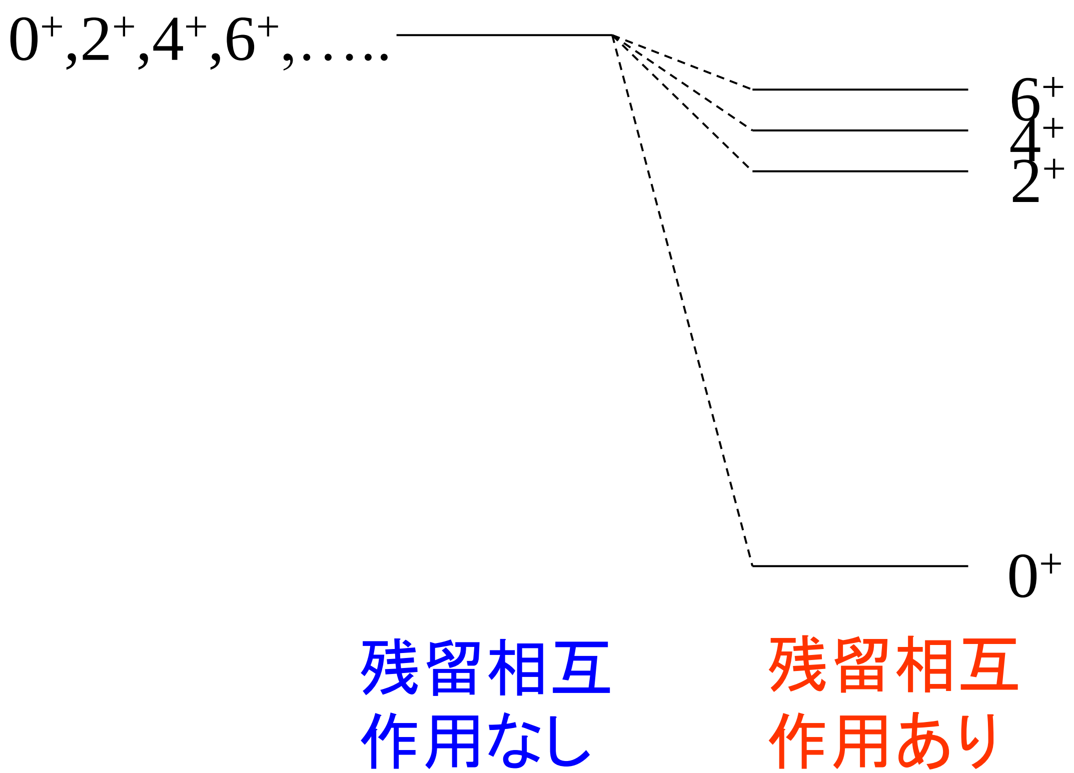
残留相互作用によるエネルギー変化:

$$\Delta E_L = \langle (ll)LM|v_{\mathrm{res}}|(ll)LM\rangle$$
$$= -g\,I_r^{(l)}\frac{(2l+1)^2}{4\pi}\begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2$$

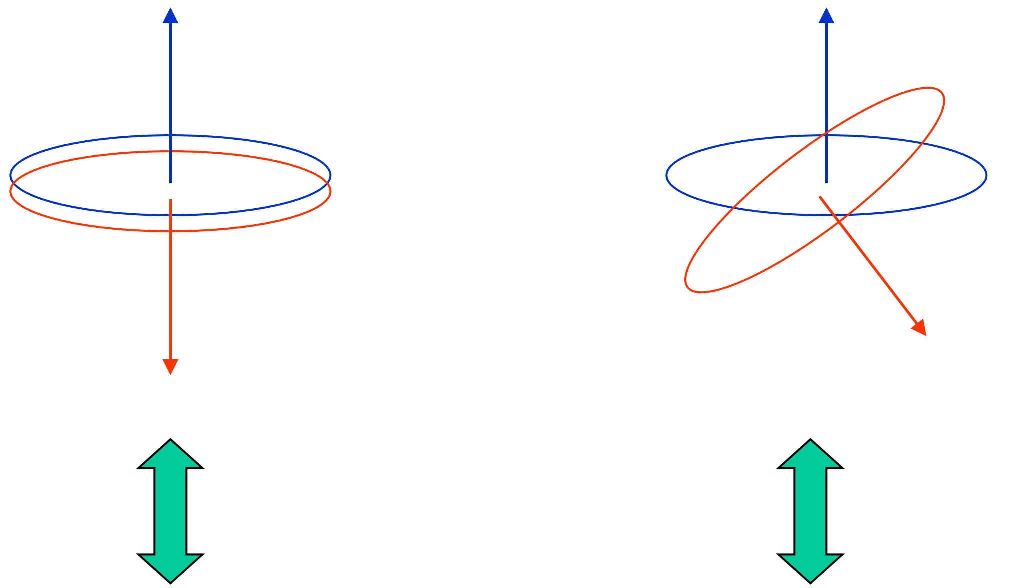
$$I_r^{(l)} = \int_0^\infty r^2 dr\,(R_l(r))^4$$

$$\Delta E_L = -g\, I_r^{(l)} \frac{(2l+1)^2}{4\pi} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 \equiv -g\, I_r^{(l)} \frac{A(ll;L)}{4\pi}$$

$A(ll;L)$	L=0	L=2	L=4	L=6	L=8
l = 2	5.00	1.43	1.43	---	---
l = 3	7.00	1.87	1.27	1.63	---
l = 4	9.00	2.34	1.46	1.26	1.81



簡単な解釈:



L=0 対 $L \neq 0$ 対

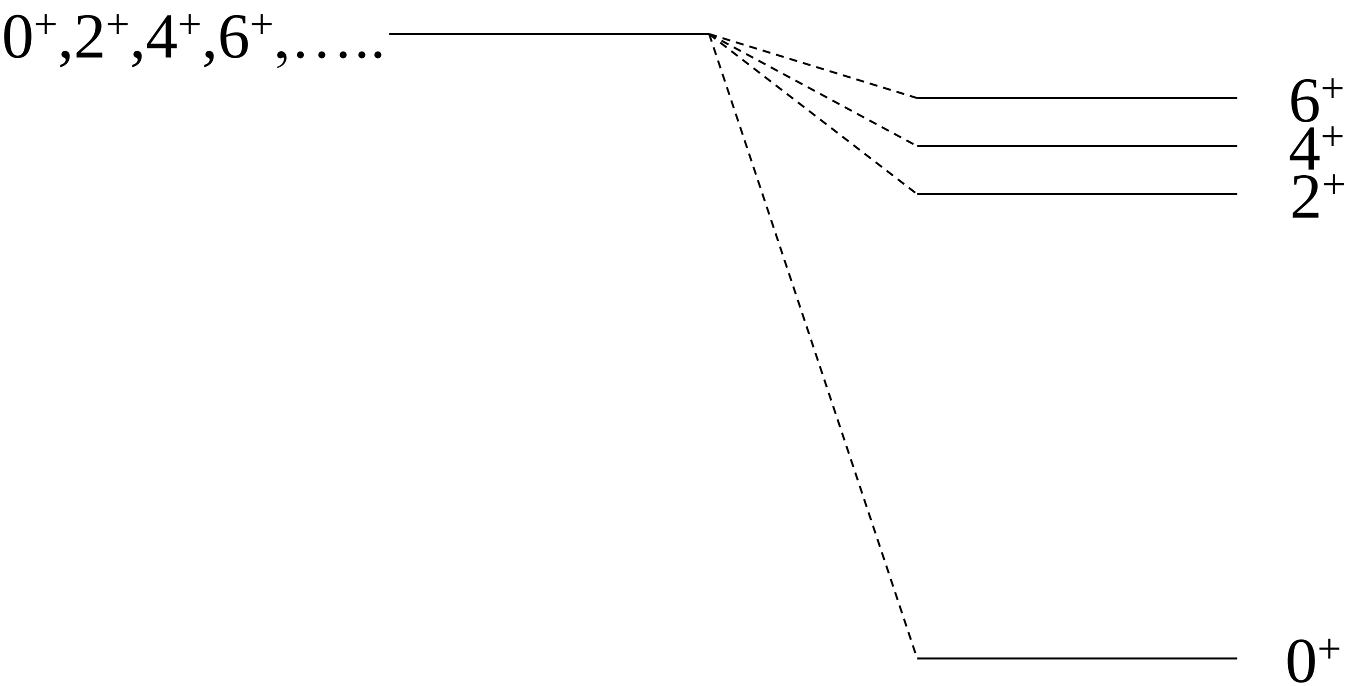
L=0 対に対して空間的重なりが最大(エネルギー的に得)

"対相関"

(note)

$$\psi(l^2; L=0) = \sum_m \langle l m l -m | L=0,0\rangle\, Y_{lm}(\hat{\boldsymbol{r}}_1) Y_{l-\mu}(\hat{\boldsymbol{r}}_2) = Y_{l0}(\theta_{12})/\sqrt{4\pi}$$

すべての m が「コヒーレント」に寄与



残留相互作用なし

残留相互作用あり

<u>原子核の基底状態のスピン</u>

- 偶々核:例外なしに 0^+
- 奇核: 最外殻核子の角運動量と一致

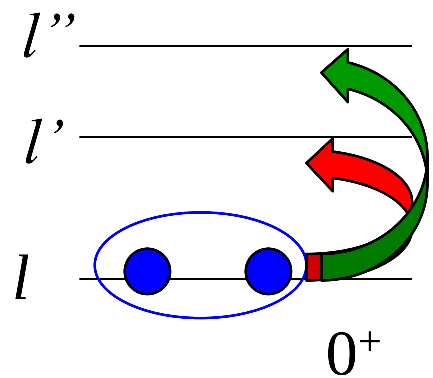
束縛エネルギー

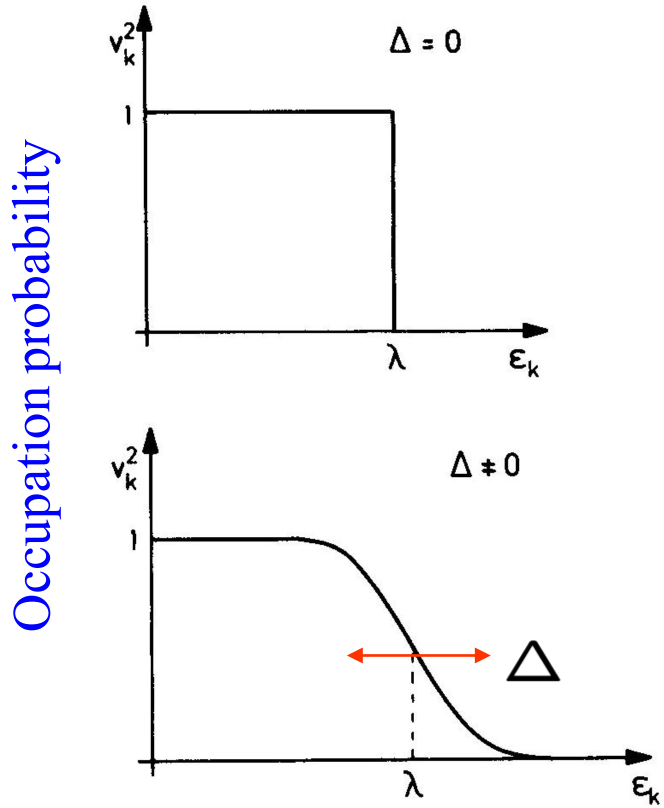
対相関のため、同種核子（2つの中性子または2つの陽子）が
角運動量ゼロを組むと安定化

例:

	束縛エネルギー (MeV)
${}^{210}_{82}Pb_{128} = {}^{208}_{82}Pb_{126}+2n$	1646.6
${}^{210}_{83}Bi_{127} = {}^{208}_{82}Pb_{126}+n+p$	1644.8
${}^{209}_{82}Pb_{127} = {}^{208}_{82}Pb_{126}+n$	1640.4
${}^{209}_{83}Bi_{126} = {}^{208}_{82}Pb_{126}+p$	1640.2

波動関数:





$$|\Psi_{0+}\rangle = |(ll)L=0\rangle + \sum_{l'} \frac{\langle (l'l')L=0|v_{\rm res}|(ll)L=0\rangle}{2\epsilon_l - 2\epsilon_{l'}} |(l'l')L=0\rangle + \cdots$$

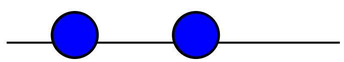
各軌道は部分的にのみ占有されることになる

cf. BCS 理論

(参考)スピンを考慮すると:

$$v_{\rm res}(\boldsymbol{r},\boldsymbol{r}') \sim -g\,\delta(\boldsymbol{r}-\boldsymbol{r}') = -g\frac{\delta(r-r')}{rr'}\sum_{\lambda\mu}Y^*_{\lambda\mu}(\hat{\boldsymbol{r}})Y_{\lambda\mu}(\hat{\boldsymbol{r}}')$$

j



$$|(jj)IM\rangle = \sum_{\mu,\mu'}\langle j\mu j\mu'|IM\rangle\psi_{j\mu}(\boldsymbol{r})\psi_{j\mu'}(\boldsymbol{r}')$$

⇩

$$\Delta E_I \sim \langle (jj)IM| - g\delta(\boldsymbol{r}-\boldsymbol{r}')|(jj)IM\rangle = -g\,F_r\,\frac{(2j+1)^2}{2}\begin{pmatrix} j & j & I \\ 1/2 & -1/2 & 0\end{pmatrix}^2$$

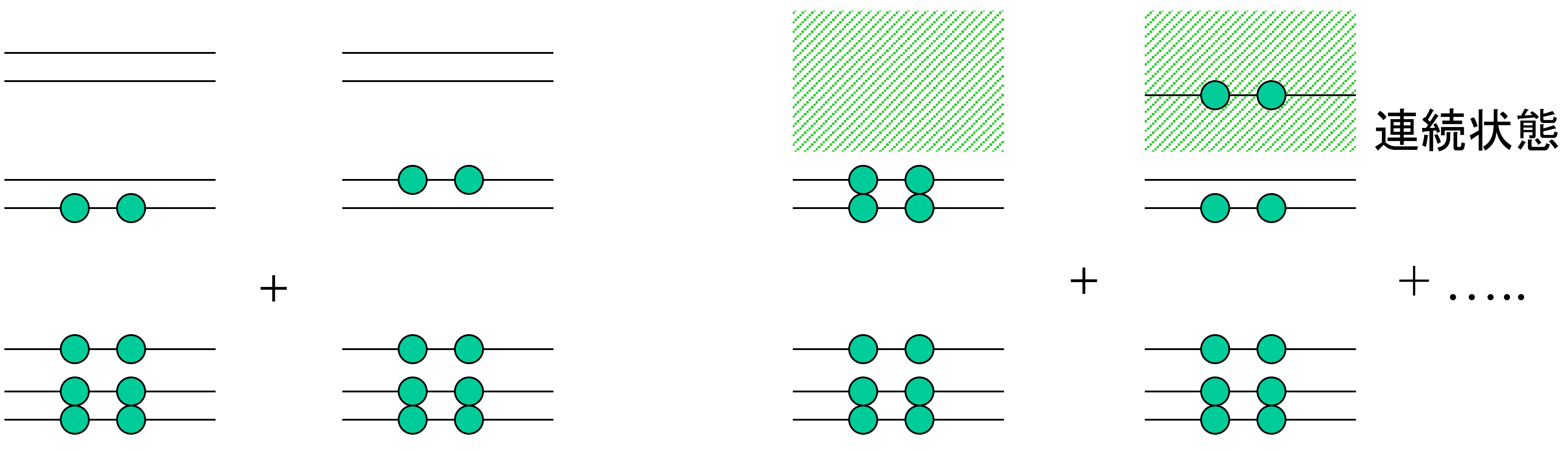
(for even I)

$$F_r = \int dr\frac{u^4_{jl}(r)}{4\pi r^2}$$ (radial integral)

弱束縛核における対相関

$$H=\sum_i T_i+\sum_{i<j}v_{ij}\rightarrow H=\sum_i(T_i+V_i)+\underbrace{\sum_{i<j}v_{ij}-\sum_i V_i}$$

平均からのずれ
（残留相互作用）



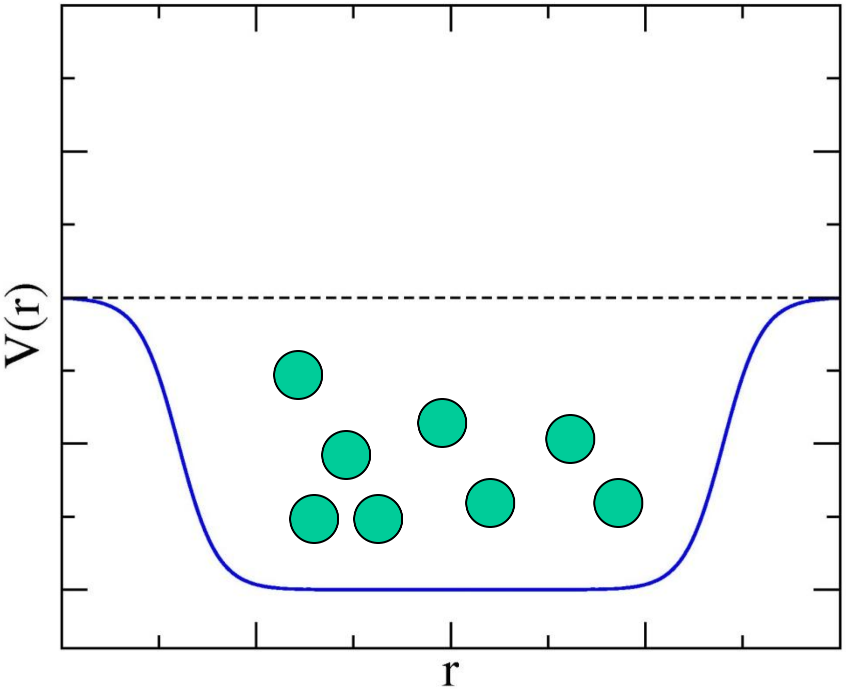
安定な原子核
→ 超流動状態

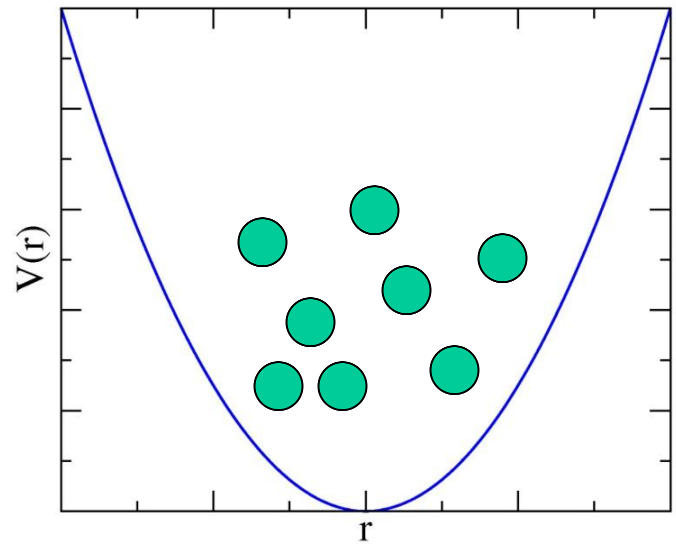
弱く束縛された系

中性子過剰核の物理

- 弱束縛系
- 残留相互作用（対相関）
- 連続状態との結合

ポテンシャルの井戸に束縛された相互作用する多フェルミオン系





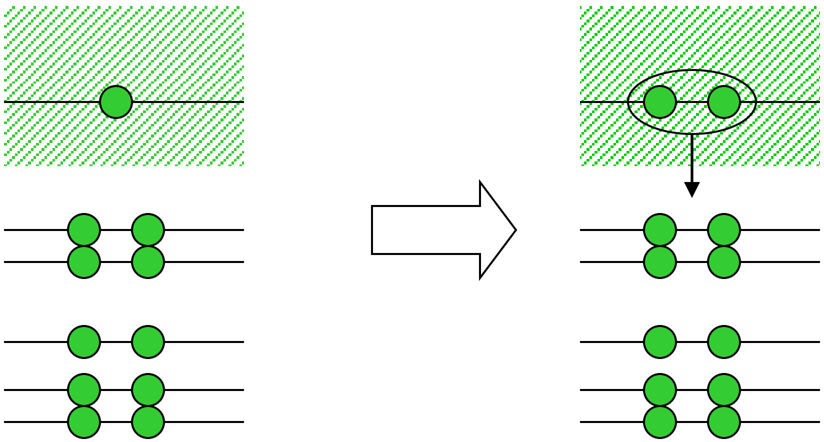
cf. a harmonic trap

- 有限の深さを持つ井戸
- 自己無撞着性

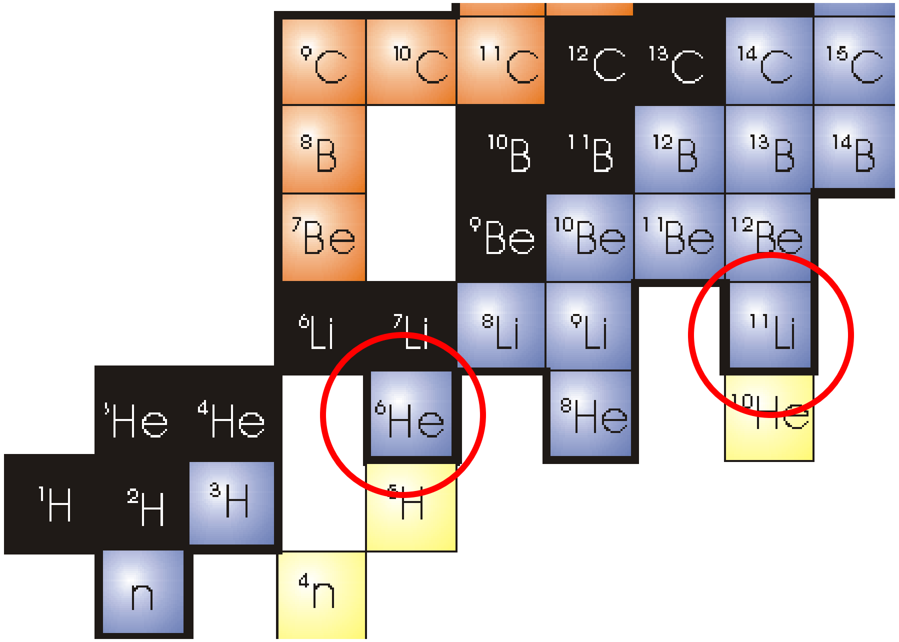
→ とてもチャレンジングな問題
（わからないことは色々ある）

ボロミアン原子核

残留相互作用 → 引力



不安定　　　　安定



"ボロミアン核"

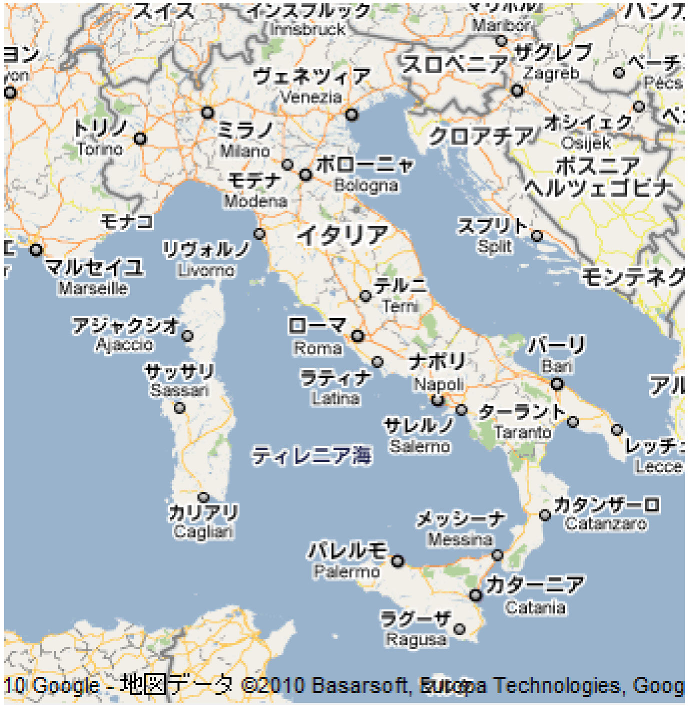
ボロミアン核の構造

✓多体相関のため non-trivial
✓多くの注目を集めている

（休憩）ボロミアンって何?

ボッロメオ諸島
（北イタリア、マッジョーレ湖）
ミラノの近く

ボッロメオ家（13世紀）の紋章



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Innsbruck
マリボル
Maribor
ヴェネツィア
Venezia
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ザグレブ
Zagreb
トリノ
Torino
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Milano
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Bologna
モデナ
Modena
クロアチア
オシイェク
Osijek
ボスニア
ヘルツェゴビナ
モナコ
マルセイユ
Marseille
リヴォルノ
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スプリト
Split
モンテネグ
テルニ
Terni
アジャクシオ
Ajaccio
ローマ
Roma
バーリ
Bari
サッサリ
Sassari
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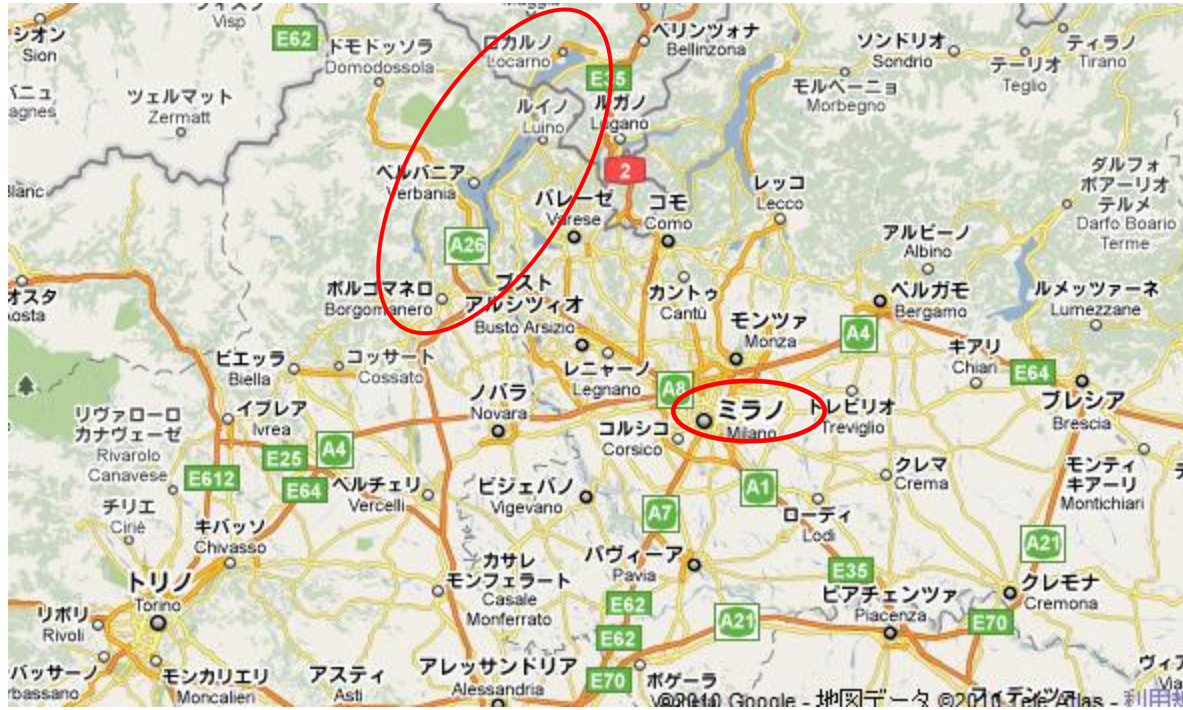

シオン
Sion
ドモドッソラ
Domodossola
ツェルマット
Zermatt
ロカルノ
Locarno
ルイノ
Luino
ルガノ
Lugano
ベリンツォナ
Bellinzona
ソンドリオ
Sondrio
ティラノ
Tirano
テーリオ
Teglio
モルベーニョ
Morbegno
ヴェルバニア
Verbania
バレーゼ
Varese
コモ
Como
レッコ
Lecco
ダルフォ
ボアーリオ
テルメ
Darfo Boario
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アルビーノ
Albino
ボルゴマネロ
Borgomanero
ブスト
アルシツィオ
Busto Arsizio
カントゥ
Cantù
モンツァ
Monza
ベルガモ
Bergamo
ルメッツァーネ
Lumezzane
オスタ
ビエッラ
Biella
コッサート
Cossato
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キアリ
Chiari
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Brescia
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Ciriè
ベルチェリ
Vercelli
ビジェバノ
Vigevano
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Crema
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Cremona
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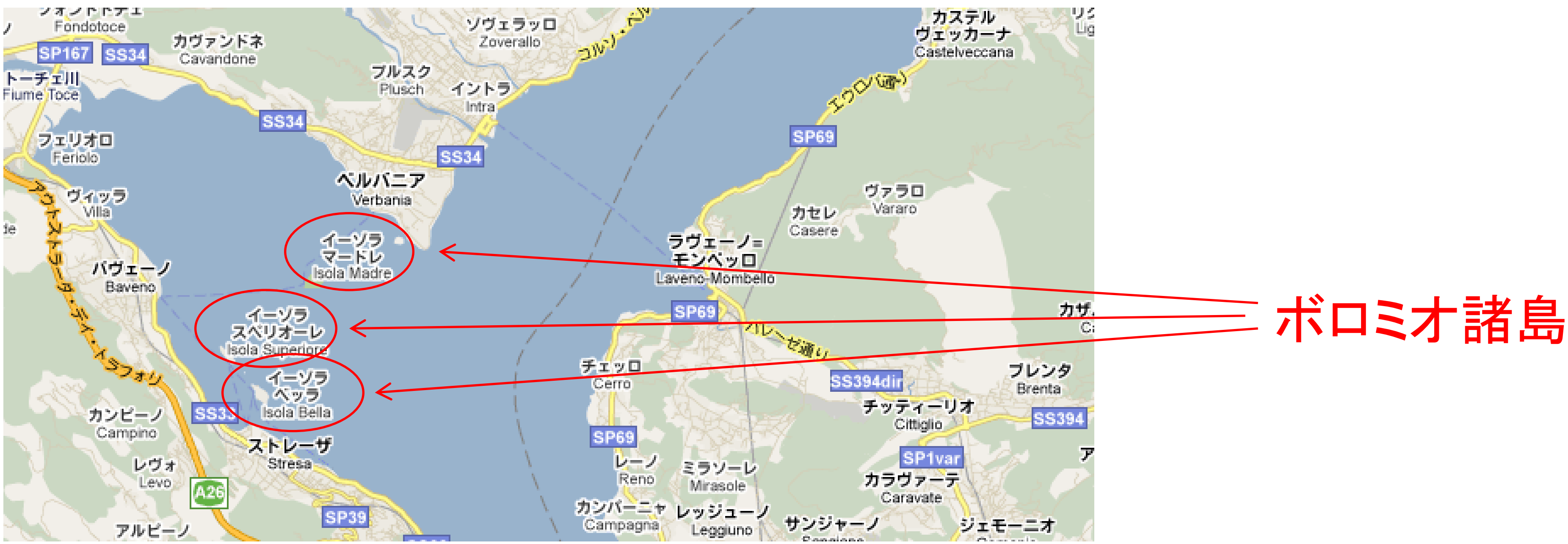

フォンドトチェ
Fondotoce
カヴァンドネ
Cavandone
ソヴェラッロ
Zoverallo
カステル
ヴェッカーナ
Castelveccana
トーチェ川
Fiume Toce
プルスク
Plusch
イントラ
Intra
フェリオロ
Feriolo
ヴェルバニア
Verbania
ヴィッラ
Villa
ヴァラロ
Vararo
カセレ
Casere
イーソラ
マードレ
Isola Madre
ラヴェーノ＝
モンベッロ
Laveno-Mombello
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Baveno
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スペリオーレ
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イーソラ
ベッラ
Isola Bella
チェッロ
Cerro
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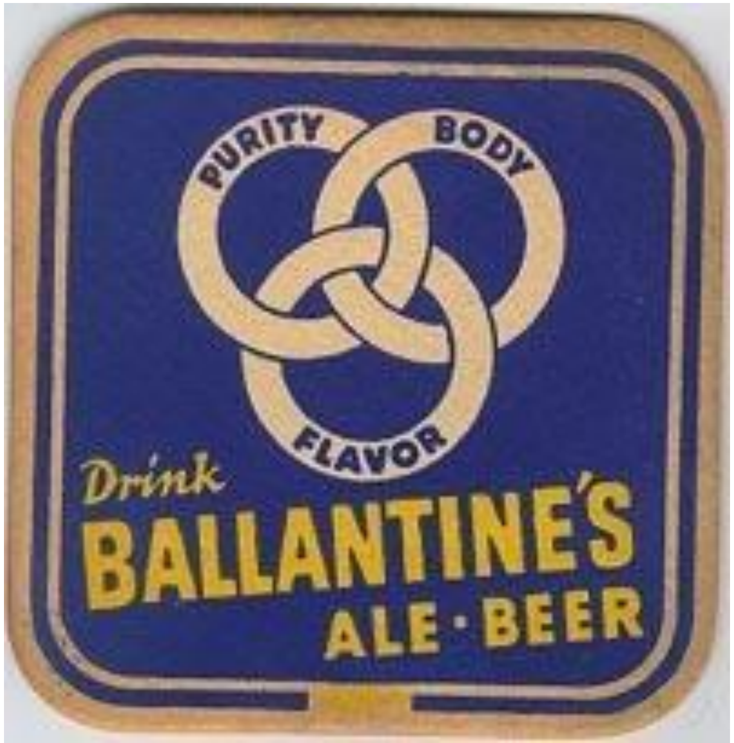
Brenta
チッティーリオ
Cittiglio
カンピーノ
Campino
ストレーザ
Stresa
レヴォ
Levo
レーノ
Reno
ミラソーレ
Mirasole
カラヴァーテ
Caravate
カンパーニャ
Campagna
レッジューノ
Leggiuno
サンジャーノ
ジェモーニオ
アルピーノ
SP167
SS34
SP69
SS394dir
SS394
SP1var
SP39
A26
ボロミオ諸島

（休憩）ボロミアンって何?

ちなみに日本でも。。。。。

三つ輪違い紋
（徳川旗本金田家の紋）

大神（おおみわ）神社
奈良県桜井市



バランタイン・エール（アメリカのビール）

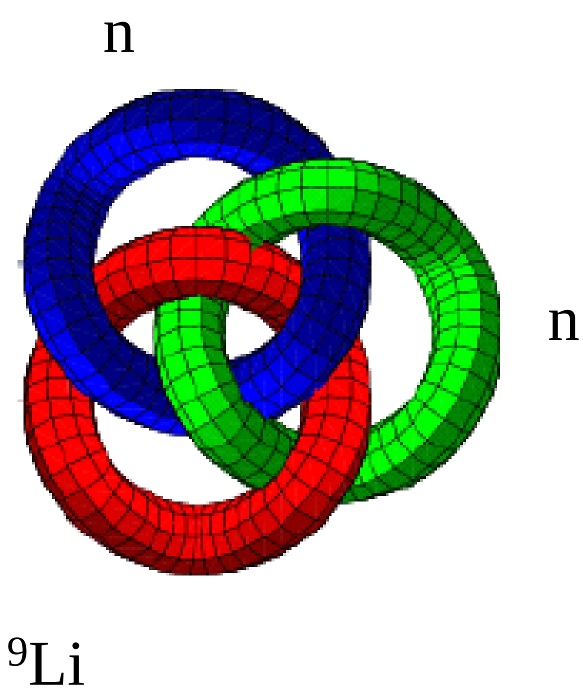
（休憩）ボロミアンって何?

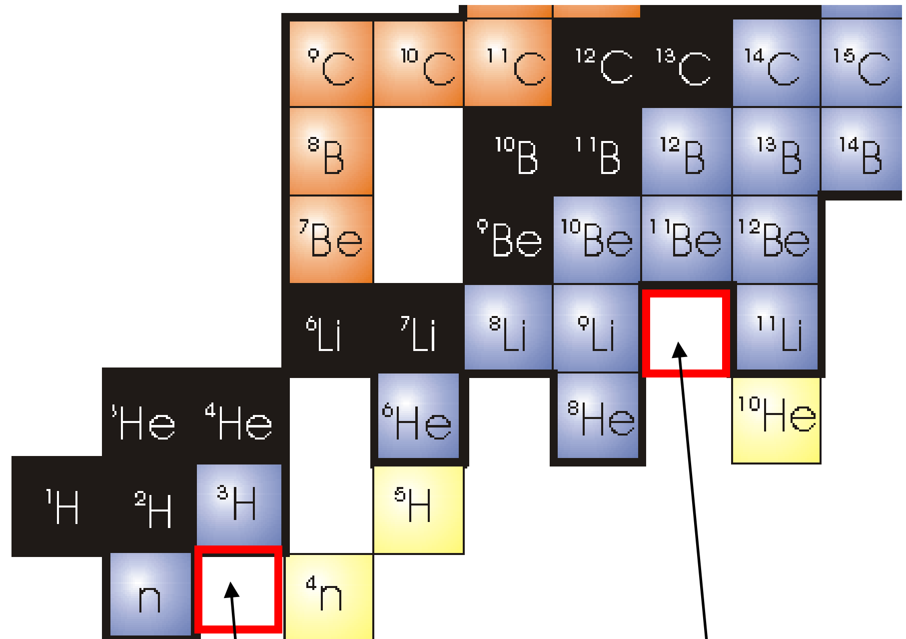
三つ輪違い紋
（徳川旗本金田家の紋）

３つの輪はつながっているけど、どれか１つをはずすとバラバラになる

「ボロミアン・リング」

ボロミアン原子核





^{10}Li (^{9}Li+n)
は存在せず

ボロミアン核

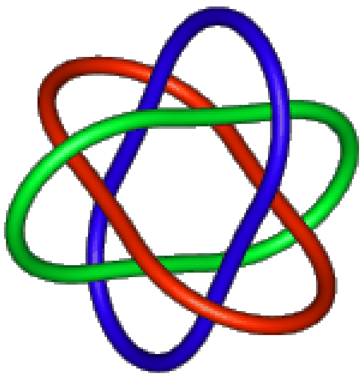
^{2}n (n+n) は存在せず

他にも、^{6}He が典型的な例

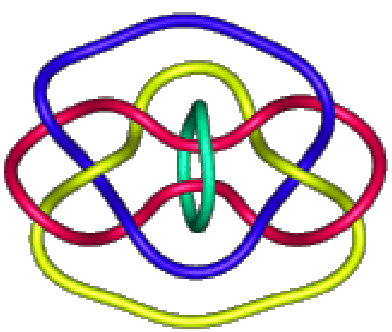
(参考)ブルニアン・リンク: 拡張されたボロミアン

結び目理論: 位相幾何学の分野(数学)

n=3: Borromean



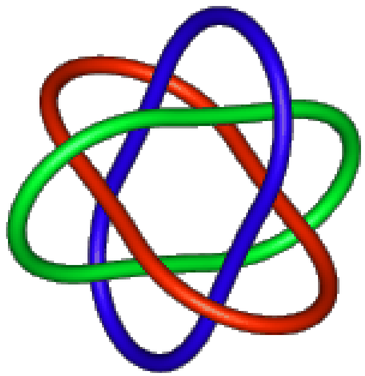
n=4



n=6

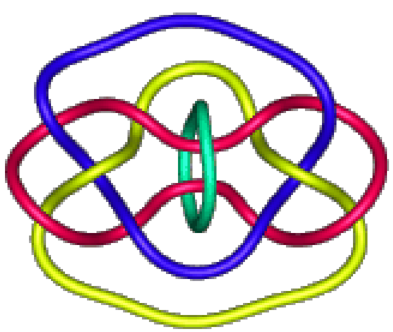
（参考）ブルニアン原子核

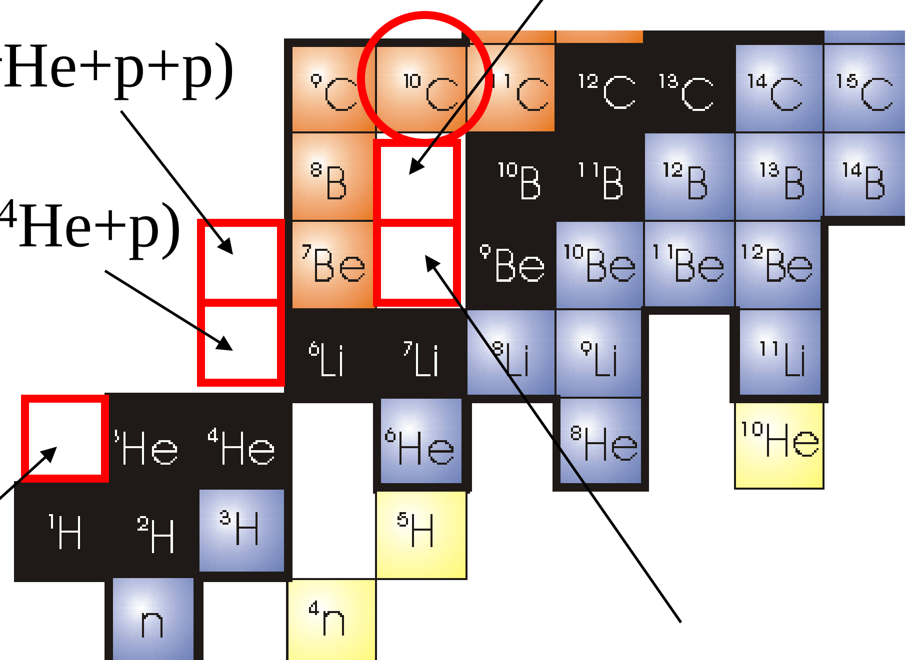
n=3: Borromean



^{11}Li, ^{6}He, etc.

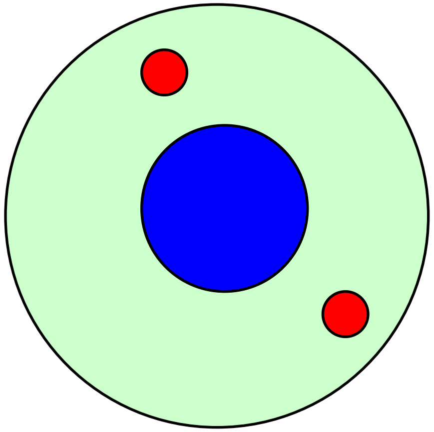
n=4: $^{10}C = {}^{4}He + {}^{4}He + p + p$





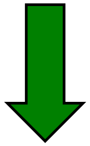
cf. N. Curtis et al., PRC77(‘08)021301(R)

双中性子 (dineutron) 相関



原子核中で2つの中性子は空間的に
どのように配置されているのか?

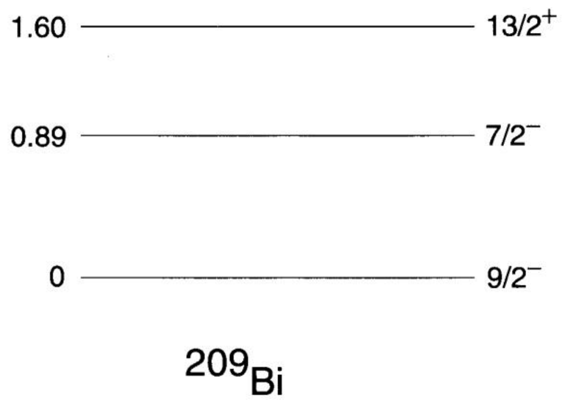
2つの中性子が独立に運動していると
すると、片方の中性子がどこにいようとも
もう片方は関知しない

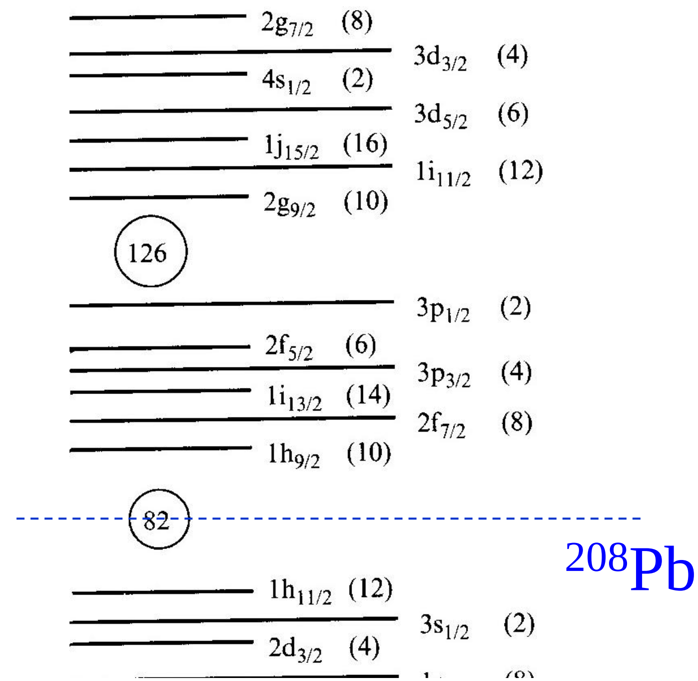


対相関が働くとどうなるか?

Pairing Correlations

$^{209}_{83}Bi_{126} = ^{208}_{82}Pb_{126} + p$





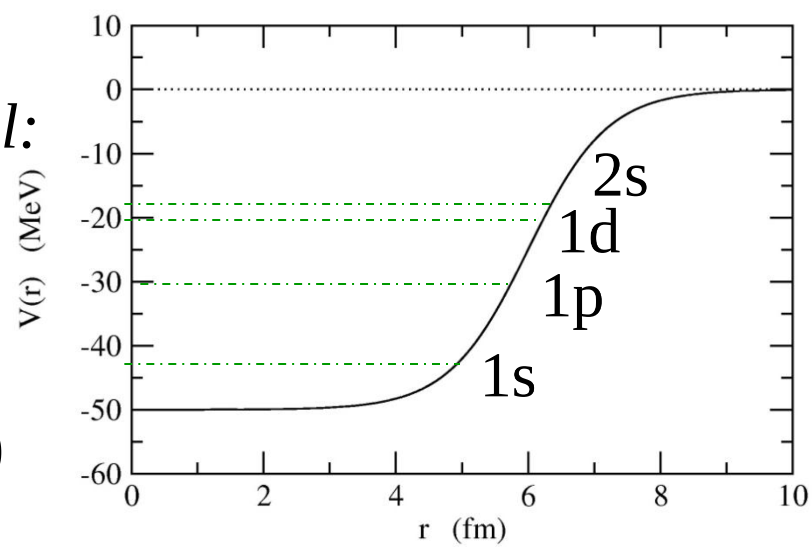
$^{210}_{84}Po_{126} = ^{208}_{82}Pb_{126} + 2p$

expectation of the indep. particle model:

E=0: $[h_{9/2} \otimes h_{9/2}]^I$ $(I=0,2,4,6,8)$

E=0.89 MeV: $[h_{9/2} \otimes f_{7/2}]^I$

$(I=1,2,3,4,5,6,7,8)$



⇨ # of states below 1 MeV: 13

$^{210}_{84}\mathrm{Po}_{126} = {}^{208}_{82}\mathrm{Pb}_{126} + 2p$

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⇨ # of states below 1 MeV: 13

observed spectra:

1.20 MeV	4^+
0.81 MeV	2^+
0	0^+

$^{210}\mathrm{Po}$

⇔ Effects of the residual interaction

$$H = \sum_{i=1}^{A} \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V_{\mathrm{HF}}(i) \right) + \frac{1}{2} \sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j) - \sum_i V_{\mathrm{HF}}(i)$$

Effects of the residual interaction

$$H = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + V_{\mathrm{HF}}(i)\right) + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j) - \sum_i V_{\mathrm{HF}}(i)$$

$$\sim -g\,\delta(\boldsymbol{r} - \boldsymbol{r}')$$ (short range force)

$$= -g\frac{\delta(r - r')}{rr'}\sum_{\lambda\mu} Y^*_{\lambda\mu}(\hat{\boldsymbol{r}})Y_{\lambda\mu}(\hat{\boldsymbol{r}}')$$

$$\Delta E_I \sim \langle [j \bigotimes j]^I | - g\delta(\boldsymbol{r} - \boldsymbol{r}') | [j \bigotimes j]^I \rangle$$

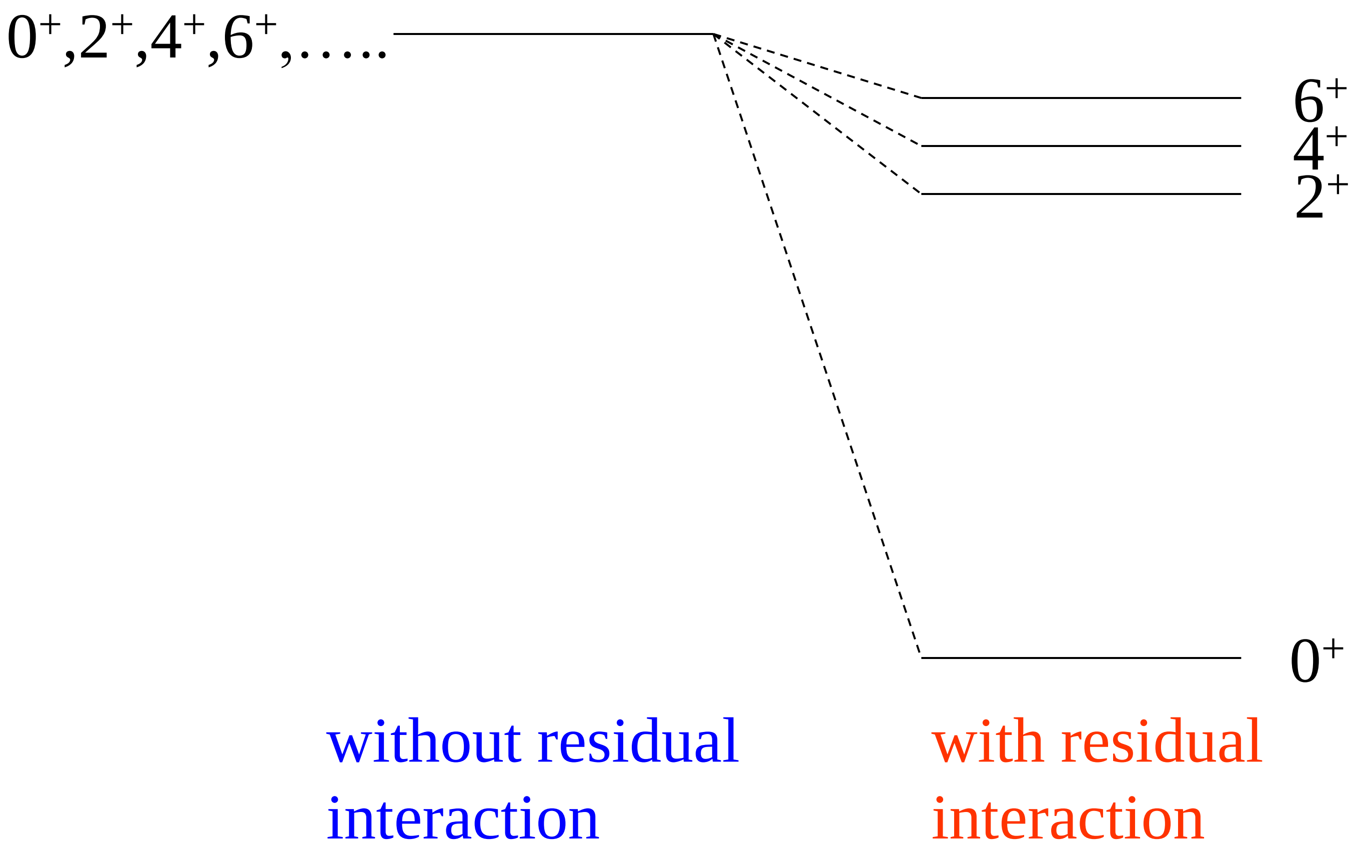
$$= -g\,F_r\,\frac{(2j+1)^2}{2}\begin{pmatrix} j & j & I \\ 1/2 & -1/2 & 0 \end{pmatrix}^2$$

(for even j)

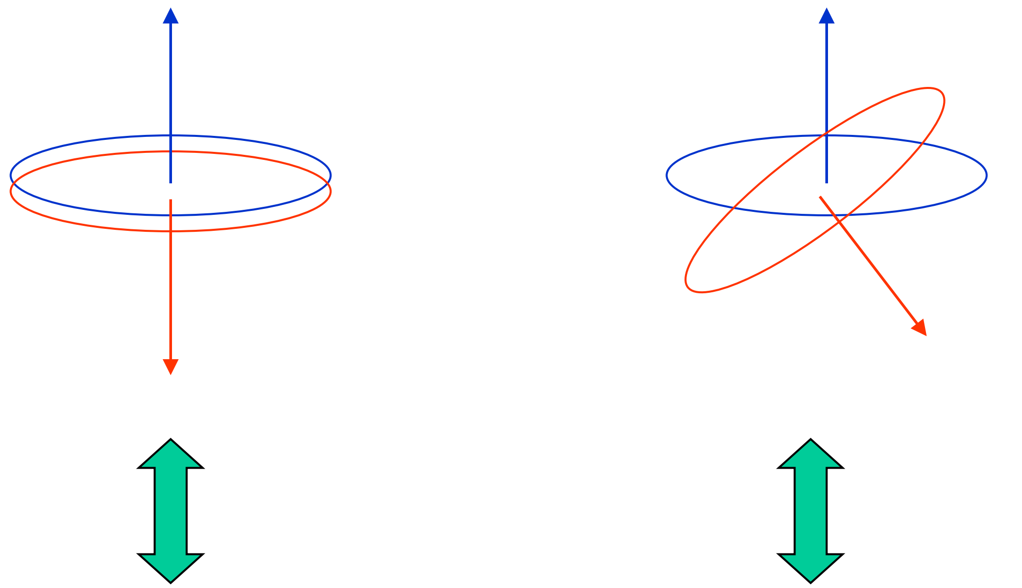
$$F_r = \int dr \frac{u_{jl}^4(r)}{4\pi r^2}$$ (radial integral)

$$\Delta E_I \sim -g\, F_r \frac{(2j+1)^2}{2} \begin{pmatrix} j & j & I \\ 1/2 & -1/2 & 0 \end{pmatrix}^2 \equiv -g\, F_r\, A(jj;I)$$

$A(jj;I)$	I=0	I=2	I=4	I=6
j=5/2	3.00	0.685	0.286	---
j=7/2	4.00	0.95	0.467	0.233



Simple interpretation:



I=0 pair

$I \neq 0$ pair

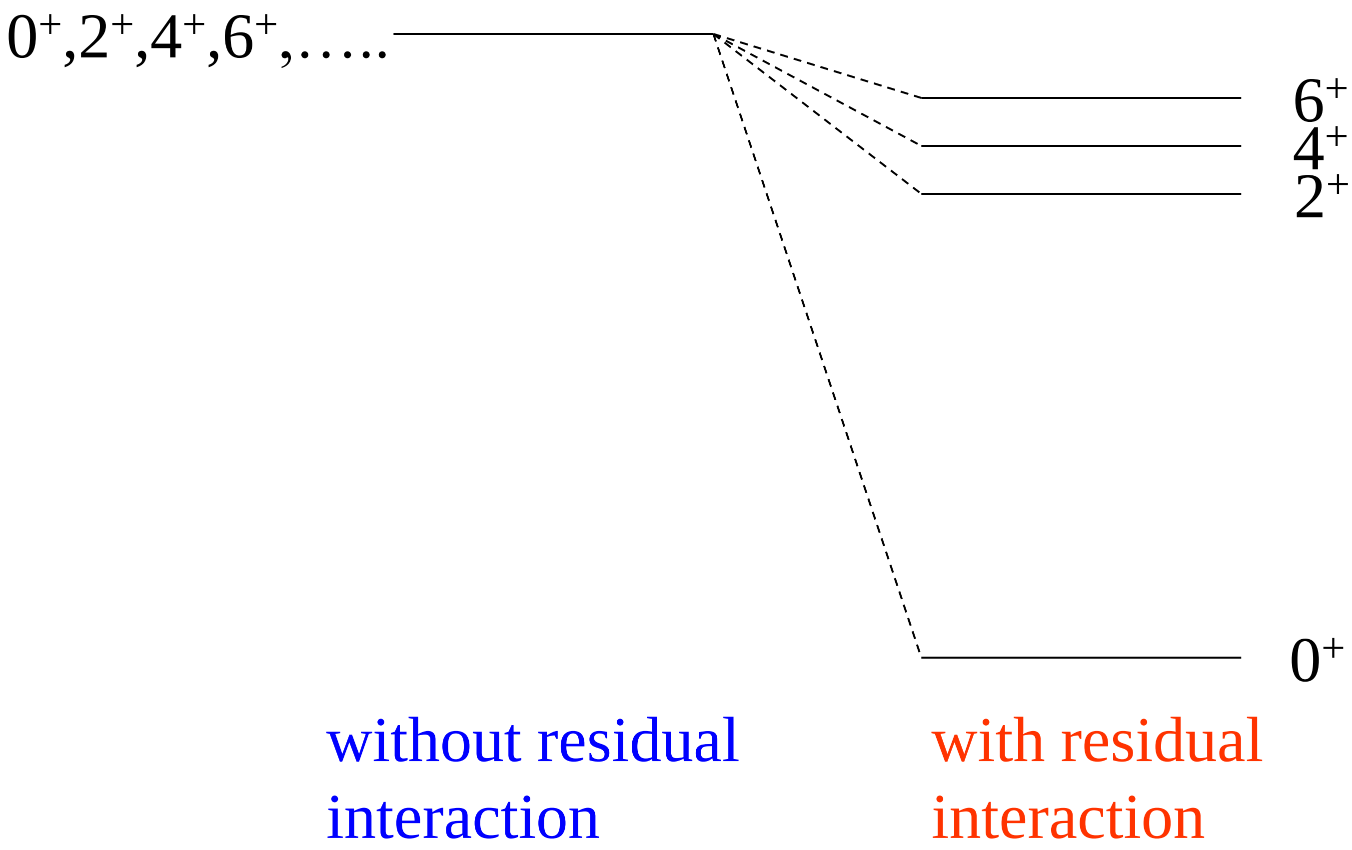
The spatial overlap is the largest for the I=0 pair.

"Pairing Correlation"

(note) The $I=2j$ pair is unfavoured due to the Pauli principle.

(note)

$$\psi(l^2; L=0) = \sum_{\mu} \langle l\mu l-\mu | L=0,0\rangle \, Y_{l\mu}(\hat{\boldsymbol{r}}_1) Y_{l-\mu}(\hat{\boldsymbol{r}}_2) = Y_{l0}(\theta_{12})/\sqrt{4\pi}$$



The ground state spin of nuclei

- Even-even nuclei: 0^+
- Even-odd nuclei: the spin of the valence particle

Mass Formula (Even-odd mass difference)

Extra binding when like nucleons form a spin-zero pair

Example:

	Binding energy (MeV)
${}^{210}_{82}Pb_{128} = {}^{208}_{82}Pb_{126} + 2n$	1646.6
${}^{210}_{83}Bi_{127} = {}^{208}_{82}Pb_{126} + n + p$	1644.8
${}^{209}_{82}Pb_{127} = {}^{208}_{82}Pb_{126} + n$	1640.4
${}^{209}_{83}Bi_{126} = {}^{208}_{82}Pb_{126} + p$	1640.2

$$
\begin{aligned}
B_{\mathrm{pair}} &= \Delta & &(\text{for even} - \text{even}) \\
&= 0 & &(\text{for even} - \text{odd}) \\
&= -\Delta & &(\text{for odd} - \text{odd})
\end{aligned}
$$

More later

The BCS theory

Many-particles in non-degenerate levels
~ mean-field approx. for the pairing channel ~

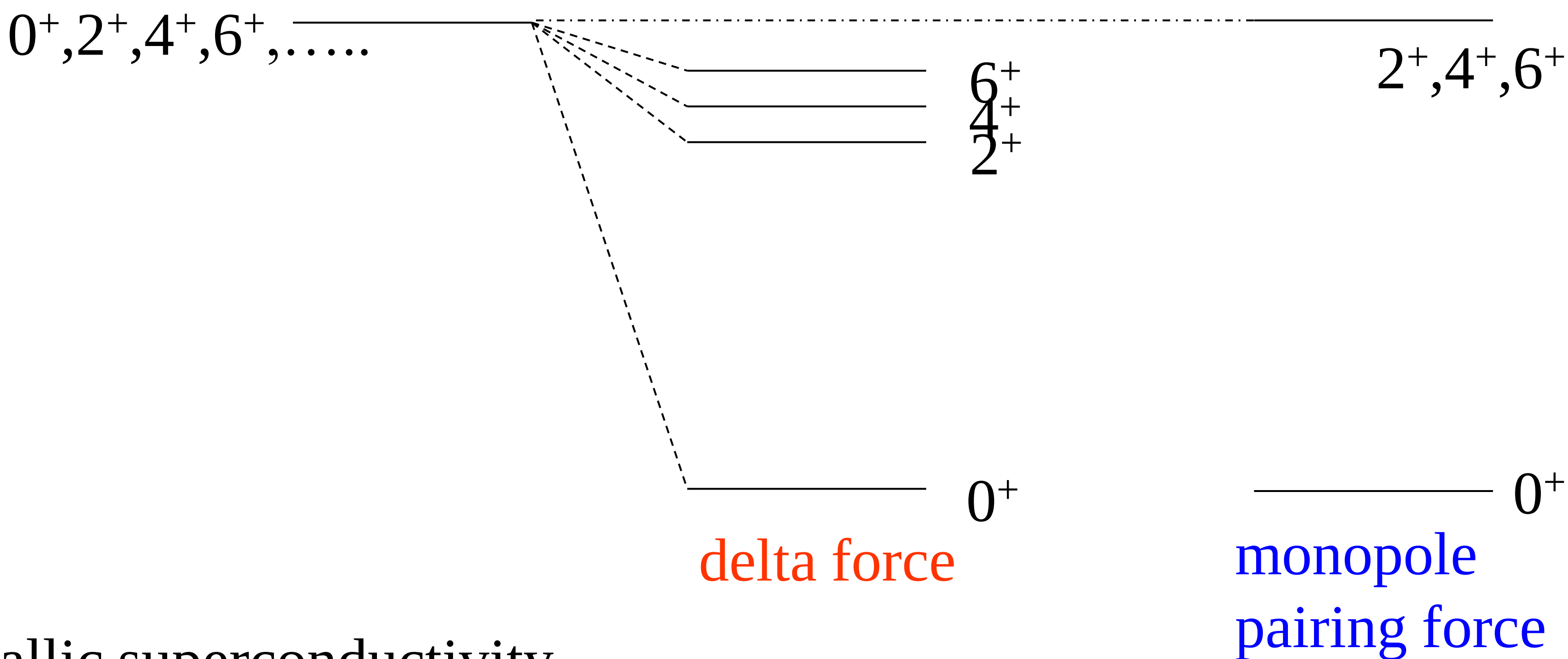
Simplified pairing interaction

$$V = -G\, P^\dagger P; \quad P^\dagger = \sum_{\nu > 0} a^\dagger_\nu a^\dagger_{\bar{\nu}}$$

$\bar{\nu}$: the time reversed state of ν

e.g.,

$$|\nu\rangle = |njlm\rangle, \quad |\bar{\nu}\rangle = |njl-m\rangle$$



Cf. Metallic superconductivity

Solve the pairing Hamiltonian

$$H = \sum_{\nu} \epsilon_\nu (a_\nu^\dagger a_\nu + a_{\bar{\nu}}^\dagger a_{\bar{\nu}}) - G \left(\sum_{\nu>0} a_\nu^\dagger a_{\bar{\nu}}^\dagger \right) \left(\sum_{\nu>0} a_{\bar{\nu}} a_\nu \right)$$

in the mean-field approximation

- Mean-field approximation:

$$V = -G\, P^\dagger P \to -G \left(\langle P^\dagger \rangle P + P^\dagger \langle P \rangle \right) = -\Delta (P^\dagger + P)$$

Cf. HF potential

$$V_H(\boldsymbol{r}) = \int v(\boldsymbol{r}, \boldsymbol{r}') \rho_{\mathsf{HF}}(\boldsymbol{r}') d\boldsymbol{r}$$

$\Longleftrightarrow$ particle number violation we consider $H' = H - \lambda\hat{N}$ instead of H :

$$H' = \sum_{k>0}(\epsilon_k - \lambda)(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - G\hat{P}^\dagger\hat{P}$$
$$\to \sum_{k>0}(\epsilon_k - \lambda)(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - \Delta(\hat{P}^\dagger + \hat{P})$$
$$= \sum_{k>0}(\epsilon_k - \lambda)(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - \Delta\sum_{k>0}(a_k^\dagger a_{\bar{k}}^\dagger + a_{\bar{k}}a_k)$$

- Transform *H'* in a form of

$$H' = \sum_{k>0} E_k(\alpha_k^\dagger\alpha_k + \alpha_{\bar{k}}^\dagger\alpha_{\bar{k}})$$

g.s.: $\alpha_k|BCS\rangle = 0$

1st excited state: $|1_k\rangle = \alpha_k^\dagger|BCS\rangle$ at E_k

…. and so on.

Bogoliubov transformation

$$\alpha^\dagger_\nu = u_\nu a^\dagger_\nu - v_\nu a_{\bar{\nu}}, \qquad \alpha^\dagger_{\bar{\nu}} = u_\nu a^\dagger_{\bar{\nu}} + v_\nu a_\nu$$

(Quasi-particle operator)

or $$a^\dagger_\nu = u_\nu \alpha^\dagger_\nu + v_\nu \alpha_{\bar{\nu}}, \qquad a^\dagger_{\bar{\nu}} = u_\nu \alpha^\dagger_{\bar{\nu}} + - v_\nu \alpha_\nu$$

(note)

$$\{\alpha_\nu, \alpha_{\nu'}\} = 0, \qquad \{\alpha_\nu, \alpha^\dagger_{\nu'}\} = \delta_{\nu,\nu'}$$

$$\longrightarrow \qquad u_\nu^2 + v_\nu^2 = 1$$

using the quasi-particle operators:

$$
\begin{aligned}
H' &\sim \sum_{k>0} (\epsilon_k - \lambda)(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - \Delta \sum_{k>0} (a_k^\dagger a_{\bar{k}}^\dagger + a_{\bar{k}} a_k) \\
&= \sum_{k>0} [(\epsilon_k - \lambda)(u_k^2 - v_k^2) + 2\Delta u_k v_k](\alpha_k^\dagger \alpha_k + \alpha_{\bar{k}}^\dagger \alpha_{\bar{k}}) \\
&\quad + \sum_{k>0} [2(\epsilon_k - \lambda) u_k v_k - \Delta (u_k^2 - v_k^2)](\alpha_k^\dagger \alpha_{\bar{k}}^\dagger + \alpha_{\bar{k}} \alpha_k)
\end{aligned}
$$

if $2(\epsilon_k - \lambda) u_k v_k - \Delta (u_k^2 - v_k^2) = 0$

then $H' = \sum_{k>0} E_k (\alpha_k^\dagger \alpha_k + \alpha_{\bar{k}}^\dagger \alpha_{\bar{k}})$

with $E_k = (\epsilon_k - \lambda)(u_k^2 - v_k^2) + 2\Delta u_k v_k$

$$\left\{\begin{array}{rcl} 0 & = & 2(\epsilon_k - \lambda)u_k v_k - \Delta(u_k^2 - v_k^2) \\ 0 & = & u_k^2 + v_k^2 \end{array}\right.$$

$$\boxed{\begin{array}{rcl} u_\nu^2 & = & \frac{1}{2}\left(1 + \frac{\epsilon_\nu - \lambda}{\sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}}\right) \\ v_\nu^2 & = & \frac{1}{2}\left(1 - \frac{\epsilon_\nu - \lambda}{\sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}}\right) \end{array}}$$

$$\begin{array}{rcl} E_k & = & (\epsilon_k - \lambda)(u_k^2 - v_k^2) + 2\Delta u_k v_k \\ & = & \sqrt{(\epsilon_k - \lambda)^2 + \Delta^2} \end{array}$$

Ground state wave function:

$$\alpha_k|BCS\rangle = 0$$

$$|BCS\rangle \propto \prod_{\nu>0} \alpha_\nu \alpha_{\bar{\nu}}|0\rangle$$

$$= \prod_{\nu>0} v_\nu \left(u_\nu + v_\nu\, a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)\Big|0\Big\rangle$$

$$|BCS\rangle = \prod_{\nu>0} \left(u_\nu + v_\nu\, a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)\Big|0\Big\rangle$$

(note) $\left\langle BCS|a^\dagger_\nu a_\nu|BCS\right\rangle = |v_\nu|^2$: occupation probability

(note)

$$E'_{\rm BCS} = \langle BCS|H'|BCS\rangle \sim 2\sum_{\nu>0}(\epsilon_\nu - \lambda)v_\nu^2 - \frac{\Delta^2}{G}$$

Gap equation

$$\begin{cases} u_\nu^2 = \frac{1}{2}\left(1+\frac{\epsilon_\nu-\lambda}{E_\nu}\right) \\ v_\nu^2 = \frac{1}{2}\left(1-\frac{\epsilon_\nu-\lambda}{E_\nu}\right) \end{cases}$$

$$E_\nu = \sqrt{(\epsilon_\nu-\lambda)^2+\Delta^2}$$

$$\Delta = G\langle BCS|\hat{P}|BCS\rangle = G\sum_{\nu>0} u_\nu v_\nu$$

$$= \frac{G}{2}\sum_{\nu>0}\frac{\Delta}{E_\nu}$$

(Gap equation)

$$N = 2\sum_{\nu>0} v_\nu^2 \qquad \leftarrow \lambda$$

Gap Equation

$$\Delta = \frac{G}{2}\sum_{\nu>0}\frac{\Delta}{\sqrt{(\epsilon_\nu-\lambda)^2+\Delta^2}}$$

i) Trivial solution: always exists

$$\Delta = 0$$

$$v_\nu^2 = \frac{1}{2}\left(1-\frac{\epsilon_\nu-\lambda}{\sqrt{(\epsilon_\nu-\lambda)^2}}\right) = 1 \quad (\epsilon_\nu \leq \lambda)$$

$$= 0 \quad (\epsilon_\nu > \lambda)$$

G a/o N ⟶ large

ii) Superfluid solution

$$1 = \frac{G}{2}\sum_{\nu>0}\frac{1}{\sqrt{(\epsilon_\nu-\lambda)^2+\Delta^2}}$$

(Note) obviously this equation cannot be satisfied for G=0

$$v_\nu^2 = \frac{1}{2}\left(1-\frac{\epsilon_\nu-\lambda}{\sqrt{(\epsilon_\nu-\lambda)^2+\Delta^2}}\right) < 1$$

i) Trivial solution: always exists

$$\Delta = 0$$

$$v_\nu^2 = 1 \quad (\epsilon_\nu \leq \lambda)$$
$$\quad = 0 \quad (\epsilon_\nu > \lambda)$$

$$|\Psi\rangle = \prod_{\nu>0} a_\nu^\dagger a_{\bar{\nu}}^\dagger |0\rangle$$

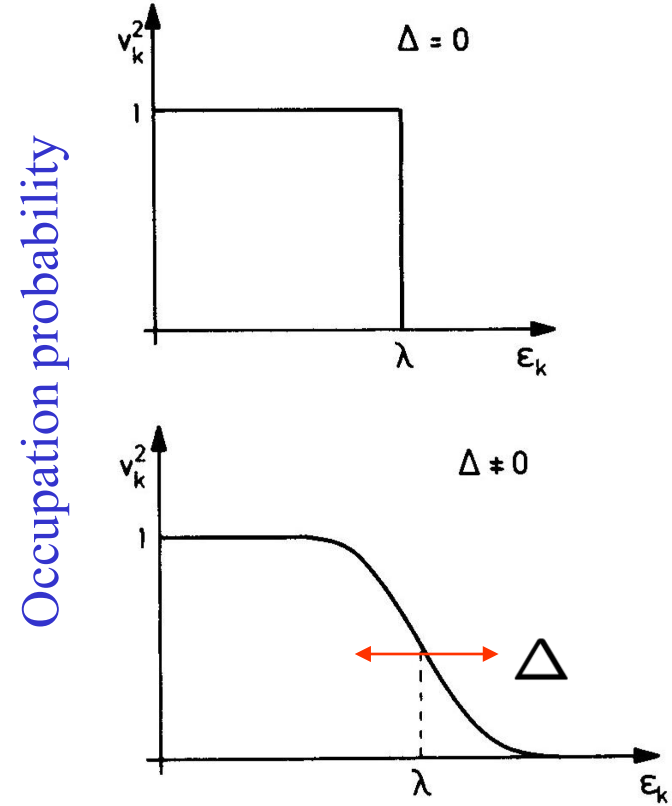
G a/o $N \longrightarrow$ large

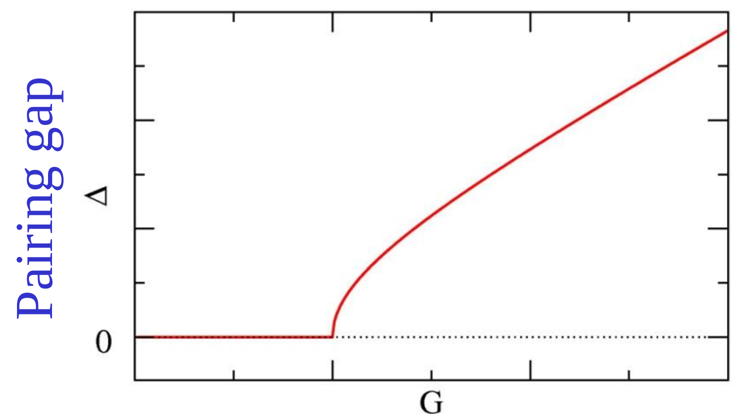
ii) Superfluid solution

$$\Delta \neq 0$$

$$v_\nu^2 < 1$$

$$|BCS\rangle = \prod_{\nu>0} \left(u_\nu + v_\nu\, a_\nu^\dagger a_{\bar{\nu}}^\dagger\right) \left|0\right\rangle$$





Number fluctuation

Normal-Superfulid phase transition

Quasi-particle excitations

$$H \sim E_{BCS} + \sum_\nu E_\nu \, \alpha^\dagger_\nu \alpha_\nu$$

- g.s. of even-even nuclei: $|BCS\rangle$
- One quasi-particle states:

$$|\nu_1\rangle = \alpha^\dagger_{\nu_1}|BCS\rangle = a^\dagger_{\nu_1} \prod_{\nu \neq \nu_1} \left(u_\nu + v_\nu \, a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)\Big|0\Big\rangle$$

Wave function for odd-mass nuclei

$$\langle \nu_1|H|\nu_1\rangle = \langle H\rangle + E_{\nu_1}$$

- Two quasi-particle states:

$$|\nu_1\nu_2\rangle = \alpha^\dagger_{\nu_1}\alpha^\dagger_{\nu_2}|BCS\rangle$$

Excited state of the even-even nuclei

$$\begin{aligned}\langle \nu_1\nu_2|H|\nu_1\nu_2\rangle - \langle H\rangle &= E_{\nu_1} + E_{\nu_2} \\ &\geq 2\Delta\end{aligned}$$

← Energy gap

(note) no pairing limit:

$$\alpha^\dagger_p \alpha^\dagger_h \to a^\dagger_p a_h, \qquad E_p + E_h \to (\epsilon_p - \lambda) + (\lambda - \epsilon_h)$$

(particle-hole excitation)

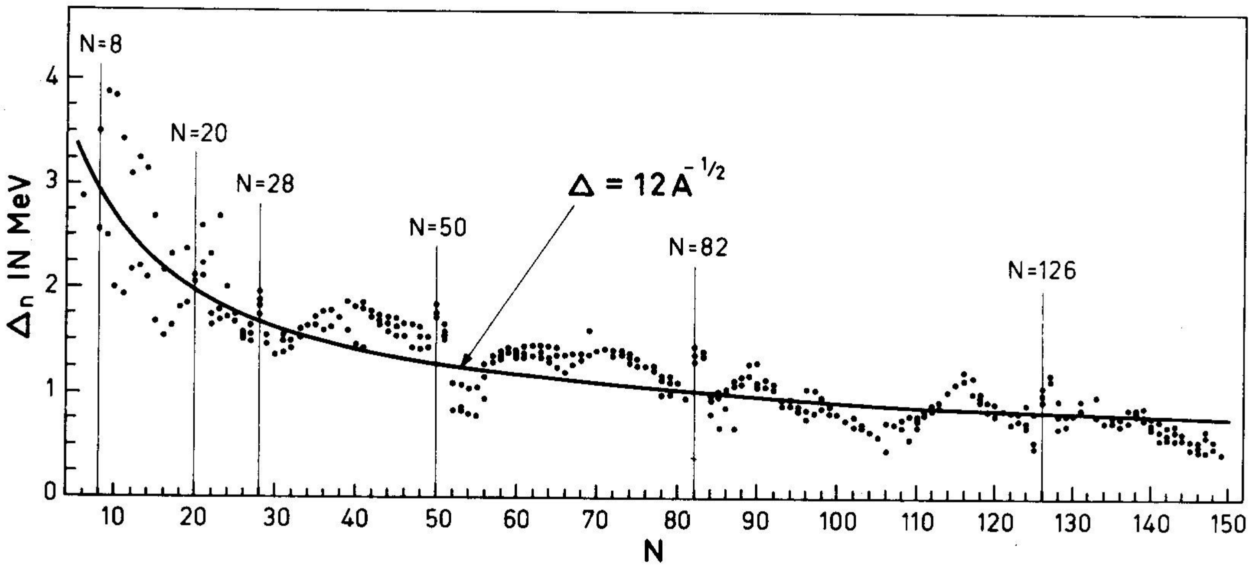
Even-odd mass difference and pairing gap

$$\begin{aligned} B_{\text{pair}} &= \Delta \quad \text{(for even – even)} \\ &= 0 \quad \text{(for even – odd)} \\ &= -\Delta \quad \text{(for odd – odd)} \end{aligned}$$

$$\begin{aligned} E(N+2,Z) &= E(N,Z) + 2\lambda \\ E(N+1,Z) &= E(N,Z) + \lambda + \Delta \end{aligned}$$

$$-\Delta_n \sim [E(N+2,Z) - 2E(N+1,Z) + E(N,Z)]/2$$

Or $\Delta_n \sim (\Delta_n(N) + \Delta_n(N-1))/2$



Bohr-Mottelson ('69)

Particle Number Projection

$$|BCS\rangle = \prod_{\nu>0}\left(u_\nu + v_\nu\, a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)|0\rangle$$: violation of the particle number

→ Particle number projection

Cf. Violation of the rot. symmetry for def. nuclei
and the angular momentum projection

Projection operator:

$$\hat{P}_N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{i\varphi(\hat{N}-N)}$$

$$(\Delta N)^2 = \langle(\hat{N}-N)^2\rangle = 4\sum_{\nu>0} u_\nu^2 v_\nu^2$$

(note) $$|BCS\rangle = \sum_{N'} C_{N'}|N'\rangle$$

$$\rightarrow |\mathrm{proj}\rangle = \hat{P}_N|BCS\rangle = C_N|N\rangle$$

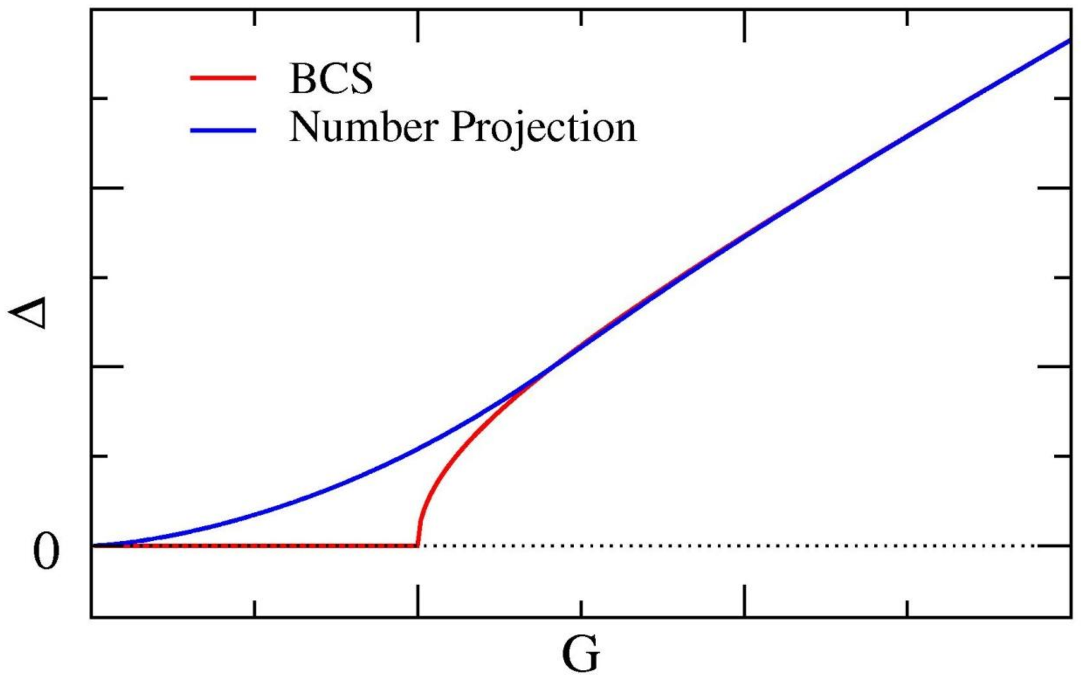
(note) $$e^{i\hat{N}\varphi}|BCS\rangle = \prod_{\nu>0}\left(u_\nu + v_\nu\, e^{2i\varphi}\, a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)|0\rangle$$ ⇐ degenerate with $|BCS\rangle$

Variation After Projection: determine v_ν by minimizing

$$E'_{\text{proj}} = \frac{\langle BCS|\hat{P}_N(\hat{H} - \lambda\hat{N})\hat{P}_N|BCS\rangle}{\langle BCS|\hat{P}_N\hat{P}_N|BCS\rangle}$$

$$\Rightarrow \quad \left(\frac{\partial}{\partial v_\nu} + \frac{\partial u_\nu}{\partial v_\nu}\frac{\partial}{\partial u_\nu}\right) E'_{\text{proj}} = 0$$

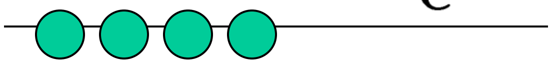
$$\Rightarrow \quad \Delta = G \sum_{\nu>0} u_\nu v_\nu$$



Seniority Scheme

$\epsilon = 0$

Particles in a single degenerate level



Degeneracy: 2Ω

$$\begin{aligned} H &= -G\, P^\dagger P; \quad P^\dagger = \sum_{m>0} a_m^\dagger a_{-m}^\dagger \\ &= -G\Omega A^\dagger A; \quad A^\dagger = P^\dagger/\sqrt{\Omega} \end{aligned}$$

- BCS approximation

$$2\Omega\, v^2 = N$$

$$\begin{aligned} v^2 &= N/2\Omega \\ u^2 &= 1 - N/2\Omega \end{aligned}$$

$$\Delta = G\Omega\, u\, v = G\Omega\sqrt{\frac{N}{2\Omega}\left(1 - \frac{N}{2\Omega}\right)}$$

$$E_{\mathrm{BCS}} = \langle H \rangle = -\Delta^2/G = -\frac{GN\Omega}{2}(1 - N/2\Omega)$$

$$\begin{aligned} H &= -G\,P^\dagger P; \qquad P^\dagger = \sum_{m>0} a_m^\dagger a_{-m}^\dagger \\ &= -G\Omega A^\dagger A; \qquad A^\dagger = P^\dagger/\sqrt{\Omega} \end{aligned}$$

•Exact solution (Seniority scheme)

(note) $$[A, A^\dagger] = 1 - \frac{\hat{N}}{\Omega}, \qquad A|0\rangle = 0, \quad \hat{N}|0\rangle = 0$$

$$[\hat{N}, A^\dagger] = 2A^\dagger$$

$$\begin{aligned} H A^\dagger|0\rangle &= -G\Omega\, A^\dagger|0\rangle \\ H(A^\dagger)^2|0\rangle &= -2G(\Omega - 1)\,(A^\dagger)^2|0\rangle \\ &\cdots \\ H(A^\dagger)^{N/2}|0\rangle &= -GN/4 \cdot (2\Omega - N + 2)\,(A^\dagger)^{N/2}|0\rangle \end{aligned}$$

↕

$$E_{\mathrm{BCS}} = -\frac{GN\Omega}{2}(1 - N/2\Omega)$$

The BCS approximation is good for large *N*.

Hartree-Fock-Bogoliubov (HFB) Theory

HF+BCS method: first solve HF, and then solve the gap equation

s.p. wave functions, occupation probabilities,
chemical potential, pairing gaps

→ wave functions do not change due to the pairing correlation.
only the occupation probabilities are modified

⇒ Hartree-Fock-Bogoliubov (HFB) theory:

both wave functions and occupation probabilities

$$\begin{pmatrix} \hat{h}(\boldsymbol{r}) - \lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}(\boldsymbol{r})^* & -\hat{h}(\boldsymbol{r}) + \lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

$$\begin{aligned} \hat{h}(\boldsymbol{r}) &= -\frac{\hbar^2}{2m}\nabla^2 + V_{\mathsf{HF}}(\boldsymbol{r}) \\ \rho(\boldsymbol{r}) &= \sum_\alpha |V_\alpha(\boldsymbol{r})|^2 \end{aligned}$$

u,*v* factors → *u*, *v* functions

Relation to the BCS approximation

$$\begin{pmatrix} \hat{h}-\lambda & \tilde{\Delta}(\boldsymbol{r}) \\ \tilde{\Delta}^*(\boldsymbol{r}) & -\hat{h}+\lambda \end{pmatrix} \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix} = E_\alpha \begin{pmatrix} U_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) \end{pmatrix}$$

Expansion on the HF basis:

$$U_\alpha(\boldsymbol{r}) = \sum_i u_i^{(\alpha)} \varphi_i(\boldsymbol{r})$$

$$V_\alpha(\boldsymbol{r}) = \sum_i v_i^{(\alpha)} \varphi_i(\boldsymbol{r})$$

where

$$\hat{h}\varphi_i = \epsilon_i\varphi_i$$

$$\sum_j \begin{pmatrix} (\epsilon_i-\lambda)\delta_{i,j} & \tilde{\Delta}_{ij} \\ \tilde{\Delta}_{ij}^* & (-\epsilon_i+\lambda)\delta_{i,j} \end{pmatrix} \begin{pmatrix} u_j^{(\alpha)} \\ v_j^{(\alpha)} \end{pmatrix} = E_\alpha \begin{pmatrix} u_i^{(\alpha)} \\ v_i^{(\alpha)} \end{pmatrix}$$

diagonalization

$$\tilde{\Delta}_{ij} = \int d\boldsymbol{r}\, \varphi_i^*(\boldsymbol{r})\tilde{\Delta}(\boldsymbol{r})\varphi_j(\boldsymbol{r})$$

BCS approximation: Take only the diagonal components in $\tilde{\Delta}_{ij}$

$$\begin{aligned}(\epsilon_i - \lambda)u_i^{(\alpha)} + \tilde{\Delta}_{ii}\, v_i^{(\alpha)} &= E_\alpha\, u_i^{(\alpha)} \\ \tilde{\Delta}_{ii}\, u_i^{(\alpha)} + (-\epsilon_i + \lambda)v_i^{(\alpha)} &= E_\alpha\, v_i^{(\alpha)}\end{aligned}$$

Solution:

$$\begin{aligned}u_i^{(\alpha)} &= u_\alpha^{\mathrm{BCS}}\,\delta_{i,\alpha} = \sqrt{\frac{1}{2}\left(1 + \frac{\epsilon_\alpha - \lambda}{E_\alpha}\right)} \\ v_i^{(\alpha)} &= v_\alpha^{\mathrm{BCS}}\,\delta_{i,\alpha} = \sqrt{\frac{1}{2}\left(1 - \frac{\epsilon_\alpha - \lambda}{E_\alpha}\right)} \\ E_\alpha &= \sqrt{(\epsilon_\alpha - \lambda)^2 + \tilde{\Delta}_{\alpha\alpha}^2}\end{aligned}$$

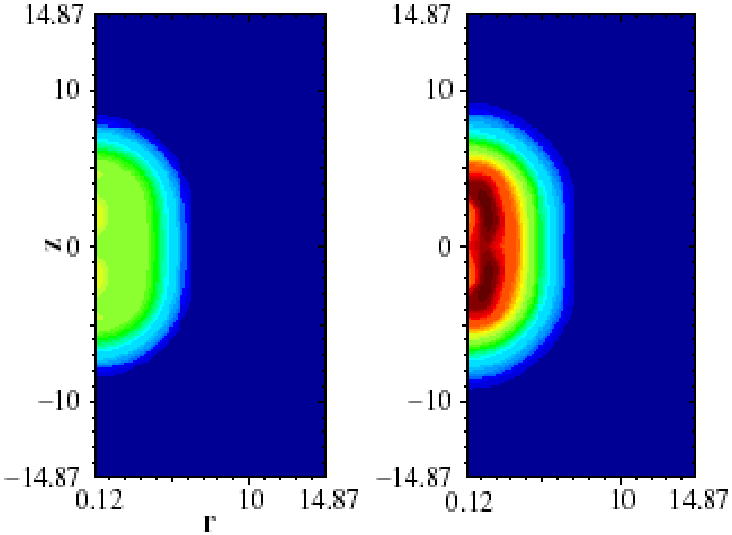
$$\begin{aligned}U_\alpha(\boldsymbol{r}) &= u_\alpha^{\mathrm{BCS}}\,\varphi_\alpha(\boldsymbol{r}) \\ V_\alpha(\boldsymbol{r}) &= v_\alpha^{\mathrm{BCS}}\,\varphi_\alpha(\boldsymbol{r})\end{aligned}$$

$U_\alpha(\boldsymbol{r})$ and $V_\alpha(\boldsymbol{r})$ have the same radial dependence in the BCS approximation.

This is not the case in HFB.

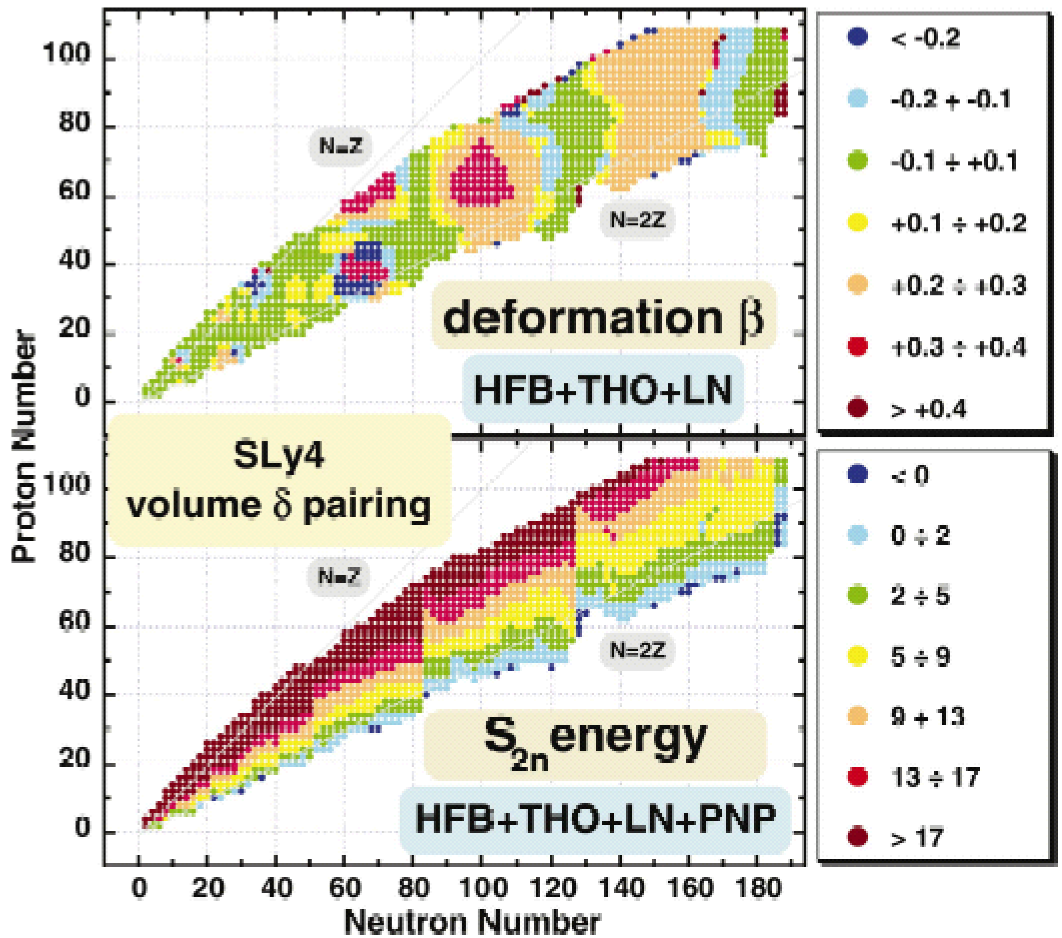
Application of the HFB method

Density of ^{110}Zr (SHFB-SLy4)

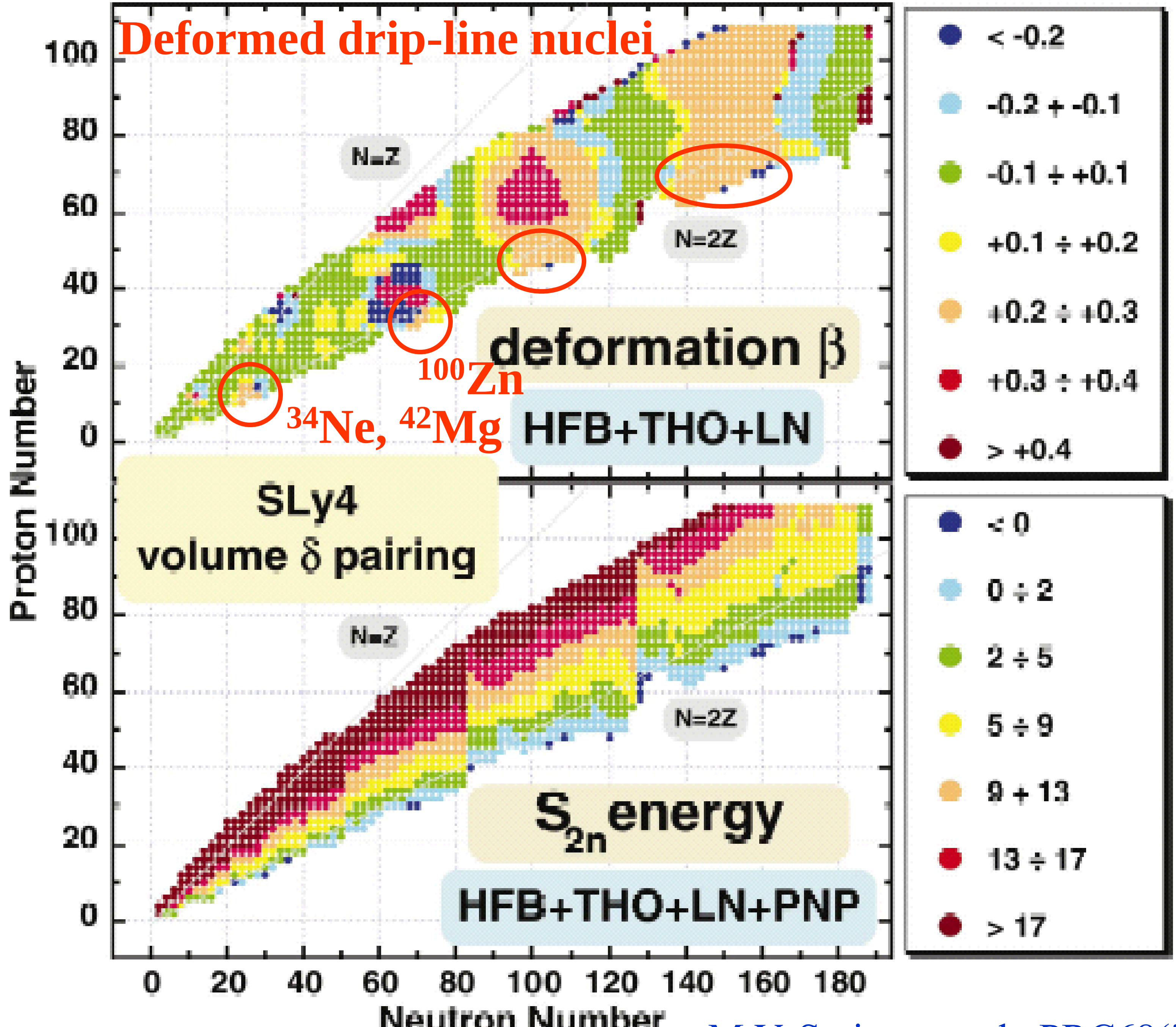


A. Blazkiewicz et al., PRC71('05)054231

Systematics of β_2 and S_{2n}



M.V. Stoitsov et al., PRC68('03)054312



M.V. Stoitsov et al., PRC68('03)054312

Back-up

The BCS theory

Many-particles in non-degenerate levels
~ mean-field approx. for the pairing channel ~

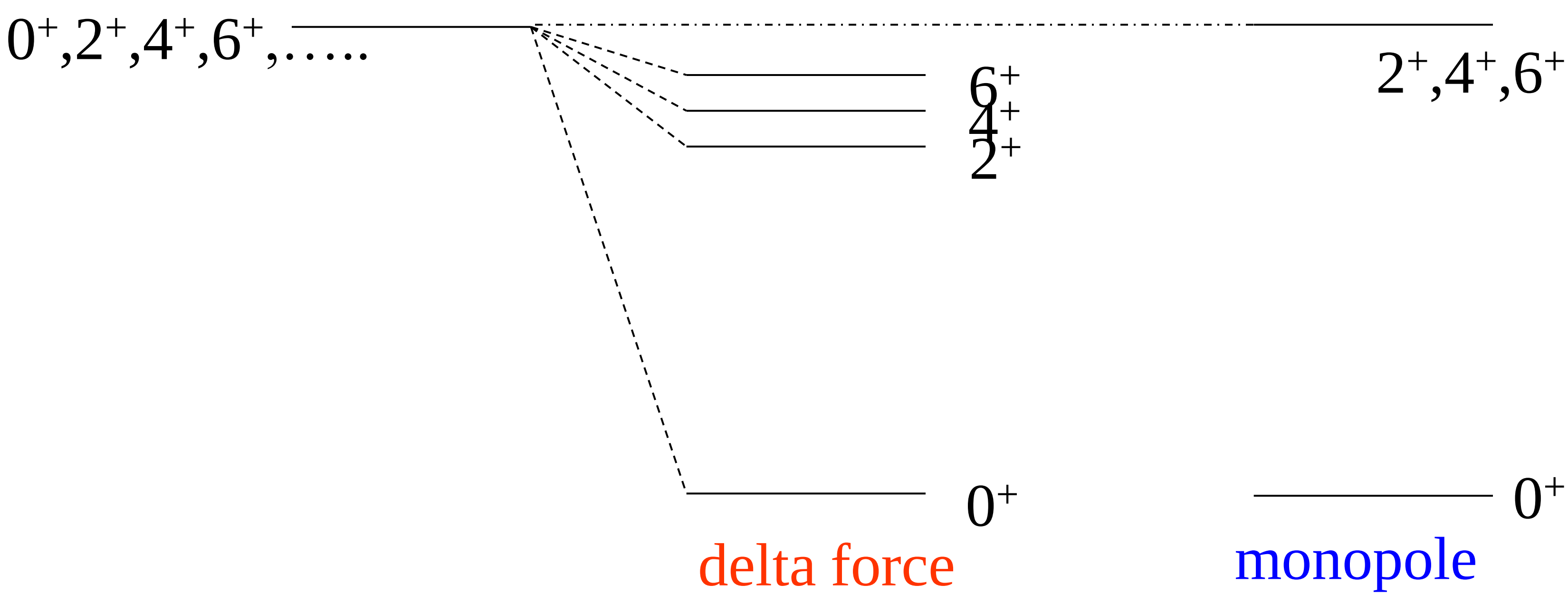
Simplified pairing interaction

$$V = -G\,P^\dagger P; \quad P^\dagger = \sum_{\nu>0} a^\dagger_\nu a^\dagger_{\bar{\nu}}$$

$\bar{\nu}$: the time reversed state of ν

e.g.,

$$|\nu\rangle = |njlm\rangle, \quad |\bar{\nu}\rangle = |njl-m\rangle$$



Cf. Metallic superconductivity

Solve the pairing Hamiltonian

$$H = \sum_\nu \epsilon_\nu (a_\nu^\dagger a_\nu + a_{\bar{\nu}}^\dagger a_{\bar{\nu}}) - G \left(\sum_{\nu>0} a_\nu^\dagger a_{\bar{\nu}}^\dagger \right) \left(\sum_{\nu>0} a_{\bar{\nu}} a_\nu \right)$$

in the mean-field approximation

- Mean-field approximation:

$$V = -G\, P^\dagger P \to -G \left(\langle P^\dagger \rangle P + P^\dagger \langle P \rangle \right) = -\Delta (P^\dagger + P)$$

Cf. HF potential

$$V_H(\boldsymbol{r}) = \int v(\boldsymbol{r}, \boldsymbol{r}') \rho_{\rm HF}(\boldsymbol{r}') d\boldsymbol{r}$$

⟺ particle number violation

- The Bardeen, Cooper, Schrieffer (BCS) ansatz

$$|\Psi\rangle = \prod_{\nu>0} \left(u_\nu + v_\nu\, a_\nu^\dagger a_{\bar{\nu}}^\dagger \right) \big| 0 \big\rangle$$

$$|u_\nu|^2 + |v_\nu|^2 = 1$$ ⟵ normalization

(note) $\left\langle a_\nu^\dagger a_\nu \right\rangle = |v_\nu|^2$: occupation probability

- The Bardeen, Cooper, Schrieffer (BCS) anzatz

$$|\Psi\rangle = \prod_{\nu>0} \left(u_\nu + v_\nu\, a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)\Big|0\Big\rangle$$

$$|u_\nu|^2 + |v_\nu|^2 = 1$$ ← normalization

(note) $\left\langle a^\dagger_\nu a_\nu \right\rangle = |v_\nu|^2$: occupation probability

(note)

BCS convention: $u_{\bar{\nu}} = u_\nu, \quad v_{\bar{\nu}} = -v_\nu$ (real numbers)

(note) $$\left(1 + \frac{v_\nu}{u_\nu} a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)\Big|0\Big\rangle = \exp\left(\frac{v_\nu}{u_\nu} a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)\Big|0\Big\rangle$$

$$|\Psi\rangle \propto \exp\left(\sum_{\nu>0} \frac{v_\nu}{u_\nu} a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)\Bigg|0\Bigg\rangle$$ (pair condensed wave function)

(note) $$|\Psi\rangle \propto \prod_{\nu>0} \alpha_\nu \alpha_{\bar{\nu}} |0\rangle$$

$$\alpha^\dagger_\nu = u_\nu a^\dagger_\nu - v_\nu a_{\bar{\nu}}$$
$$\alpha^\dagger_{\bar{\nu}} = u_\nu a^\dagger_{\bar{\nu}} + v_\nu a_\nu$$

$$H = \sum_\nu \epsilon_\nu (a_\nu^\dagger a_\nu + a_{\bar\nu}^\dagger a_{\bar\nu}) - G\left(\sum_{\nu>0} a_\nu^\dagger a_{\bar\nu}^\dagger\right)\left(\sum_{\nu>0} a_{\bar\nu} a_\nu\right)$$

- Mean-field approximation:

$$V = -G\,P^\dagger P \to -G\left(\langle P^\dagger\rangle P + P^\dagger \langle P\rangle\right) = -\Delta(P^\dagger + P)$$

- The Bardeen, Cooper, Schrieffer (BCS) anzatz

$$|\Psi\rangle = \prod_{\nu>0}\left(u_\nu + v_\nu\, a_\nu^\dagger a_{\bar\nu}^\dagger\right)\big|0\big\rangle \qquad |u_\nu|^2 + |v_\nu|^2 = 1$$

(note) $\left\langle a_\nu^\dagger a_\nu \right\rangle = |v_\nu|^2, \qquad \Delta = G\langle P^\dagger\rangle = G\sum_{\nu>0} u_\nu v_\nu$

Minimize $\langle H'\rangle = \left\langle \sum_\nu \epsilon_\nu (a_\nu^\dagger a_\nu + a_{\bar\nu}^\dagger a_{\bar\nu}) - GP^\dagger P - \lambda\hat N \right\rangle$

with $\langle\Psi|\hat N|\Psi\rangle = 2\sum_{\nu>0} v_\nu^2 = N$

$$\hat N = \sum_\nu (a_\nu^\dagger a_\nu + a_{\bar\nu}^\dagger a_{\bar\nu})$$

$$E' = \langle\Psi|H'|\Psi\rangle \sim 2\sum_{\nu>0}(\epsilon_\nu - \lambda)v_\nu^2 - \Delta^2/G$$

$$E' = 2\sum_{\nu>0}(\epsilon_\nu - \lambda)v_\nu^2 - \left(G\sum_{\nu>0}u_\nu v_\nu\right)^2 / G$$

Minimization:

$$\begin{aligned} 0 &= \left(\frac{\partial}{\partial v_\nu} + \frac{\partial u_\nu}{\partial v_\nu}\frac{\partial}{\partial u_\nu}\right)E' \\ &= 2(\epsilon_\nu - \lambda)u_\nu v_\nu + \Delta(v_\nu^2 - u_\nu^2) \end{aligned}$$

$$u_\nu^2 + v_\nu^2 = 1$$

$$\begin{aligned} u_\nu^2 &= \frac{1}{2}\left(1 + \frac{\epsilon_\nu - \lambda}{E_\nu}\right) \\ v_\nu^2 &= \frac{1}{2}\left(1 - \frac{\epsilon_\nu - \lambda}{E_\nu}\right) \end{aligned}$$

$$E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta^2}$$

$$\Delta = \frac{G}{2}\sum_{\nu>0}\frac{\Delta}{E_\nu}$$

(Gap equation)

Gap Equation

$$\Delta = \frac{G}{2}\sum_{\nu>0}\frac{\Delta}{\sqrt{(\epsilon_\nu-\lambda)^2+\Delta^2}}$$

i) Trivial solution: always exists

$$\Delta = 0$$

$$v_\nu^2 = \frac{1}{2}\left(1-\frac{\epsilon_\nu-\lambda}{\sqrt{(\epsilon_\nu-\lambda)^2}}\right) = 1 \quad (\epsilon_\nu \leq \lambda)$$

$$= 0 \quad (\epsilon_\nu > \lambda)$$

G a/o *N* ⟶ large

ii) Superfluid solution

$$1 = \frac{G}{2}\sum_{\nu>0}\frac{1}{\sqrt{(\epsilon_\nu-\lambda)^2+\Delta^2}}$$

⇦ (Note) obviously this equation cannot be satisfied for *G*=0

$$v_\nu^2 = \frac{1}{2}\left(1-\frac{\epsilon_\nu-\lambda}{\sqrt{(\epsilon_\nu-\lambda)^2+\Delta^2}}\right) < 1$$

i) Trivial solution: always exists

$$\Delta = 0$$

$$v_\nu^2 = 1 \quad (\epsilon_\nu \le \lambda)$$
$$\quad = 0 \quad (\epsilon_\nu > \lambda)$$

$$|\Psi\rangle = \prod_{\nu>0} a_\nu^\dagger a_{\bar{\nu}}^\dagger |0\rangle$$

G a/o $N \longrightarrow$ large

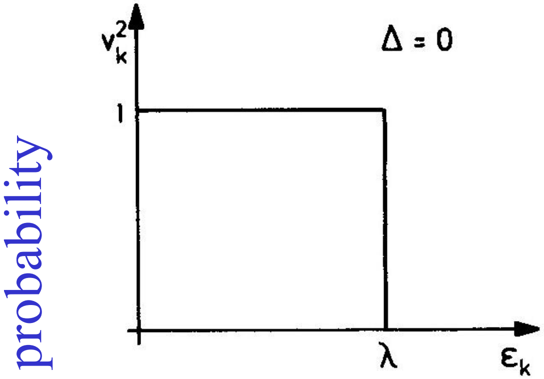
ii) Superfluid solution

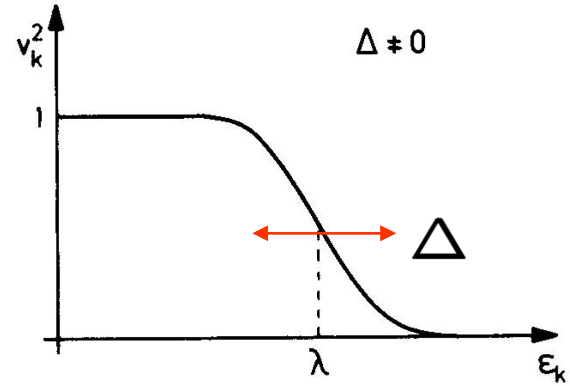
$$\Delta \neq 0$$

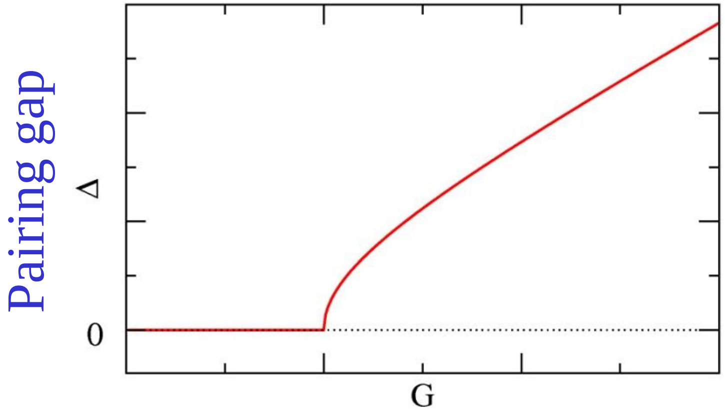
$$v_\nu^2 < 1$$

$$|BCS\rangle = \prod_{\nu>0} \left(u_\nu + v_\nu\, a_\nu^\dagger a_{\bar{\nu}}^\dagger\right) \Big| 0 \Big\rangle$$

Number fluctuation







Normal-Superfulid phase transition