CNSSS18

Systematic Treatment of Odd-mass Nuclei in Hartree-Fock-Bogoliubov Calculation

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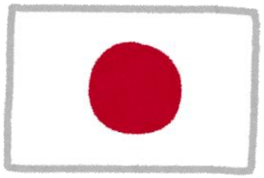


ODD

EVEN

Outline

1. HFB theory and the conventional treatment of odd-particle systems
2. Symmetry and a new treatment of odd-particle systems
3. HF calculation using my own code and the calculation result
4. Summary and future direction

Original idea :

George Bertsch, Jacek Dobaczewski, Witold Nazarewicz, and Junchen Pei
Phys. Rev. A 79, 043602 (2009)

HFB theory and the conventional treatment

Quasiparticle

$$\begin{pmatrix}\beta_\mu \\ \beta_\mu^\dagger\end{pmatrix} = \sum_k W_{\mu k}^\dagger \begin{pmatrix} c_k \\ c_k^\dagger \end{pmatrix} \qquad W \equiv \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \quad \text{unitary}$$

Vacuum

$$|\Phi\rangle \ \text{ s.t. } \ \beta_\mu |\Phi\rangle = 0 \qquad \text{for } \forall \mu$$

Density

$$\rho_{ij} \equiv \langle \Phi | c_j^\dagger c_i | \Phi \rangle \qquad \kappa_{ij} \equiv \langle \Phi | c_j c_i | \Phi \rangle$$

Variation

$$\delta \langle \Phi | H - \lambda \hat{N} | \Phi \rangle = 0 \qquad \hat{N} = \sum_k c_k^\dagger c_k$$

Mean field

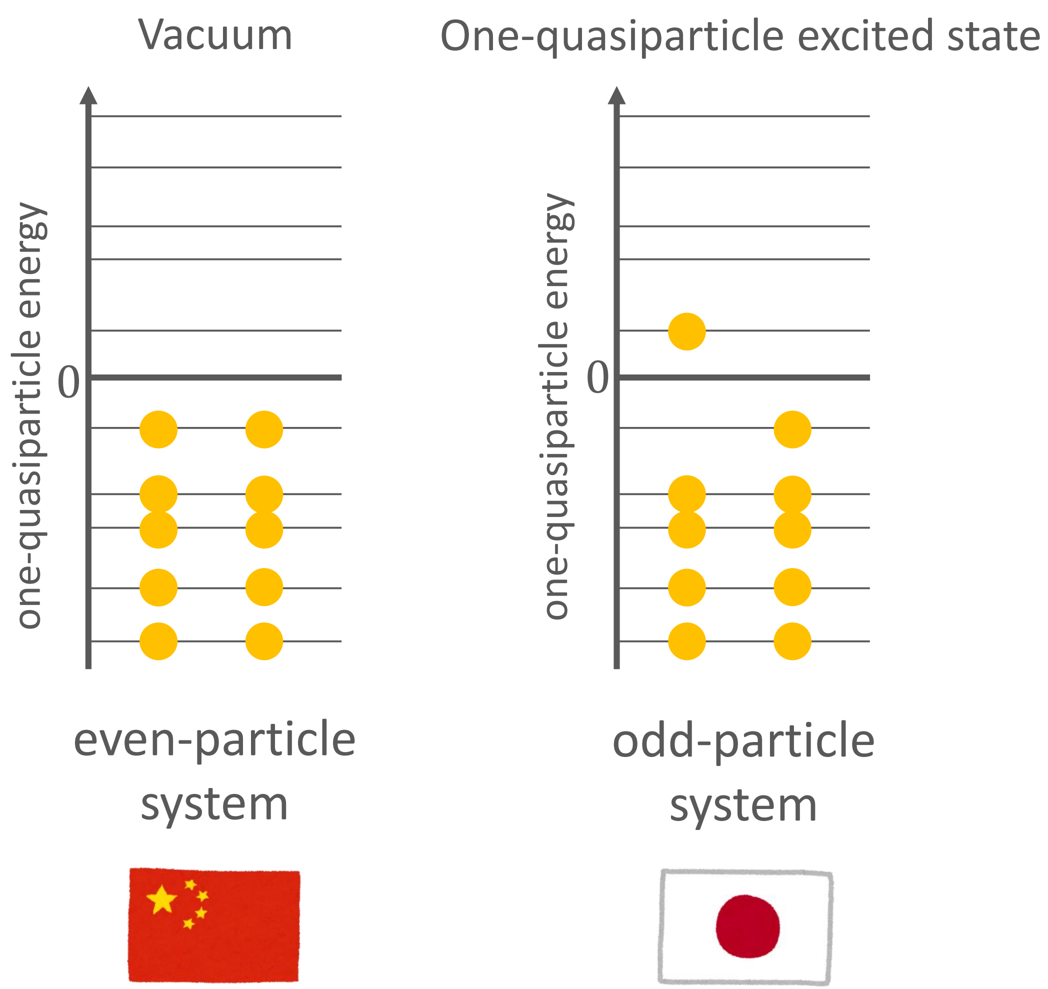
$$\mathcal{H} \equiv \begin{pmatrix} h - \lambda 1 & \Delta \\ -\Delta^* & -h^* + \lambda 1 \end{pmatrix}$$

$$h_{ij} = \frac{\delta \langle \Phi | H | \Phi \rangle}{\delta \rho_{ji}} \qquad \Delta_{\mathrm{ij}} = \frac{\delta \langle \Phi | H | \Phi \rangle}{\delta \kappa_{ij}^*}$$

Equation

$$W^\dagger \mathcal{H} W = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

HFB theory and the conventional treatment



The vacuum $|\Phi\rangle$ usually represents an even-particle system because of the pairing. Then an odd-particle system is represented as a one-quasiparticle excited state on the vacuum.

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Symmetry and a new treatment

Quasiparticle	$\begin{pmatrix}\beta_\mu \\ \beta_\mu^\dagger\end{pmatrix} = \sum_k W_{\mu k}^\dagger \begin{pmatrix} c_k \\ c_k^\dagger \end{pmatrix}$ $\quad W \equiv \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$ unitary
Vacuum	$\lvert\Phi\rangle$ s.t. $\beta_\mu \lvert\Phi\rangle = 0$ for $\forall\mu$
Density	$\rho_{ij} \equiv \langle\Phi\rvert c_j^\dagger c_i \lvert\Phi\rangle \quad \kappa_{ij} \equiv \langle\Phi\rvert c_j c_i \lvert\Phi\rangle$
Variation	$\delta\langle\Phi\rvert H - \lambda\hat{N} \lvert\Phi\rangle = 0 \quad \hat{N} = \sum_k c_k^\dagger c_k$
Mean field	$\mathcal{H} \equiv \begin{pmatrix} h - \lambda 1 & \Delta \\ -\Delta^* & -h^* + \lambda 1 \end{pmatrix}$ $\quad h_{ij} = \frac{\delta\langle\Phi\rvert H \lvert\Phi\rangle}{\delta\rho_{ji}} \quad \Delta_{\mathrm{ij}} = \frac{\delta\langle\Phi\rvert H \lvert\Phi\rangle}{\delta\kappa_{ij}^*}$
Equation	$W^\dagger \mathcal{H} W = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$

Symmetry and a new treatment

$$\delta\langle\Phi|H-\lambda\hat{N}-\lambda_s\hat{S}|\Phi\rangle=0$$

$$[H,\hat{S}]=0 \quad \text{s.t.} \quad T\hat{S}T^{-1}=-\hat{s}$$

$$\mathcal{H}'=\begin{pmatrix} h-\lambda 1-\lambda_s s & \Delta \\ -\Delta^* & -h^*+\lambda 1+\lambda_s s^* \end{pmatrix}$$
$$=\begin{pmatrix} h-\lambda 1-\lambda_s s & \Delta \\ -\Delta^* & -h^*+\lambda 1-\lambda_s s \end{pmatrix}$$

$$s_{ij}^*=(\langle i|\hat{s}|j\rangle)^*=(\langle i|T^{-1})(T\hat{s}T^{-1})(T|j\rangle)$$
$$=-\langle i|\hat{s}|j\rangle=-s_{ij}$$

$\because$ $T\hat{s}T^{-1}=-\hat{s}$

$T|i\rangle=|i\rangle$ (The part of the definition of T)

In general $T|i\rangle=F|i\rangle$ (F:unitary). In that case we can make a similar discussion.

Since $[H,\hat{S}]=0$, we can take the simultaneous eigenstate of $\mathcal{H}$ and s.

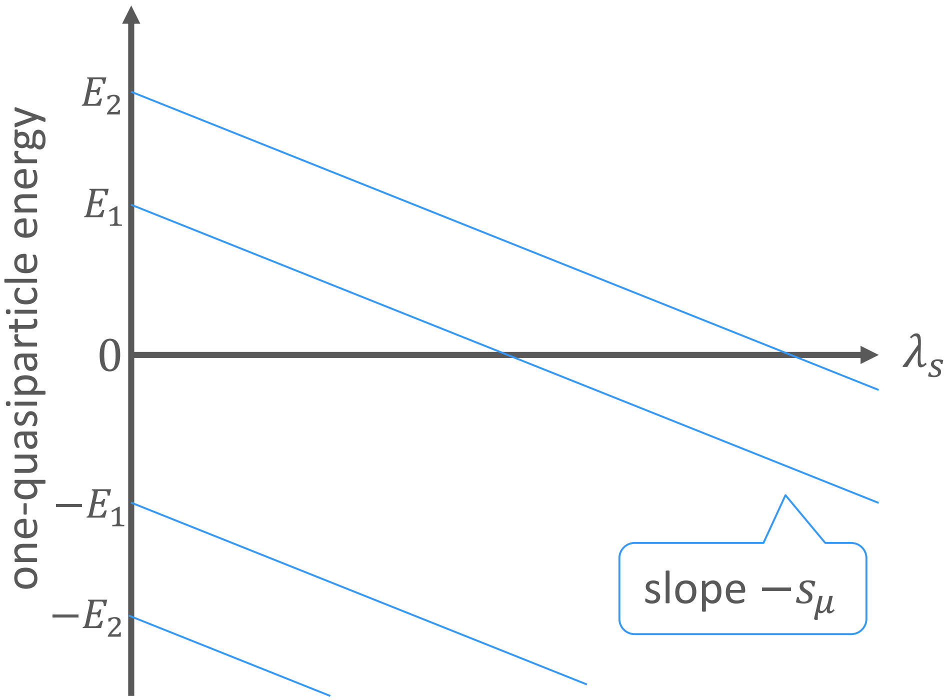
$$\mathcal{H}'\rightarrow\begin{pmatrix} h-\lambda 1-\lambda_s s_\mu 1 & \Delta \\ -\Delta^* & -h^*+\lambda 1-\lambda_s s_\mu 1 \end{pmatrix}$$
$$=\begin{pmatrix} h-\lambda 1 & \Delta \\ -\Delta^* & -h^*+\lambda 1 \end{pmatrix}-\lambda_s s_\mu \mathbf{1}$$

s_μ: eigenvalue of s

Using $\hat{s}$ is time-odd and the symmetry of the system, $\mathcal{H}'$ turns to be the original $\mathcal{H}$ plus a constant × identity.

Symmetry and a new treatment

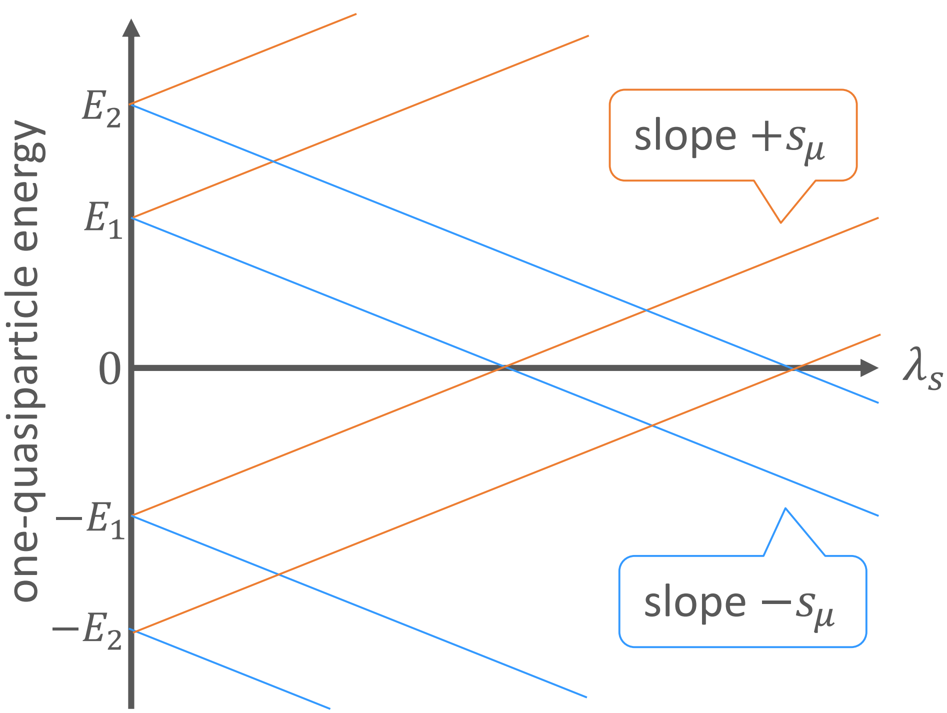
$\mathcal{H}'$	eigenvector	eigenvalue
$\mathcal{H} - \lambda_s s_\mu \mathbf{1}$	$\begin{pmatrix} U_{i\mu} \\ V_{i\mu} \end{pmatrix}$ $\begin{pmatrix} V_{i\bar{\mu}}^* \\ U_{i\bar{\mu}}^* \end{pmatrix}$	$E_\mu^{\lambda_s=0} - \lambda_s s_\mu$ $-E_{\bar{\mu}}^{\lambda_s=0} - \lambda_s s_\mu$



The one-quasiparticle energies are shifted uniformly while the eigenstates don't change.

Symmetry and a new treatment

$\mathcal{H}'$	eigenvector	eigenvalue
$\mathcal{H} - \lambda_s s_\mu \mathbf{1}$	$\begin{pmatrix} U_{i\mu} \\ V_{i\mu} \end{pmatrix}$ $\begin{pmatrix} V^*_{i\bar{\mu}} \\ U^*_{i\bar{\mu}} \end{pmatrix}$	$E_\mu^{\lambda_s=0} - \lambda_s s_\mu$ $-E_{\bar{\mu}}^{\lambda_s=0} - \lambda_s s_\mu$
$\mathcal{H} + \lambda_s s_\mu \mathbf{1}$	$\begin{pmatrix} U_{i\bar{\mu}} \\ V_{i\bar{\mu}} \end{pmatrix}$ $\begin{pmatrix} V^*_{i\mu} \\ U^*_{i\mu} \end{pmatrix}$	$E_{\bar{\mu}}^{\lambda_s=0} + \lambda_s s_\mu$ $-E_\mu^{\lambda_s=0} + \lambda_s s_\mu$



Since $\hat{s}$ is time odd, the time reversed states are also eigenstates of $\mathcal{H}'$.

Symmetry and a new treatment

$\mathcal{H}'$	eigenvector	eigenvalue
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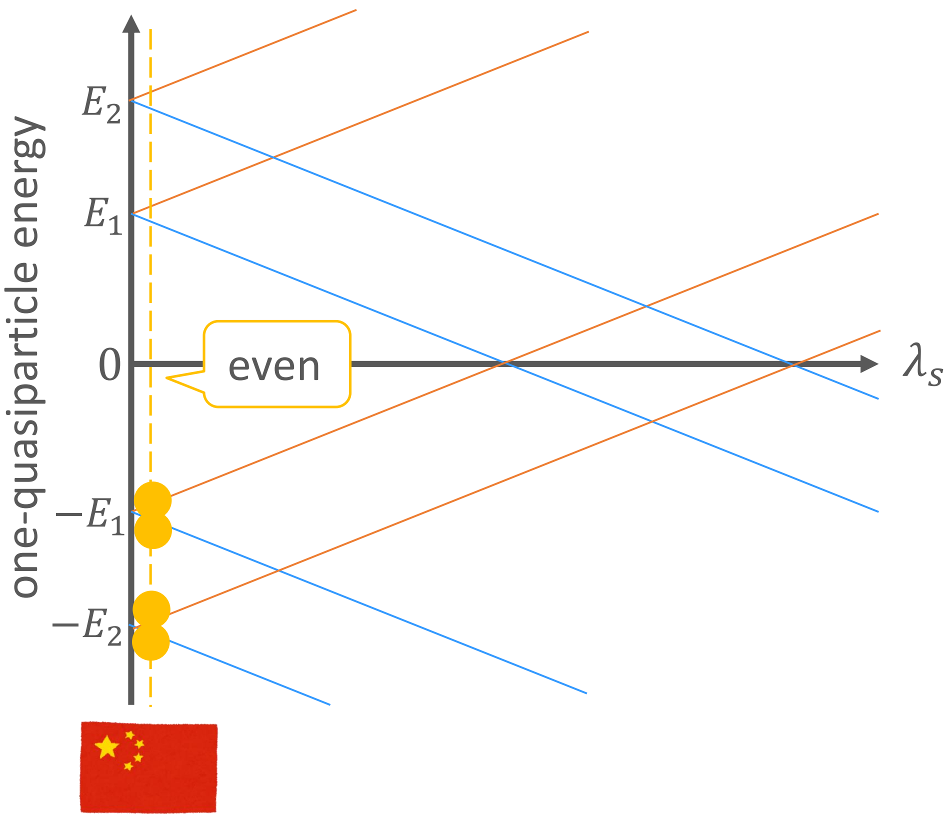

Symmetry and a new treatment

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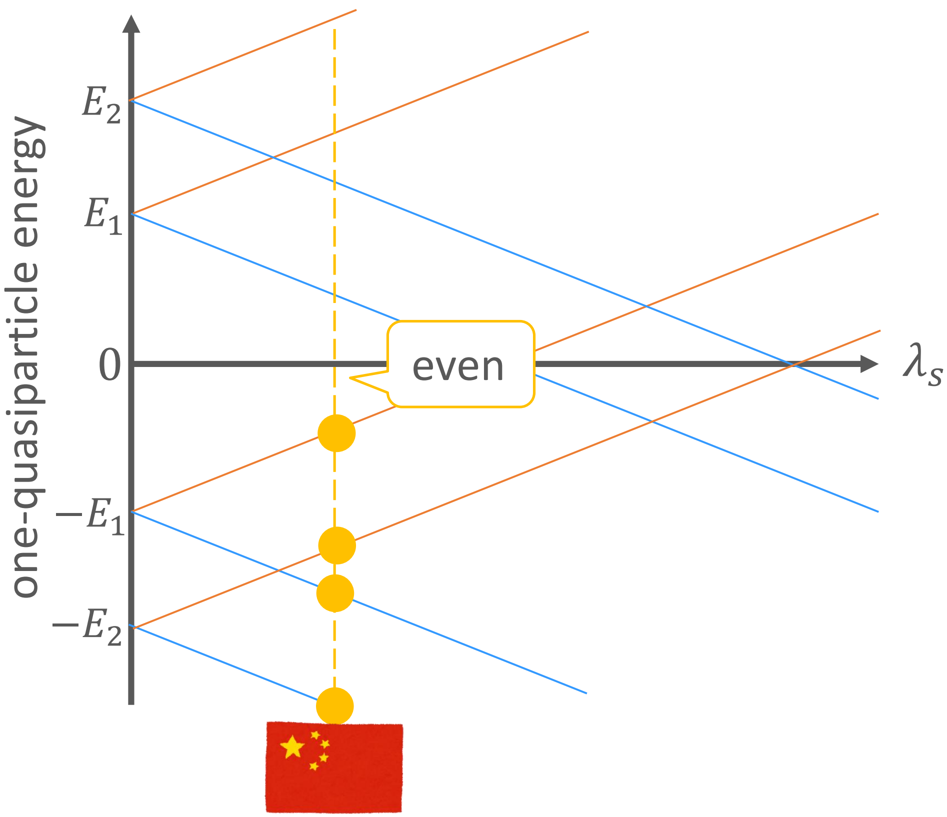

Symmetry and a new treatment

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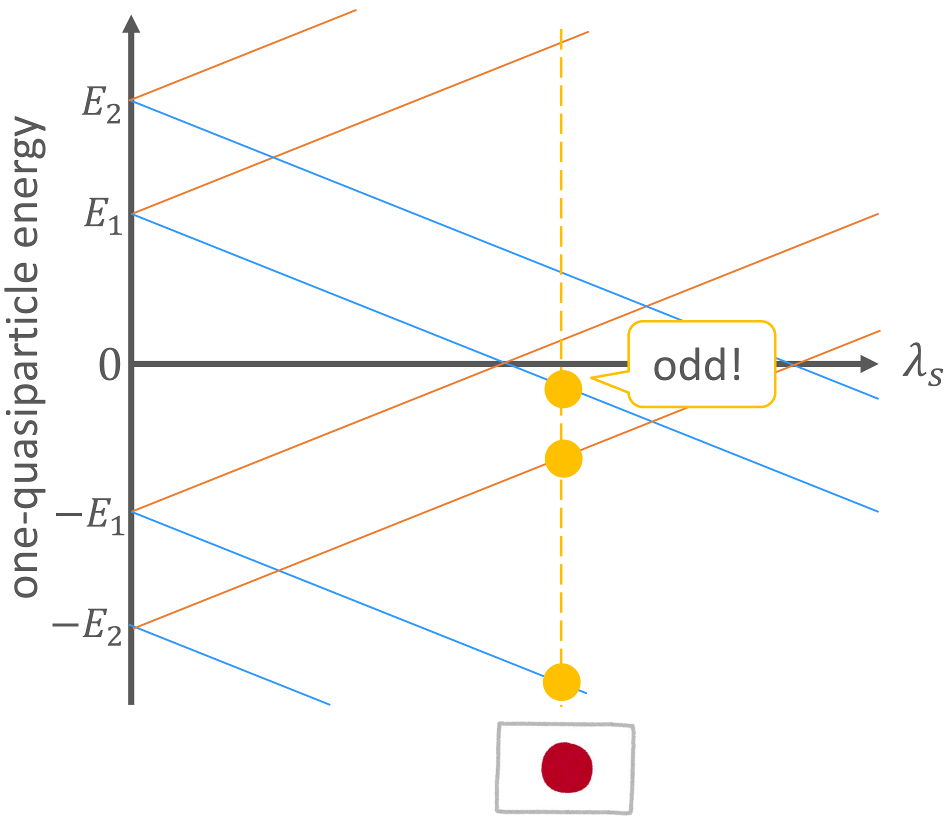

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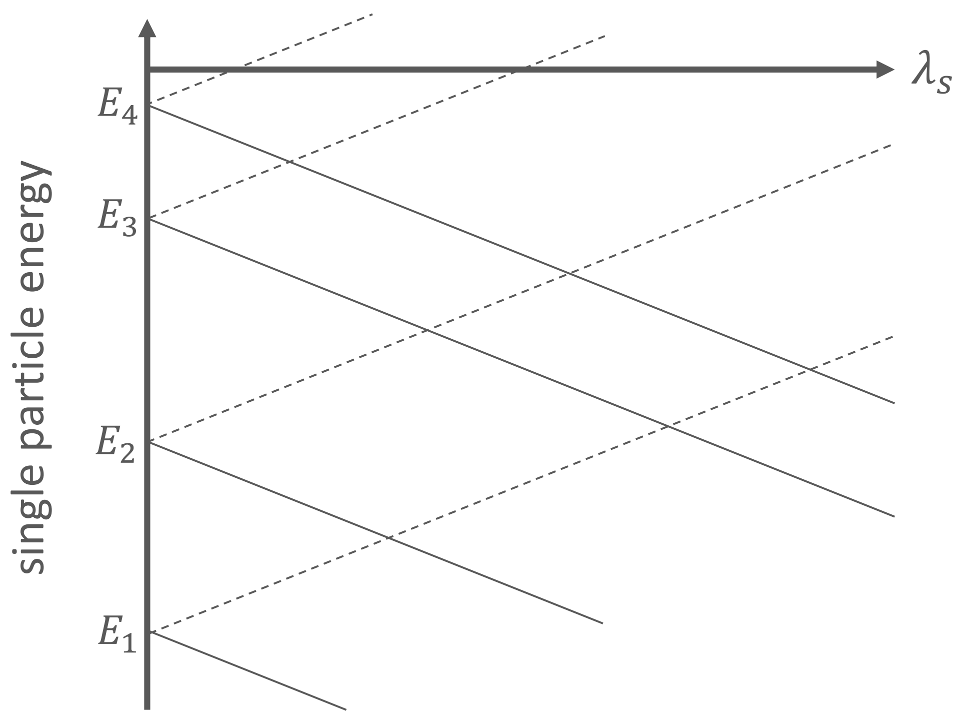
HF calculation and the result

$$\delta\langle\Phi|H-\lambda_s\hat{S}|\Phi\rangle = 0$$

$$a_k^\dagger = \sum_j D_{jk}\, c_j^\dagger \qquad a_k|\Phi\rangle = 0$$

h'	eigenvector	eigenvalue
$h-\lambda_s s_k 1$	D_{ik}	$E_k^{\lambda_s=0} - \lambda_s s_k$
$h+\lambda_s s_k 1$	$D_{i\bar{k}}$	$E_{\bar{k}}^{\lambda_s=0} + \lambda_s s_k$



HF calculation and the result

$$\delta\langle\Phi|H-\lambda_s\hat{S}|\Phi\rangle = 0$$

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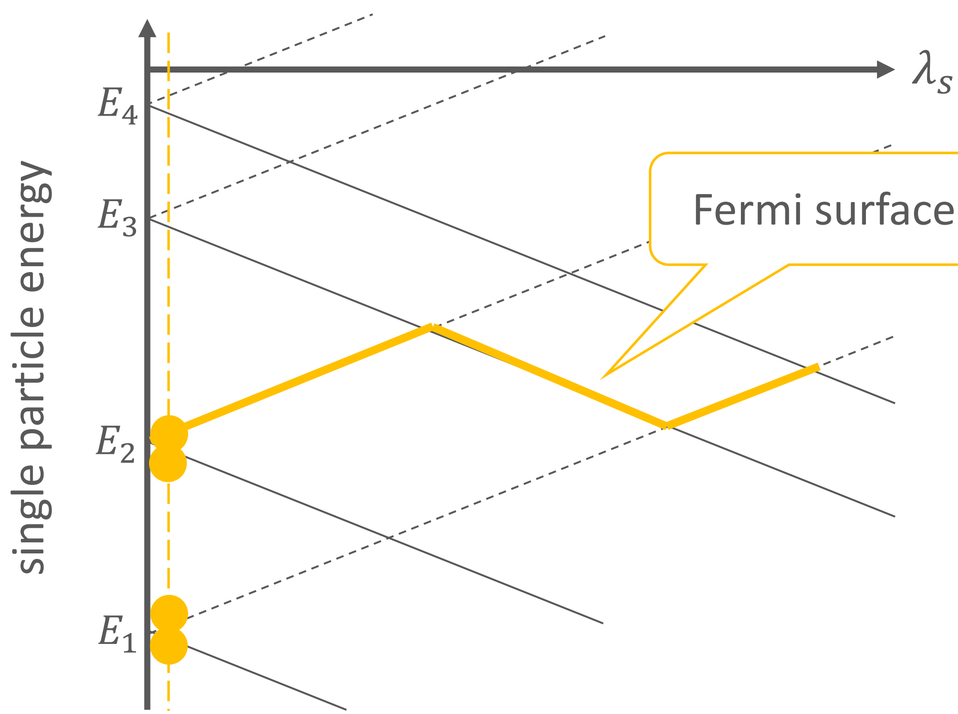

HF calculation and the result

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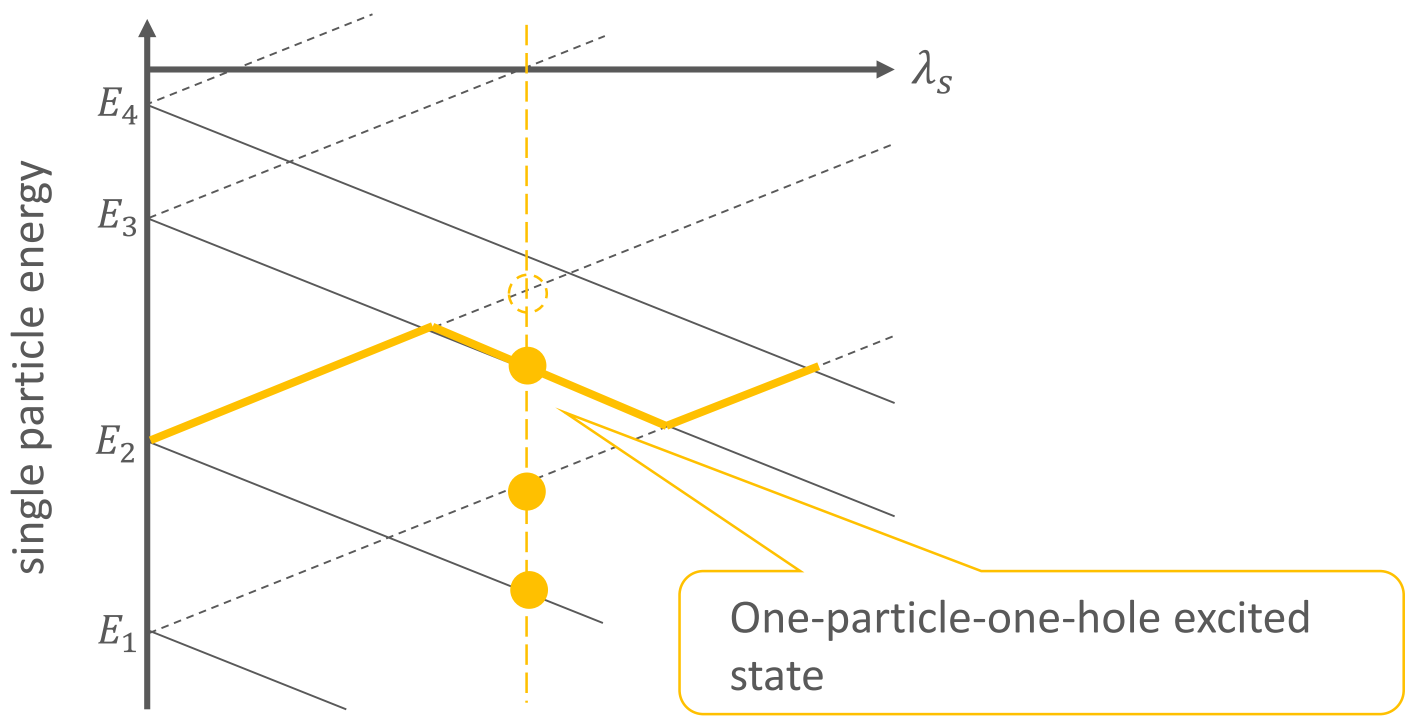


HF calculation and the result

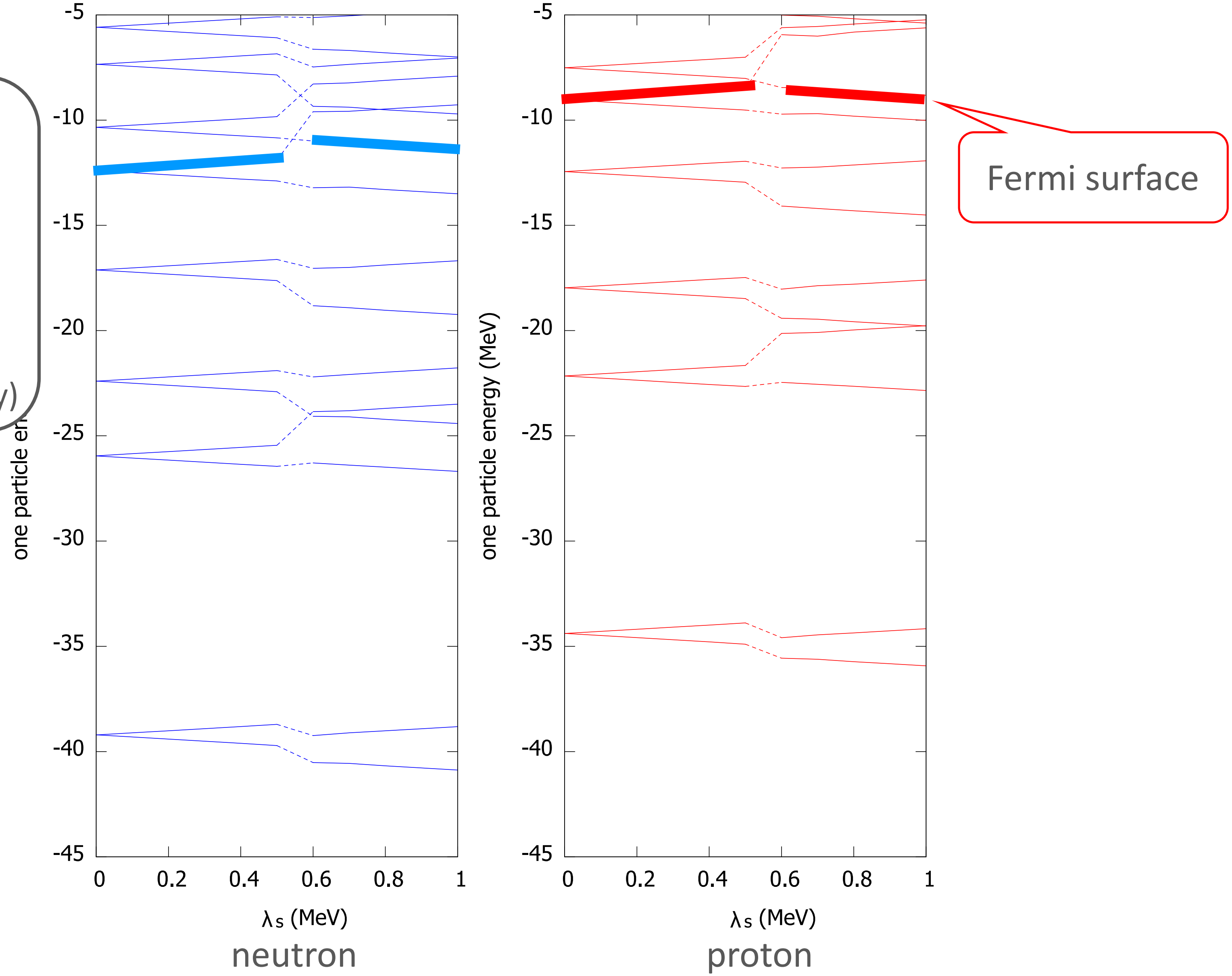
^{20}Ne

Symmetry

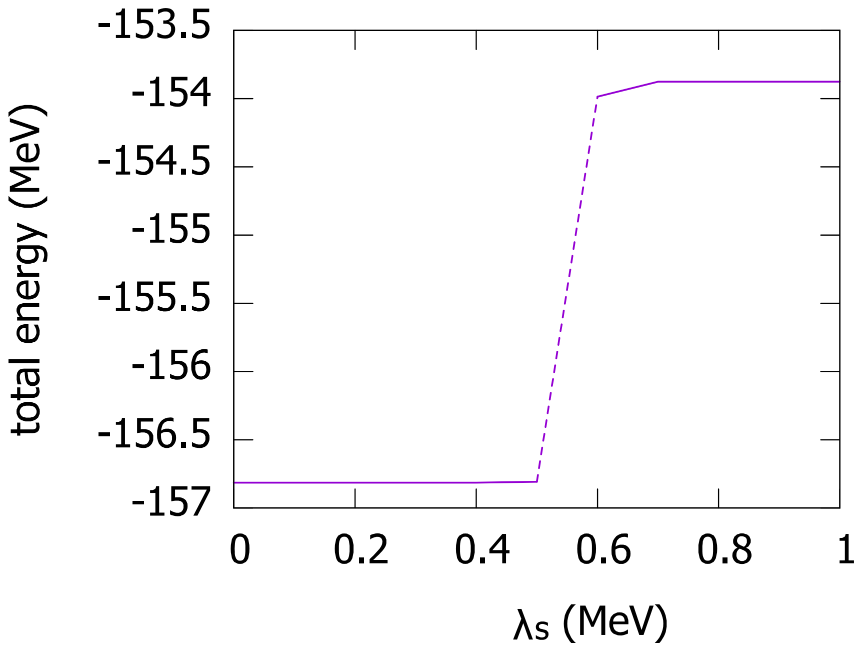
Axial
Space reflection

$$\hat{s} = iPe^{-i\pi J_z}$$

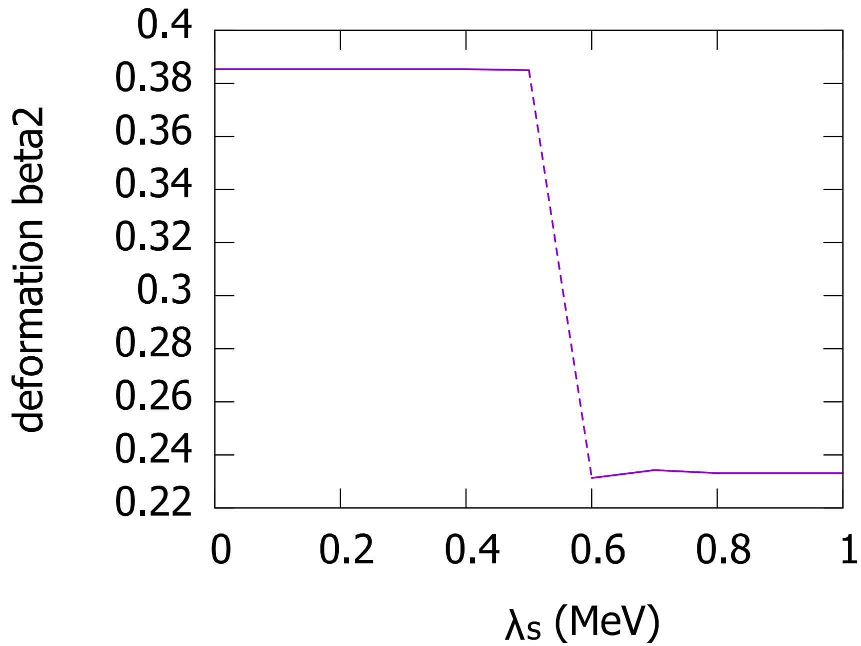
(P:parity)



HF calculation and the result



Total energy



Quadrupole deformation

The structure has changed around $\lambda_s \sim 0.5$ MeV.

Conclusion

Summary

1. In the HFB theory odd-mass nuclei are conventionally treated as the "excited state" on the neighbor even-even nuclei.
2. A constraint related to the symmetry of the system can make an odd-particle system the vacuum.
3. HF calculation result with the constraint suggests that the structure of the nucleus has changed.

Future

1. HFB calculation with the constraint and the systematic study of odd-mass nuclei
2. Application to the many-quasiparticle excited state such as high-K isomer

My HF(B) code

Base	$\|\boldsymbol{r}\sigma\tau\rangle$
Symmetry	Axial, Space reflection
Interaction	Skyrme (SLy4)
Initial state	Nilsson (Non-isotropic HO+LS+ℓ^2)

$iPe^{-i\pi J_z}$ is taken as $\hat{s}$

Calculation result on $^{20}\mathrm{Ne}$

	HFBTHO	My code
total B.E. (MeV)	-157.1	-156.2
deformation β_2	0.387	0.385
neutron rms radius (fm)	2.901	2.893
proton rms radius (fm)	2.929	2.921

Skyrme EDF

$$\langle\Phi|H|\Phi\rangle = \int d\boldsymbol{r}\, H(\boldsymbol{r})$$

$$H(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\boldsymbol{r}) + \mathcal{H}_1(\boldsymbol{r})$$

$$\rho_0 = \rho_n + \rho_p$$

$$\rho_1 = \rho_n - \rho_p$$

$$\mathcal{H}_t(\boldsymbol{r}) = \mathcal{H}_t^{\text{even}}(\boldsymbol{r}) + \mathcal{H}_t^{\text{odd}}(\boldsymbol{r})$$

$$\mathcal{H}_t^{\text{even}}(\boldsymbol{r}) = C_t^{\rho}\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J}J_t^2 + C_t^{\nabla J}\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t$$

$$\mathcal{H}_t^{\text{odd}}(\boldsymbol{r}) = C_t^{s}\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C_t^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\nabla j}\boldsymbol{s}_t\cdot(\boldsymbol{\nabla}\times\boldsymbol{j}_t)$$

$$\rho_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\langle\sigma'|1|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\rho(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = \left\langle\Phi\middle|c^\dagger_{\boldsymbol{r}'\sigma'\tau'}c_{\boldsymbol{r}\sigma\tau}\middle|\Phi\right\rangle$$

$$\boldsymbol{s}_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\langle\sigma'|\boldsymbol{\sigma}|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\tau_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \{\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|1|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\boldsymbol{T}_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \{\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|\boldsymbol{\sigma}|\sigma\rangle\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$\boldsymbol{j}_q(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \frac{1}{2i}\{(\boldsymbol{\nabla} - \boldsymbol{\nabla}')\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|1|\sigma\rangle\,\delta(\boldsymbol{r}' - \boldsymbol{r})$$

$$J_{q\,\mu\nu}(\boldsymbol{r}) = \int dr' \sum_{\sigma\sigma'} \frac{1}{2i}\{(\nabla_\mu - \nabla'_\mu)\rho(\boldsymbol{r}\sigma q, \boldsymbol{r}'\sigma' q)\}\langle\sigma'|\sigma_\nu|\sigma\rangle\,\delta(\boldsymbol{r}' - \boldsymbol{r})$$