On the non-Unitarity of the Bogoliubov Transformation due to the Quasiparticle Space Truncation

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Collaboration:

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Pairing (I)

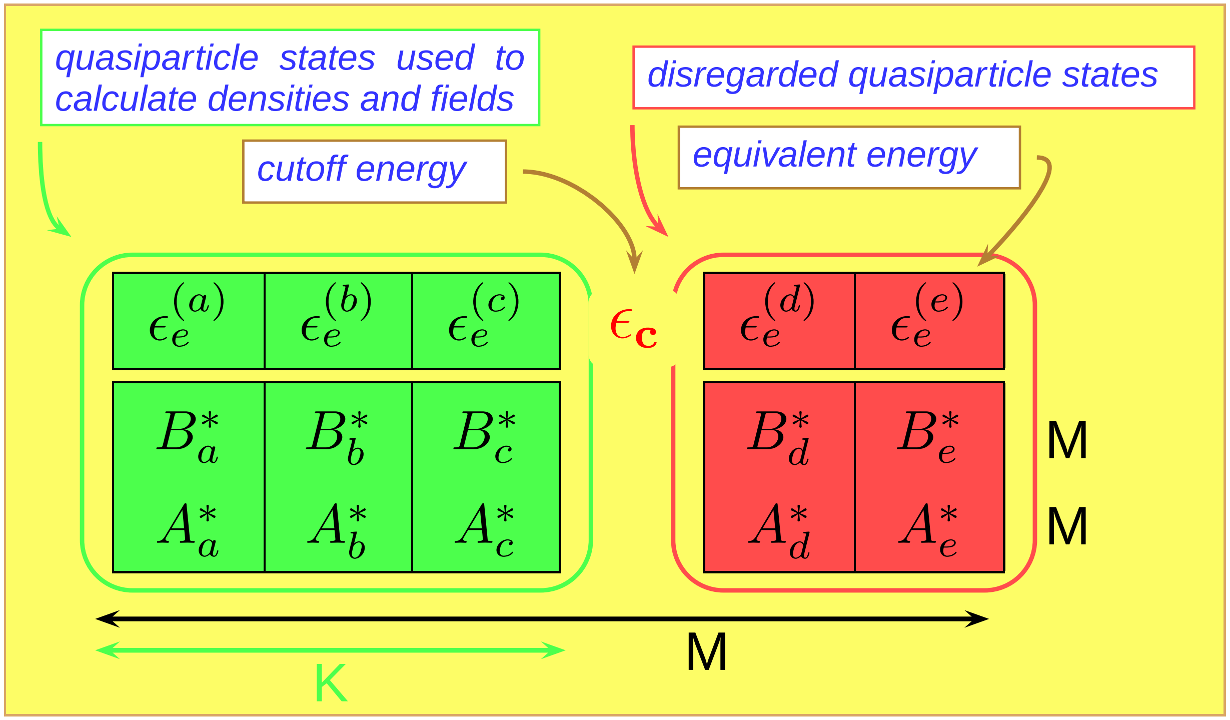
The *density dependent delta* pairing interaction, usually used in the Skyrme-HFB calculations:

$$V_p(\vec{r}, \vec{r}') = V_0 \left(1 - \boxed{\chi} \frac{\rho(\vec{r})}{\rho(0)}\right) \boxed{\delta(\vec{r} - \vec{r}')}$$

$\chi = 0$ *volume pairing*

$\chi = 1/2$ *mixed pairing*

zero range in the coordinate space corresponds to infinite range in the momentum space



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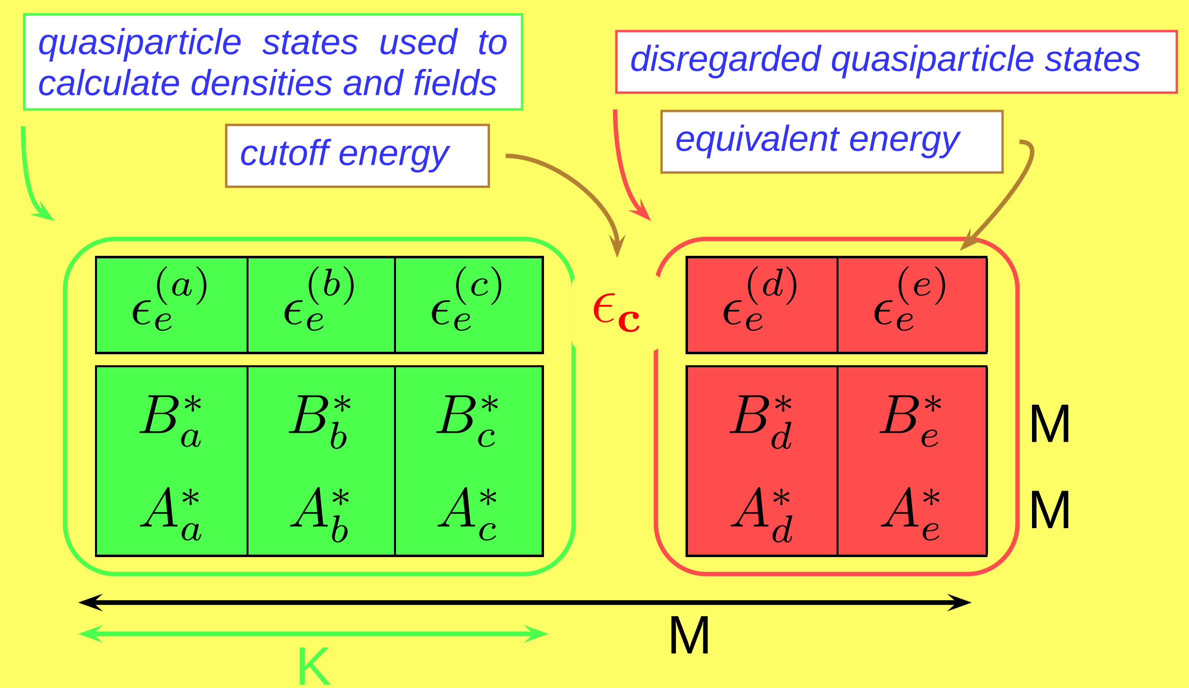


PROBLEMS:

1. pairing renormalization scheme
2. unitarity of the Bogoliubov transformation

Pairing (II)

Skyrme density functional is a sum of two terms:

$$
\begin{aligned}
E[\rho, \kappa] &= E_{Sk}[\rho] + E_{pairing}[\kappa], \\
\rho &= B^* B^T, \\
\kappa &= B^* A^T.
\end{aligned}
$$

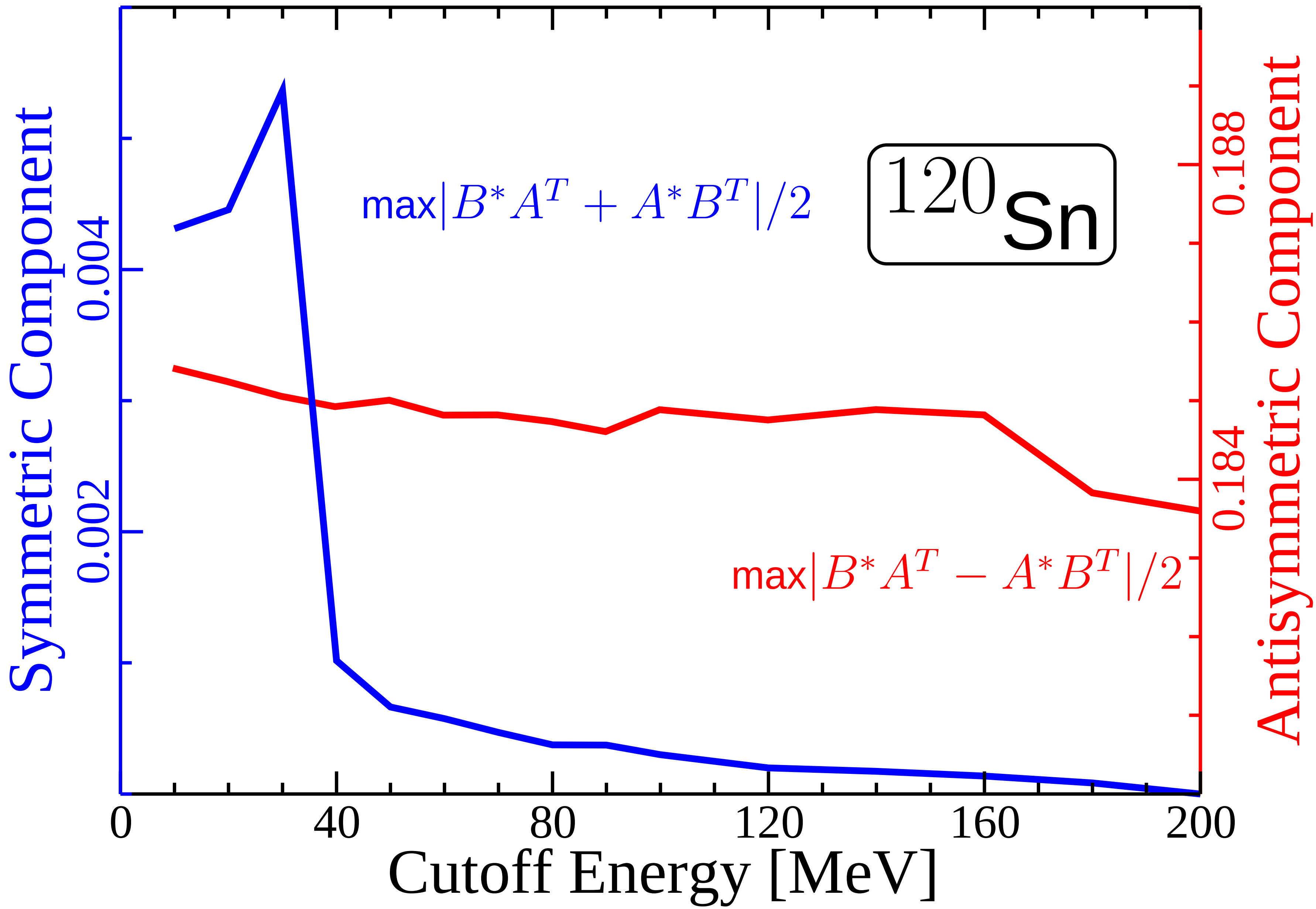
Unitarity of the Bogoliubov transformation guarantees that:

- ρ is hermitian — *density matrix*
- κ is antisymmetric — *pairing tensor*

The energy cutoff procedure does not affect ρ significantly, since removed states correspond to very small singular values of B. However, since

$$v_{Ai}^2 + v_{Bi}^2 = 1,$$

repercussions of the cutoff for κ are more severe: the pairing tensor is no longer antisymmetric, but it develops a finite symmetric part. Usually one disregards this symmetric part in the HFB calculations.


max$|B^*A^T + A^*B^T|/2$
^{120}Sn
max$|B^*A^T - A^*B^T|/2$
Symmetric Component
0.002
0.004
Antisymmetric Component
0.184
0.188
0
40
80
120
160
200
Cutoff Energy [MeV]

Antisymmetricity of the Pairing Tensor

However, the smallness of symmetric component of the pairing tensor may be deceiving:

- In EDF approach densities ρ and κ are independent dynamical variables.
- In HFB generalized density matrix $\mathcal{R}$ must be projective.

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} \longleftarrow$$

constrain within HFB theory

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- Antisymmetricity of the pairing tensor is a result of fermionic commutation relations for particle and quasiparticle operators.

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- Antisymmetricity of the pairing tensor is a result of fermionic commutation relations for particle and quasiparticle operators.

Therefore, symmetric component of the pairing tensor is not just a minor disturbance to be discarded.

The Background of the Method

We propose a method of restoring the unitarity by introducing a truncated single-particle Hilbert space, in which the HFB equations are to be solved.

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We propose a method of restoring the unitarity by introducing a truncated single-particle Hilbert space, in which the HFB equations are to be solved.

- We want to fi nd a new particle basis, in which the truncated (B_i^*, A_i^*) HFB results are best reproduced.
- There are two sets of K vectors to be expanded in (B^*, A^*).

A **singular value decomposition** of an $(M \times N)$, $M \geq N$ matrix A is any factorization of the form

$$A = SVD^T,$$

where S $(M \times M)$, D $(N \times N)$ are orthogonal matrices and V $(M \times N)$ is a diagonal matrix with matrix elements $v_i = V_{ii} \geq 0$.

SVD matrices

- ❋ D^T rotates to the 'singular' reference frame
- ❋ V 'stretches' vectors by the factor of corresponding singular values v_i
- ❋ S rotates the reference frame

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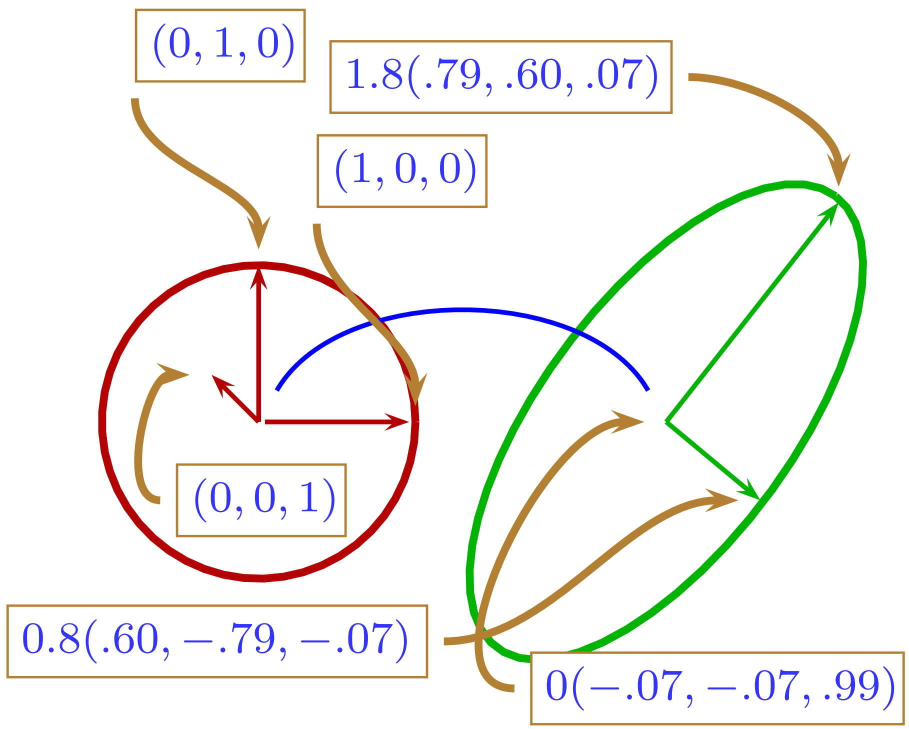
Example:

$$\underbrace{\begin{bmatrix} 1.24 & .85 \\ .14 & 1.25 \\ -.12 & -.07 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} .79 & .60 & .07 \\ .60 & -.79 & -.07 \\ -.07 & -.07 & .99 \end{bmatrix}}_{S} \times \underbrace{\begin{bmatrix} 1.8 & 0 \\ 0 & .8 \\ 0 & 0 \end{bmatrix}}_{V} \underbrace{\begin{bmatrix} .6 & .8 \\ .8 & -.6 \end{bmatrix}}_{D^T}$$



SVD is a convenient method of orthogonalization of a set of vectors. In a M-dimensional space:

- SVD of two sets of K orthogonal vectors, one proportional to each other (i.e. BCS), gives K 'singular' states corresponding to non-zero singular value.

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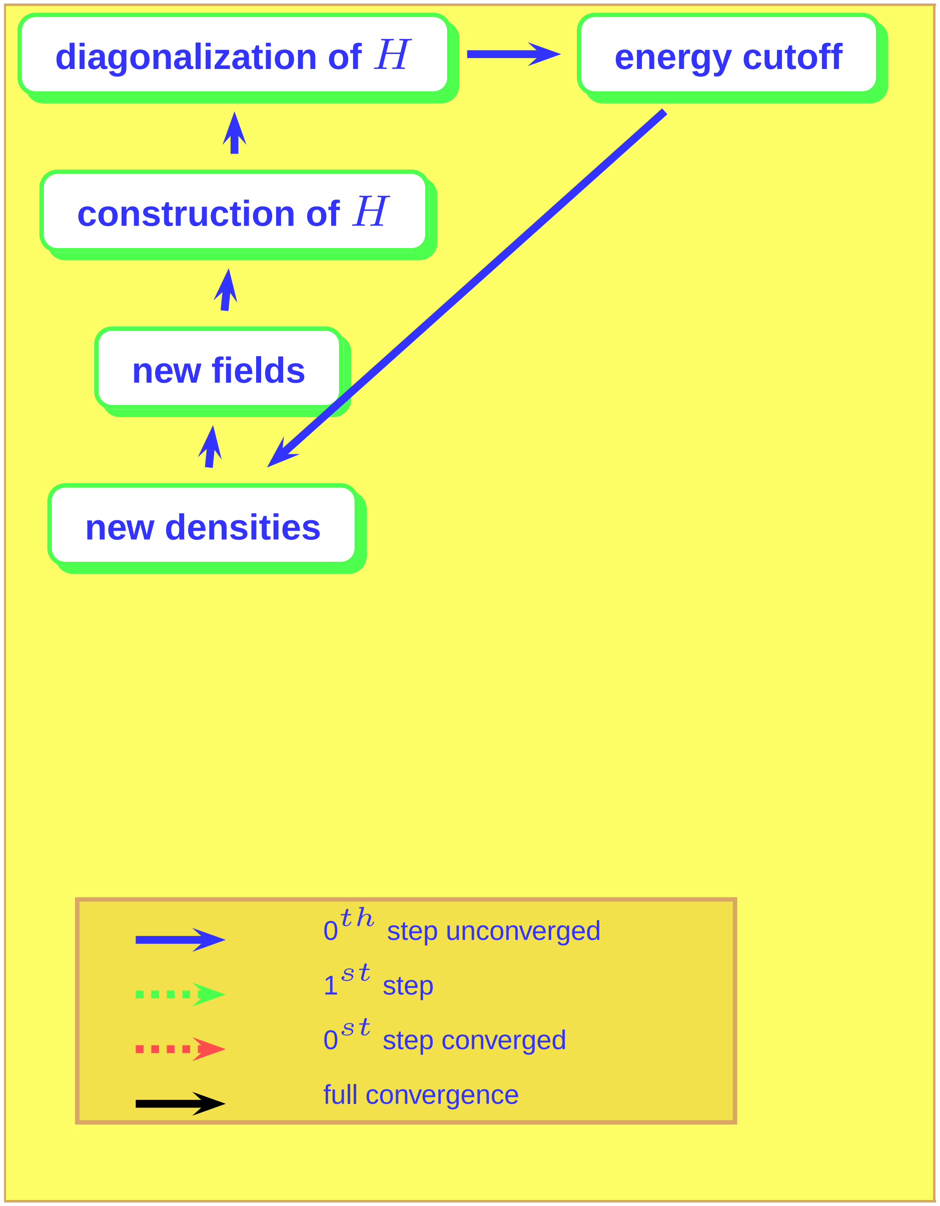
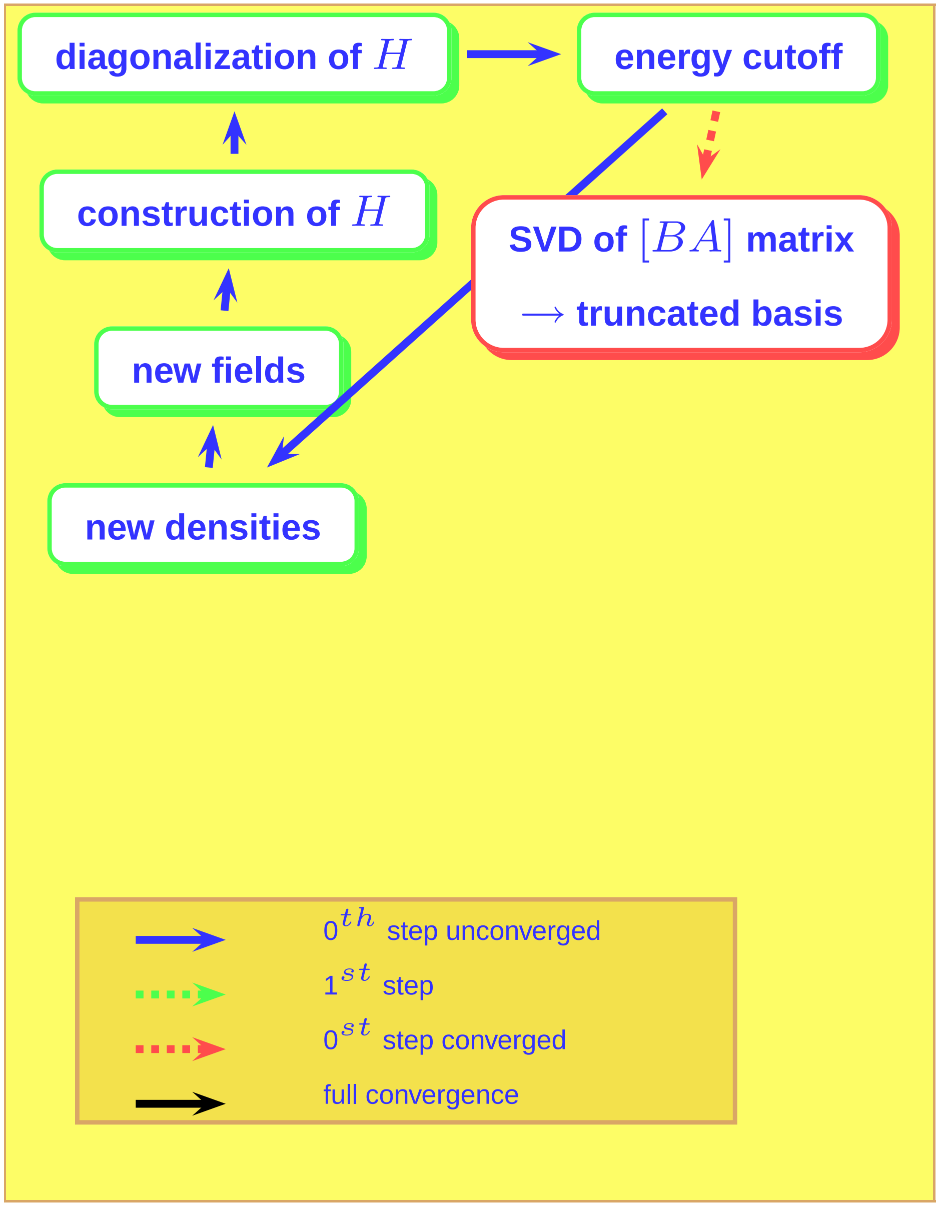
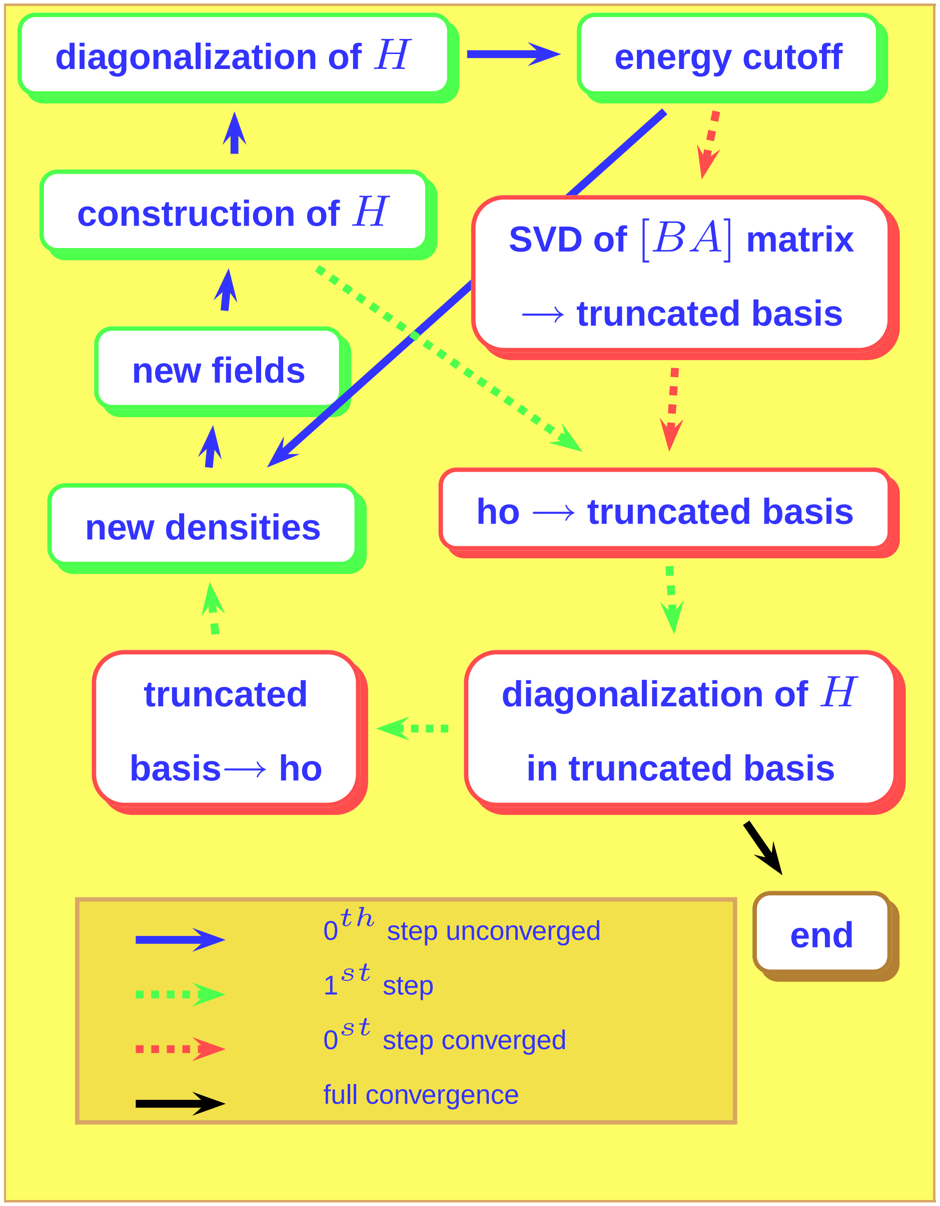
- SVD of A, B matrices is more general than the Bloch-Messiah decomposition.
- Gives canonical basis with higher precision than the diagonalization of ρ.

Method

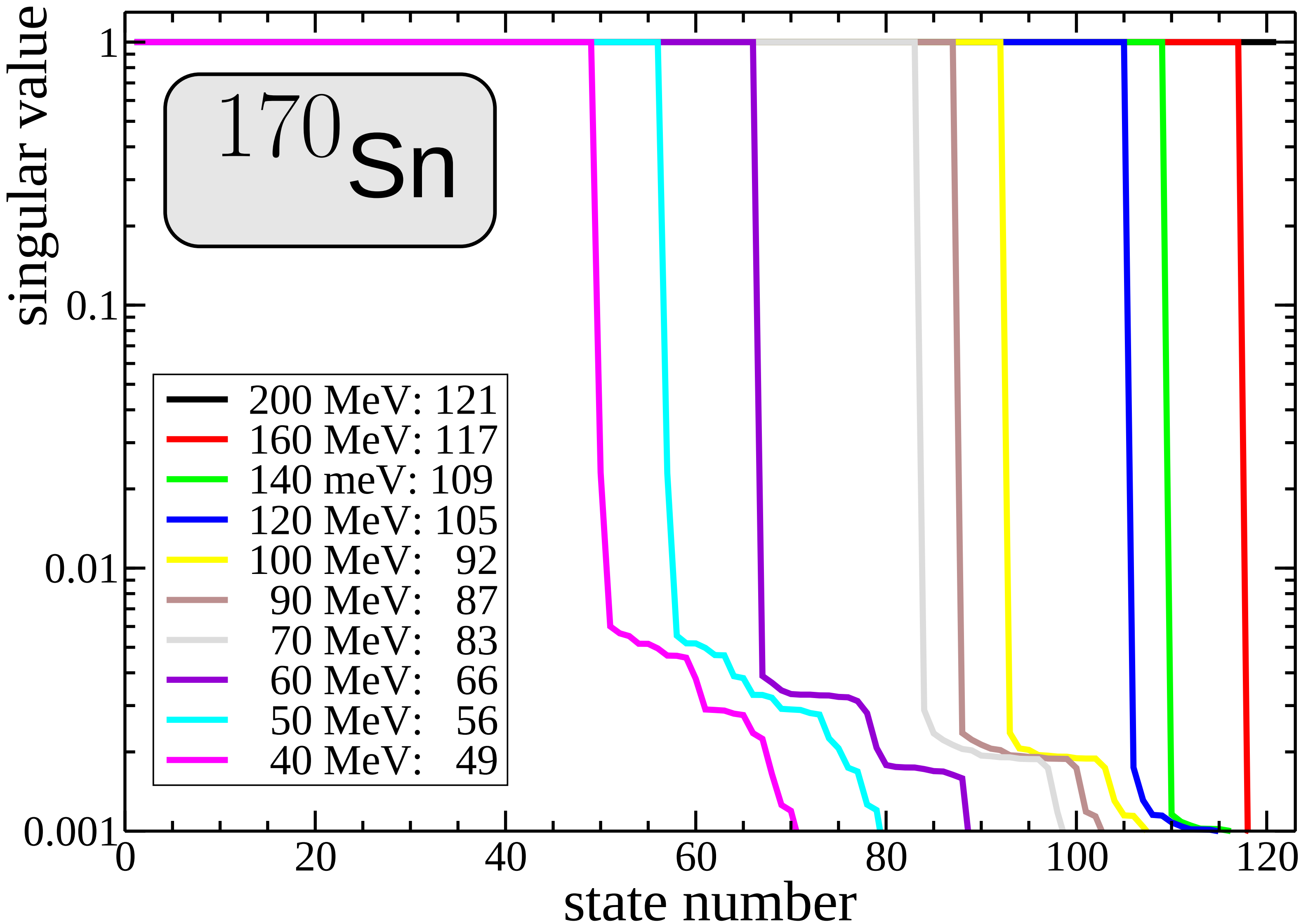

diagonalization of H
energy cutoff
construction of H
new fields
new densities
0^{th} step unconverged
1^{st} step
0^{st} step converged
full convergence


diagonalization of H
energy cutoff
construction of H
SVD of $[BA]$ matrix
$\longrightarrow$ truncated basis
new fields
new densities
0^{th} step unconverged
1^{st} step
0^{st} step converged
full convergence



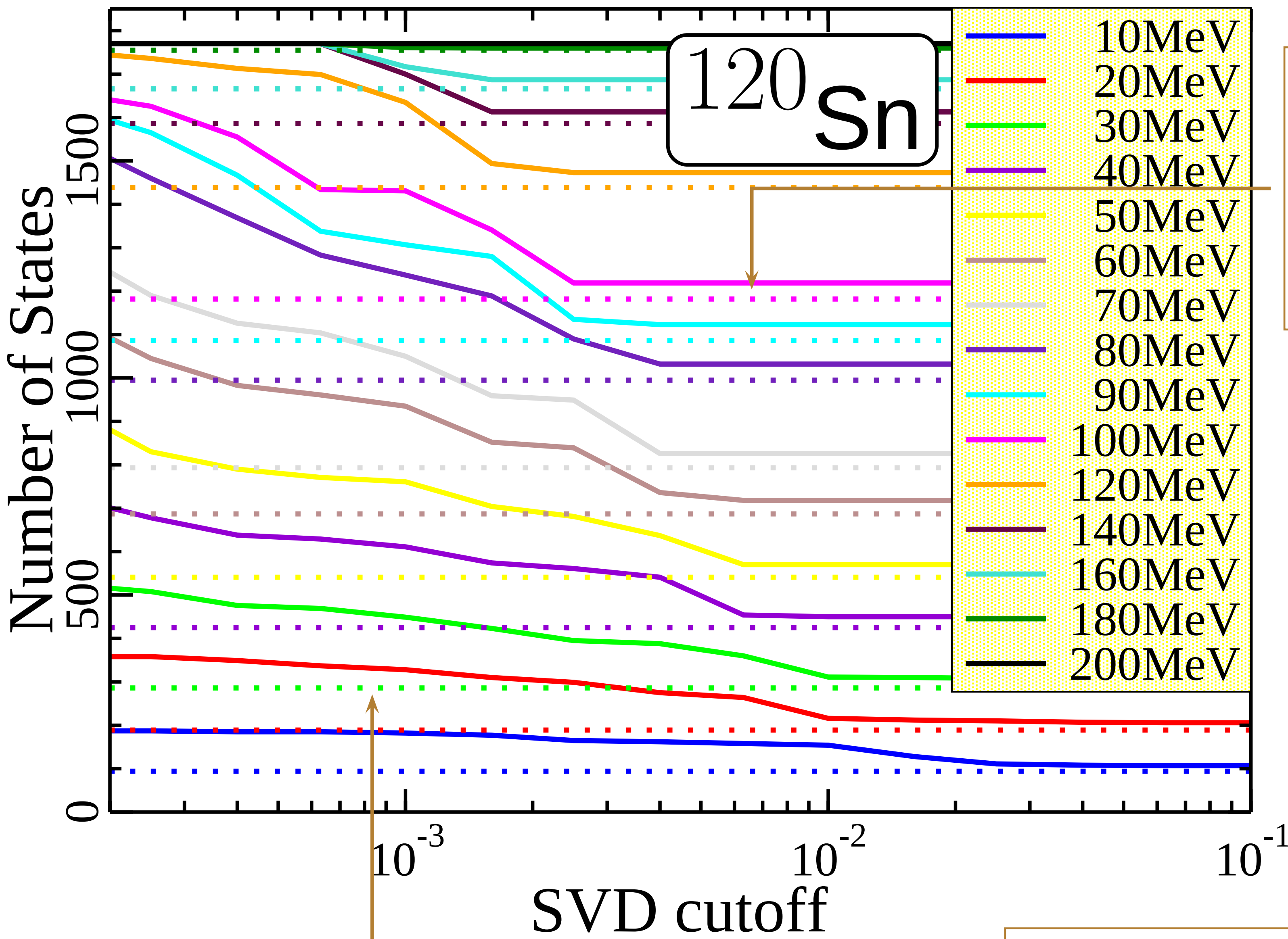
- \+ step 0^{th} generates input for step 1^{st} - parameters are easy to adjust
- \+ the dimensionality of the problem may be reduced by the consistent use of the 'truncated' basis in step 1^{st}
- \+ self-consistent minimalization in a given truncated basis - variational method
- \- 'singular' basis may not be self-consistent with the final solution

Singular Values of $[B^*A^*]$ - example



Singular values of $[B^*A^*]$ in $1/2^+$ block for neutrons in ^{170}Sn.

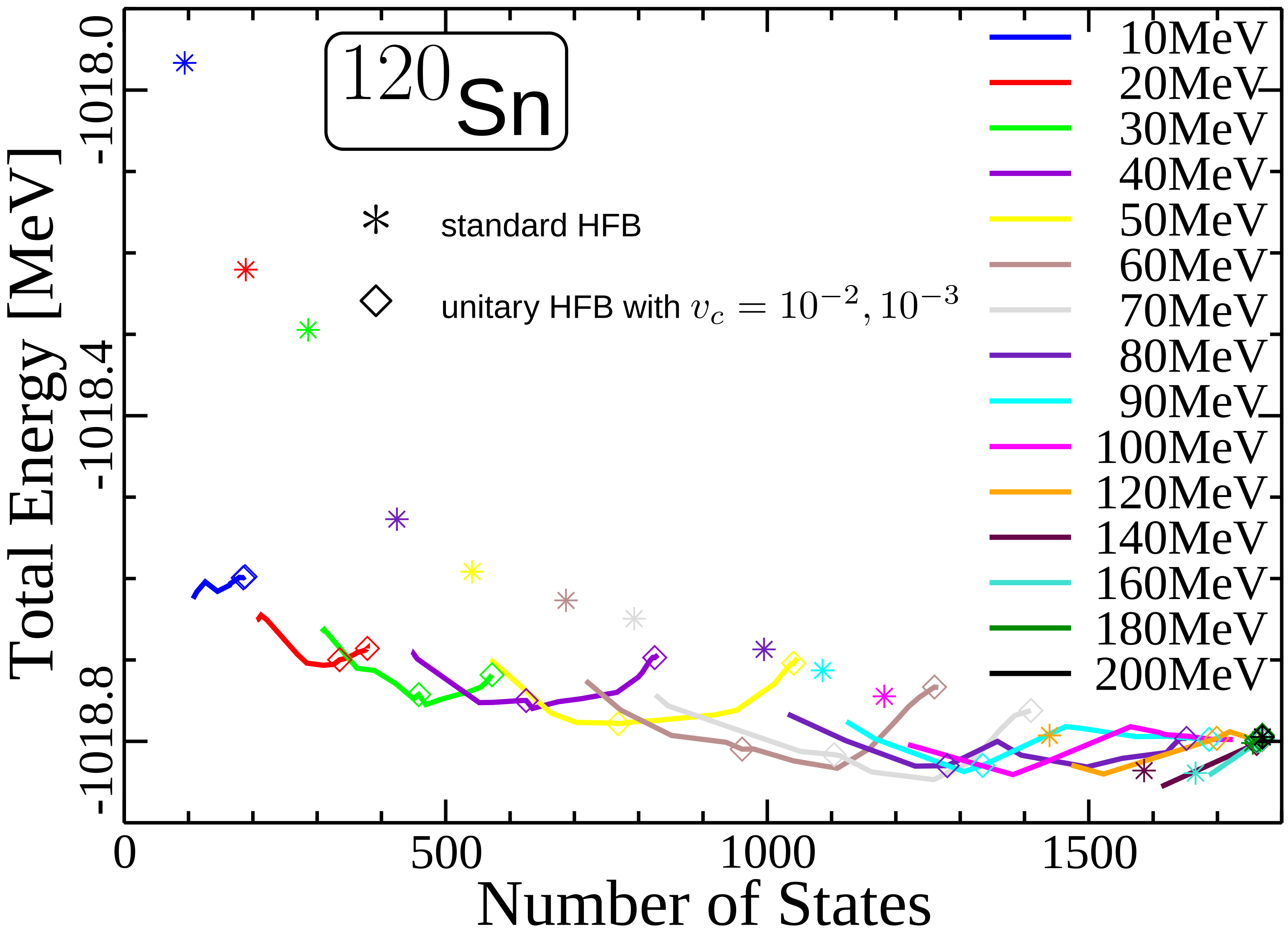
Particle Space Truncation - Results (I)



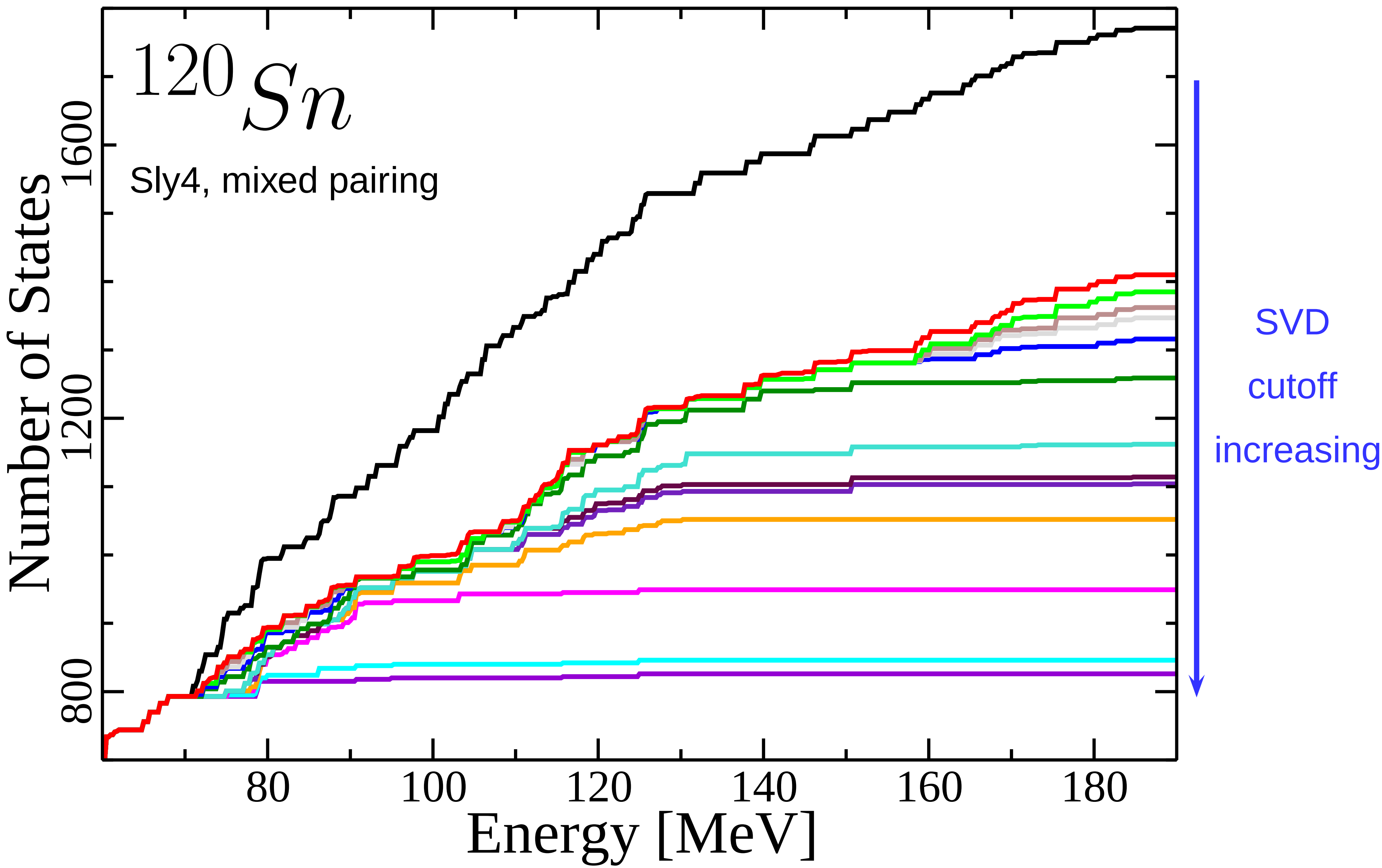
minimal number of states - close to BCS limit $B^* \sim A^*$

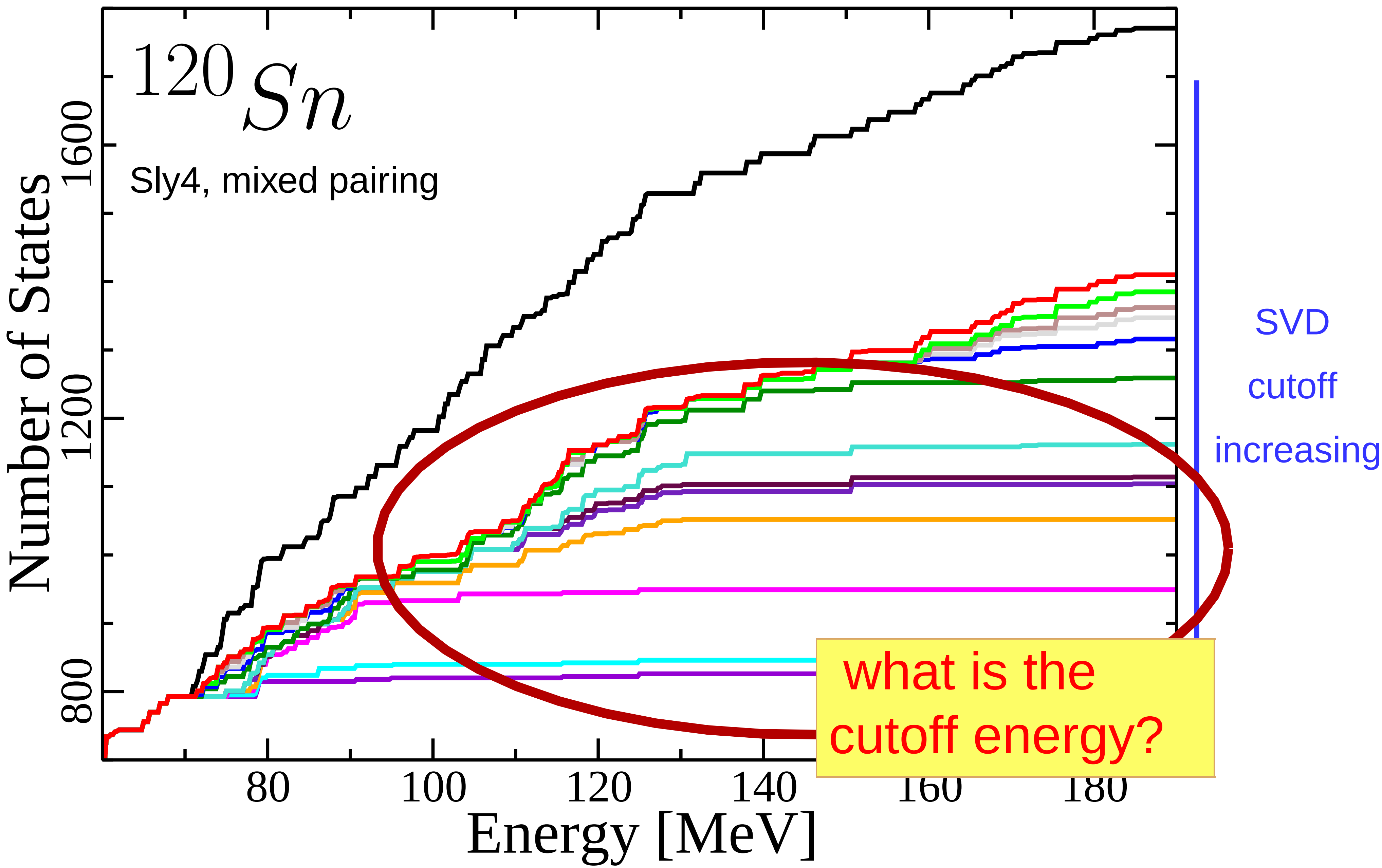
more states - more redundancy

Particle Space Truncation - Results (II)



Regularization in Truncated Space




^{120}Sn
Sly4, mixed pairing
Number of States
800
1200
1600
80
100
120
140
160
180
Energy [MeV]
SVD
cutoff
increasing
what is the
cutoff energy?