Deformed Coordinate-Space HFB: Finite-Temperature Fission Barriers

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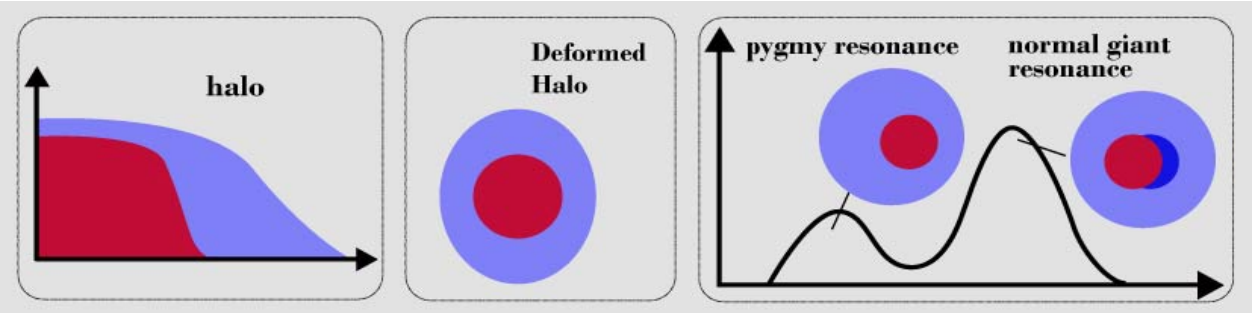
MSU, Nov. 21, 2008

OAK RIDGE National Laboratory

Outline

Purpose of Coordinate-Space HFB-AX



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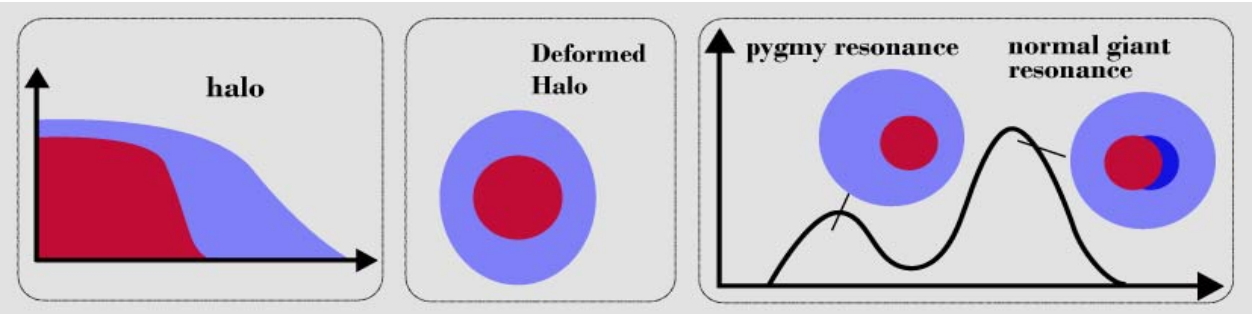

- Correct treat the surface properties and better convergence: halo structure, deformed halo, hot nuclei
- Provide better input for HFB+QRPA: pygmy resonance
- A general purpose tool for nuclear, atomic systems: Skyrme, Gogny, SLDA
- Large scale calculation utilizing the new generation computer

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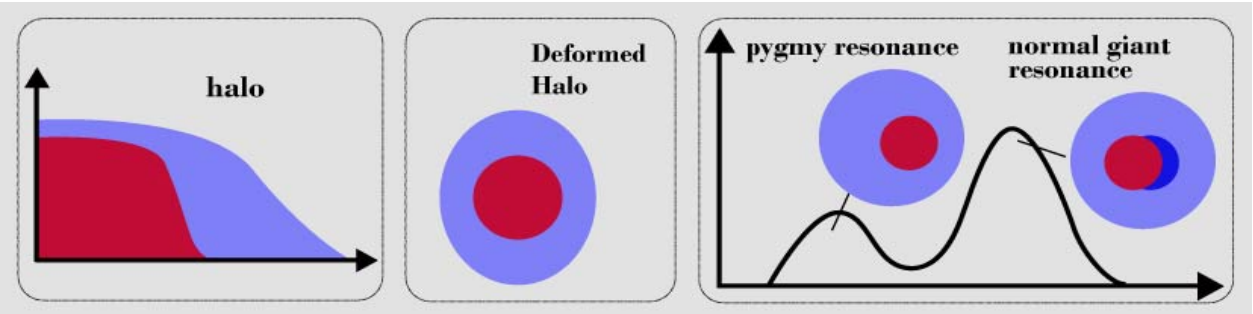

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HFB codes based on HO basis expansion

HFB codes based on HO basis (have been strictly tested):

1. 2D HFB-THO
   - based on transformed HO basis to improve the description of drip-line nuclei
   - very efficient in calculating the whole mass table

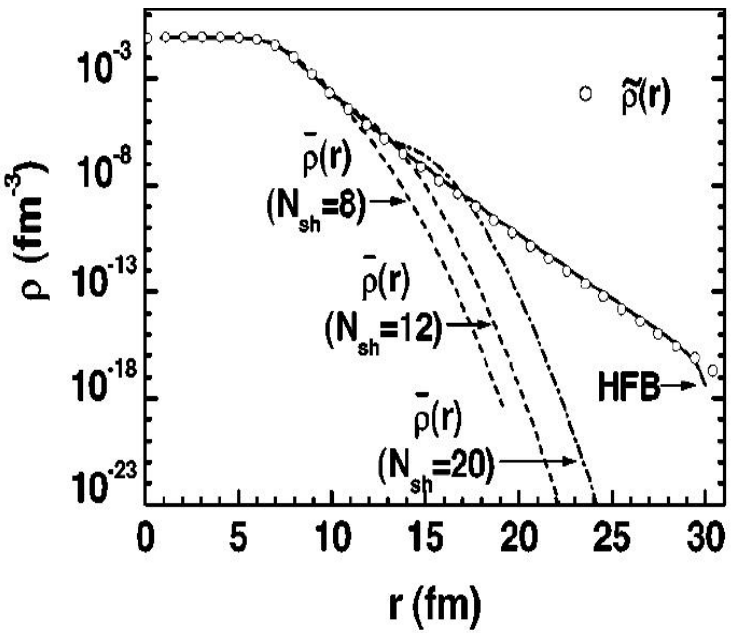
   M.V. Stoitsov, J. Dobaczewski, W. Nazarewicz, P. Ring, Comp. Phys. Commun. **167**, *43(2005).*

2. 3D HFODD
   - based on 3D Cartesian HO basis
   - proper code to calculate the asymmetric and triaxial fission paths
   - time-reversal symmetry broken

   J. Dobaczewski and P. Olbratowski, Comp. Phys. Commun., **167**, *214(2004)*

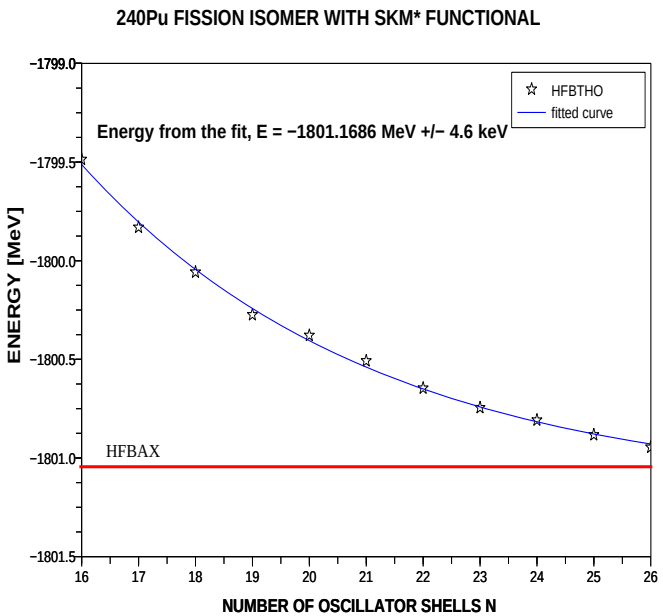
Advantages of Coordinate-Space HFB codes

Gauss-type vs exponential asymptotics:



M. Stoitsov, PRC, 2003

Convergence of HO basis:



plot by N. Nikolov

Various Coordinate-Space HFB codes

1. 1D HFBRAD: finite-difference method
   standard tool for benchmarking others codes at spherical cases
   K. Bennaceur, and J. Dobaczewski, Compt. Phys. Comm. **168**, *96 (2005).*
2. 2D HFB-Lattice: B-spline direct diagonalization method
   useful for studying deformation at drip-lines but very time consuming *E. Terán, V.E. Oberacker, and A.S. Umar, Phys. Rev. C* **67**, *064314 (2003).*
3. 2D HFB-AX: B-spline direct diagonalization method
   numerical optimized to be as fast as HFODD; parallel; accurate
   J.C. Pei, M.V. Stoitsov, G. I. Fann, W. Nazarewicz, N. Schunck, and F.R. Xu, arXiv:0807.3036
4. 3D HFB
   two-basis method: *B. Gall, P.Bonche, J. Dobaczewski, et al. Z. Phys. A 348, 183(1994)*
   canonical basis: *N. Tajima, Physical Review C, vol.69, 034305 (2004)*
5. 3D Madness-HFB: adaptive multi-resolution wavelets
   error is controllable; spin-orbit has been implemented
   3D HFB is still in progress (succeed for fixed potential recently)
   G.I. Fann, R.J. Harrison, G. Beylkin, J. Jia, R. Hartman-Baker, W.A. Shelton, and S. Sugiki, J. Phys. Conf. Ser. **78**, *012018 (2007)*

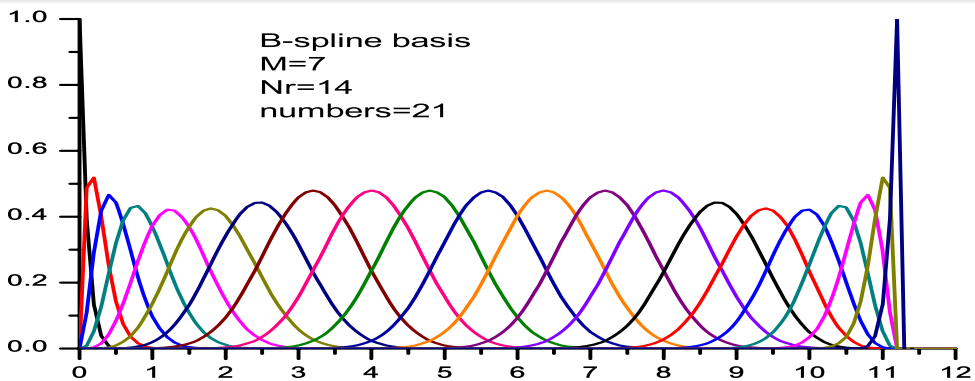
B-Spline techniques

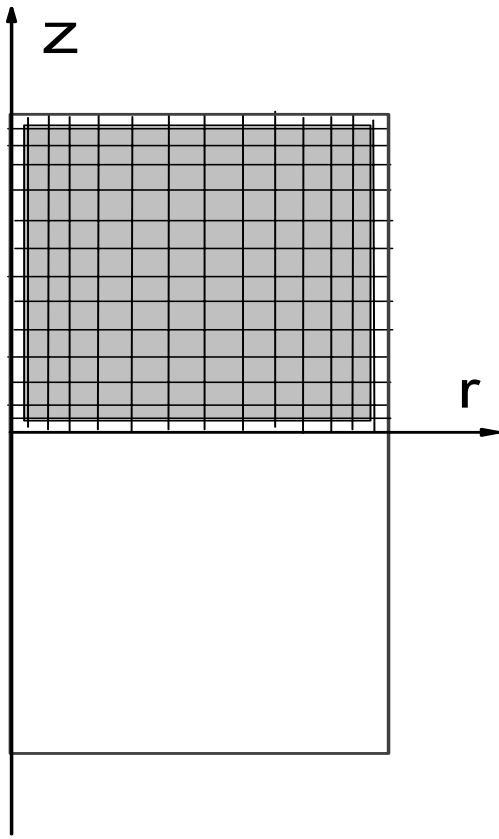
In HFBAX, the wave functions are discretized on a 2D grid (r_α, z_β) with the M-order B-splines:

$$\psi^{(1,2)}_{n\Omega^\pi q}(\rho_\alpha, z_\beta) = \sum_{i,j} B^M_i(\rho_\alpha) B^M_j(z_\beta) C^{ij(1,2)}_{n\Omega^\pi q},$$

where C^{ij} is the matrix of expansion coefficients; $\alpha = 1, \ldots, N_\rho$ and $\beta = 1, \ldots, N_z$.

The mesh point numbers:
$N_z = N_\rho = \frac{R}{h} + (M-1) - 2$, for a box of size R, max mesh size h, and M-order B-Splines.





Operators

Define matrix from Galerkin method:

$$\mathcal{O}(kl,ij) = \int v(r,z)B_k(r)B_l(z)\mathcal{O}B_i(r)B_j(z)drdz$$
$$G(kl,ij) = \int v(r,z)B_k(r)B_l(z)B_i(r)B_j(z)drdz$$

Operators $[\frac{\partial}{\partial r}, \frac{\partial}{\partial z}, \frac{\partial^2}{\partial r^2}, \frac{\partial^2}{\partial z^2}]$ are constructed with boundary conditions:

$$\mathcal{O}^{\alpha\beta}_{\delta\gamma} = \sum_{ij,kl,i'j'} \tilde{B}^r_{\delta i'} \tilde{B}^z_{\gamma j'} G^{i'j',kl} \mathcal{O}_{kl,ij} \tilde{B}^{\alpha i}_r \tilde{B}^{\beta j}_z$$

HFB equation becomes:

$$\sum_{\alpha\beta} \mathcal{H}^{\alpha\beta}_{\delta\gamma} f_{\alpha\beta} = g_{\delta\gamma}$$

We diagonalize the operators (non-symmetric), not actually the Hamiltonian matrix $< \psi_i|H|\psi_j >$ like the basis expansion method.

Diagonalization Speedup

- Instead of diagonalizing the full HFB matrix, it is equivalent to diagonalize half of the matrix:

$$\begin{pmatrix} (h-\lambda+i\tilde{h})(h-\lambda-i\tilde{h}) & 0 \\ 0 & (-h+\lambda+i\tilde{h})(-h+\lambda-i\tilde{h}) \end{pmatrix} \begin{pmatrix} U' \\ V' \end{pmatrix} = E_\alpha^2 \begin{pmatrix} U' \\ V' \end{pmatrix}$$

- The resulting energy spectrum can be several GeV. We want an energy cut-off in LAPACK. For non-symmetric matrix: Hessenberg form–>eigenvalues–>eigenvectors (selection cutoff)

Broyden method

The convergence estimation:

$$\boldsymbol{F}^{(m)} = \boldsymbol{V}_{out}^{(m)} - \boldsymbol{V}_{in}^{(m)},$$

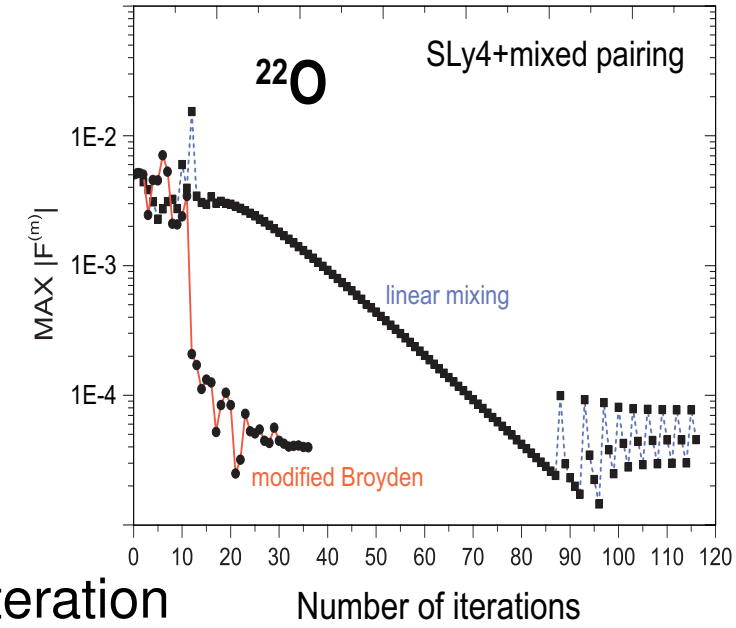
The linear mixing:

$$\boldsymbol{V}_{in}^{(m+1)} = \boldsymbol{V}_{in}^{(m)} + \alpha \boldsymbol{F}^{(m)},$$

The Broyden mixing:

$$\boldsymbol{V}_{in}^{(m+1)} = \boldsymbol{V}_{in}^{(m)} + \mathrm{B}^{(m)} \boldsymbol{F}^{(m)},$$

$\mathrm{B}^{(m)}$ is a matrix that includes several previous iteration information.



Andrzej Baran, et al. Phys. Rev. C 78, 014318 (2008)

In HFB-AX,

$$\boldsymbol{V} \equiv \left\{ \rho_q, \tau_q, \boldsymbol{\nabla} \cdot \mathbf{J}_q, \tilde{\rho}_q, \nabla^2 \rho_q, \nabla_\rho \rho_q, \nabla_z \rho_q \right\}.$$

^{120}Sn

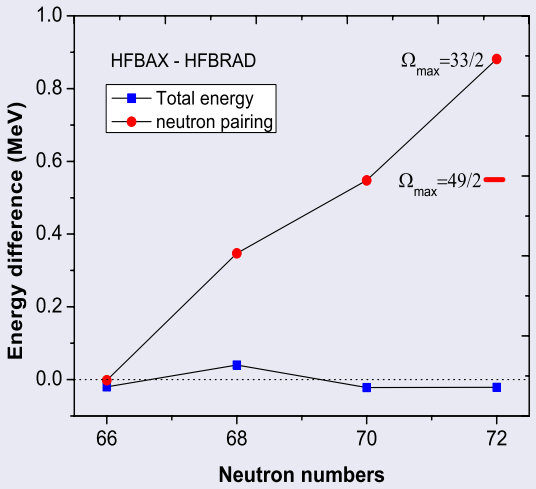
(MeV)	HFB-AX h=0.6	HFBRAD h=0.1	HFBTHO N_{sh}=25
E_{tot}	−1018.795	−1018.791	−1018.777
E_C	347.442	347.400	347.370
E^p_{kin}	830.856	830.848	830.735
E^n_{kin}	1340.675	1340.668	1340.458
E^n_{pair}	−12.491	−12.467	−12.467
$\tilde{E}^n_{kin}$	1328.184	1328.201	1327.991
Δ_n	1.2448	1.2446	1.2447
λ_n	−8.0186	−8.0181	−8.0168

The renormalized kinetic energy $\tilde{E}_{kin} = E_{kin} + E_{pair}$ is less sensitive to the actual discretization of quasi-particle continuum.

Ni isotopes

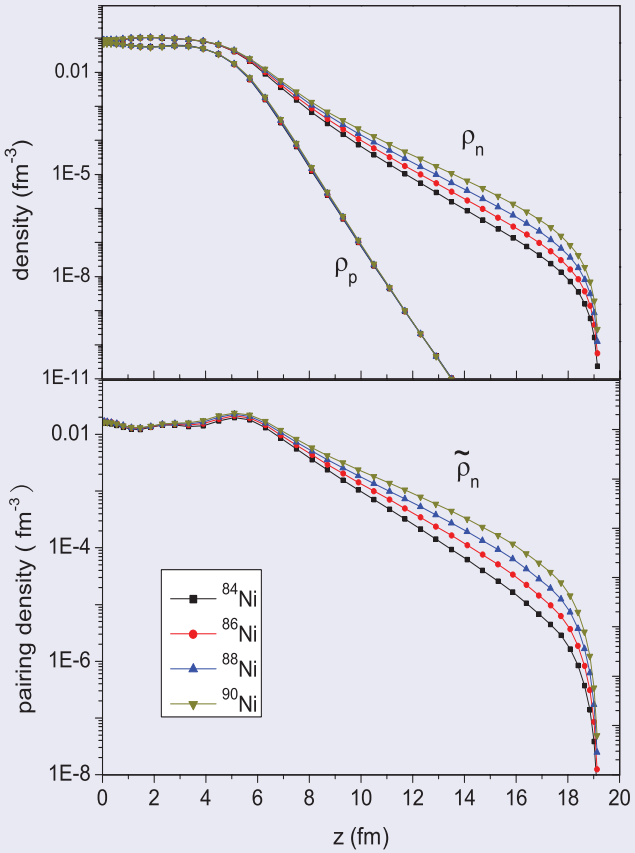
Pairing properties

HFBRAD: J_{max}; HFBAX: Ω_{max}



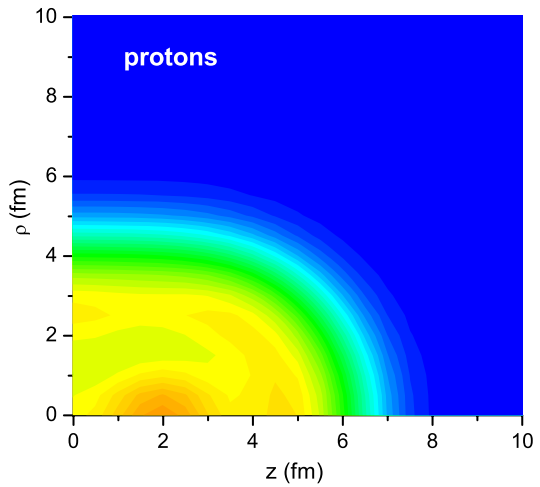
Conclusion: Neutron drip-line nuclei with surface pairing require very large angular momentum cutoff.

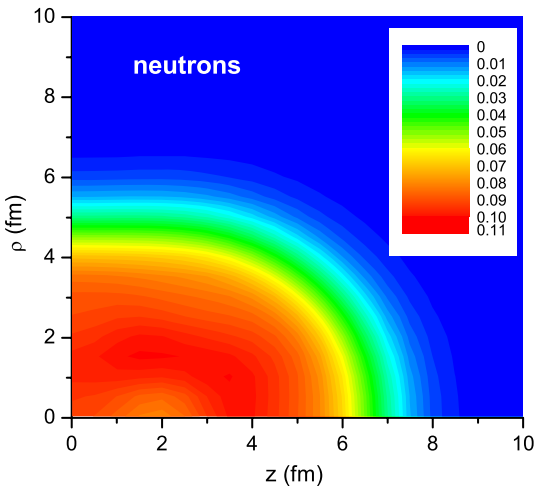
Densities



^{110}Zr

	HFB-AX	HFBTHO		HFB-AX	HFBTHO
E_{tot}	−893.983	−893.840	$\tilde{E}^n_{kin}$	1365.006	1364.878
E_C	226.758	226.712	Δ_n	0.636	0.652
E^p_{kin}	632.115	631.882	λ_n	−3.552	−3.543
E^n_{kin}	1368.206	1368.201	Q^p_{20}	444.02	443.90
E^n_{pair}	−3.200	−3.323	Q^n_{20}	788.32	786.63

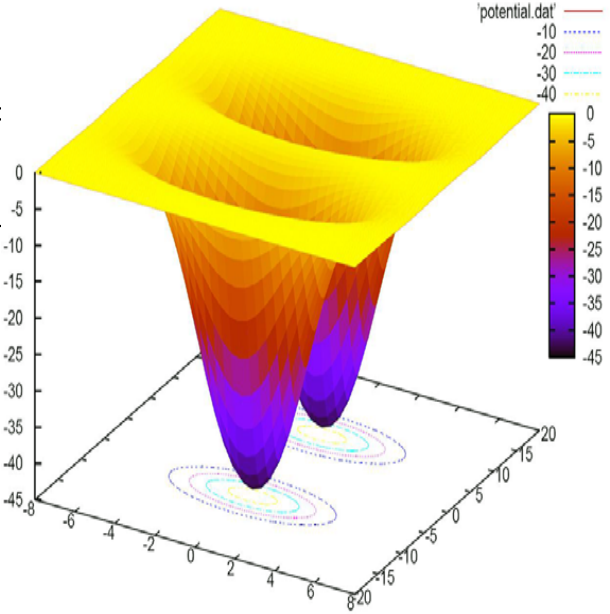




Two-center Potential Test

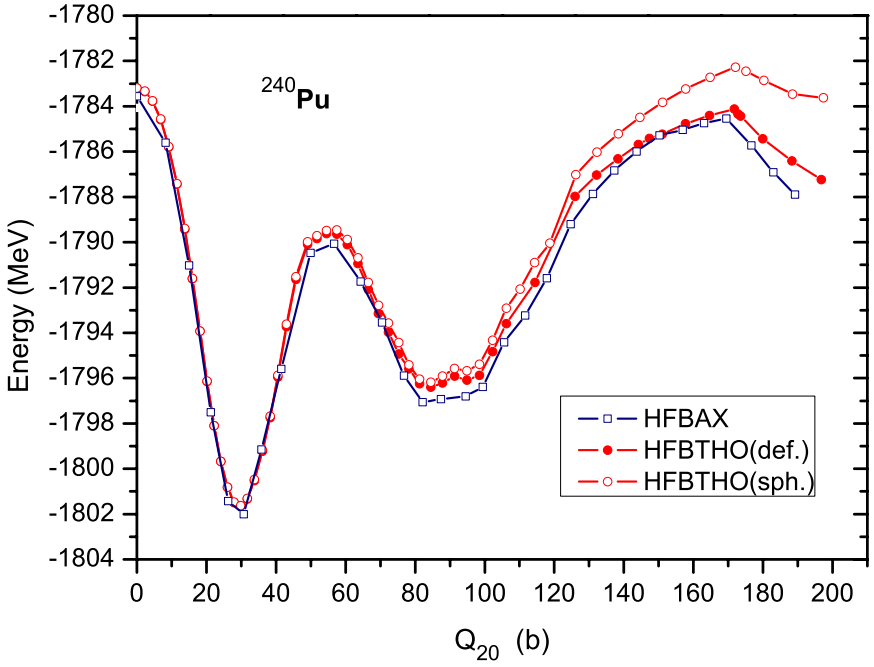
The two-center separated potential provides a good test for different numerical methods at very large deformations:

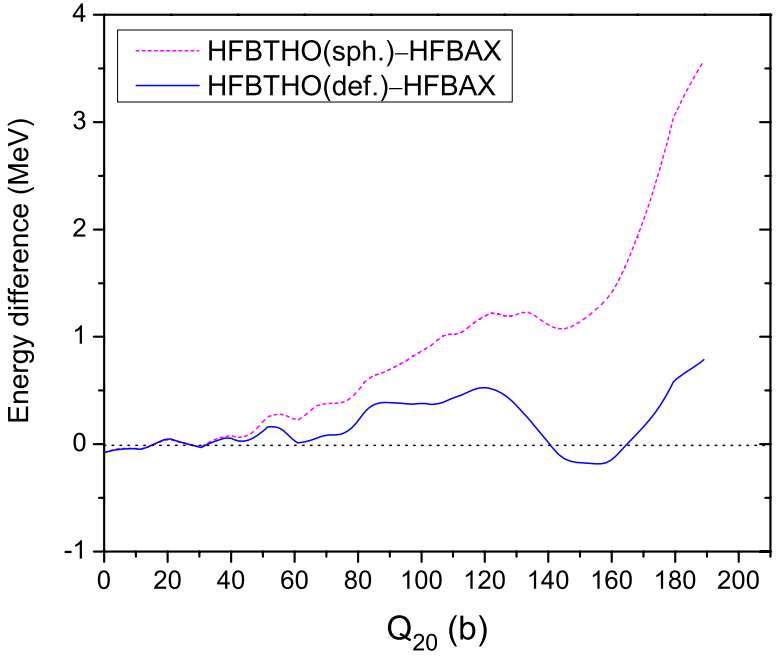
Ω^π	HO N_{sh}=20	HO N_{sh}=30	B-spline h=0.6	Wavelets
$1/2^+$	−22.23916	−22.24008	−22.24011	−22.24011
$1/2^-$	−22.23816	−22.23995	−22.23998	−22.23998
$1/2^+$	−9.43145	−9.43659	−9.43663	−9.43662
$3/2^-$	−9.42314	−9.43199	−9.43203	−9.43202
$3/2^+$	−9.42561	−9.43078	−9.43081	−9.43080
$1/2^-$	−9.41931	−9.42783	−9.42788	−9.42788
$1/2^+$	−8.77250	−8.77825	−8.77828	−8.77828
$1/2^-$	−8.76475	−8.77380	−8.77384	−8.77383
$1/2^+$	−1.70727	−1.72405	−1.72506	−1.72516
$1/2^-$	−1.49222	−1.52490	−1.52675	−1.52693



Fission Pathways

The HO basis HFB can have several hundreds of KeV differences in the prediction of fission barriers at large deformations.





Atomic calculations

Superfluid Local Density Approximation(SLDA) for Fermi system description: no spin-orbit coupling *Aurel Bulgac, arXiv:cond-mat/0703526*

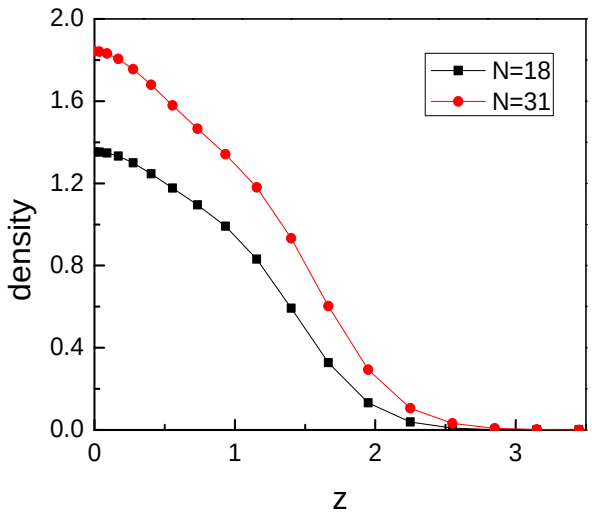
$$\mathcal{E}(\mathbf{r}) = \alpha\frac{\tau_c(\mathbf{r})}{2} + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\mathbf{r})}{10} + g_{eff}(\mathbf{r})|\nu_c(\mathbf{r})|^2 + V_{ext}(\mathbf{r})n(\mathbf{r})$$

where $g_{eff}(\mathbf{r})$ is renormalized pairing. Similarly the HFB equation with two components: spin up and down,

$$\begin{cases} [h(\mathbf{r}) - \mu]u_k(\mathbf{r}) + \Delta(\mathbf{r})v_k(\mathbf{r}) = E_k u_k(\mathbf{r}), \\ \Delta^*(\mathbf{r})u_k(\mathbf{r}) - [h(\mathbf{r}) - \mu]v_k(\mathbf{r}) = E_k v_k(\mathbf{r}), \end{cases}$$

Recently we have implemented that in HFBAX.

G. Bertsch, J. Dobaczewski, w. Nazarewicz, J. Pei, arXiv:0808.1874



Outline

Important SHE experiments

1. cold-fusion in **GSI**
   $(^{70}\mathrm{Zn}+^{208}\mathrm{Pb})^{278}112 \rightarrow ^{277}112+n$

   S. Hofmann and G. Münzenberg, Rev. Mod. Phys. **7**

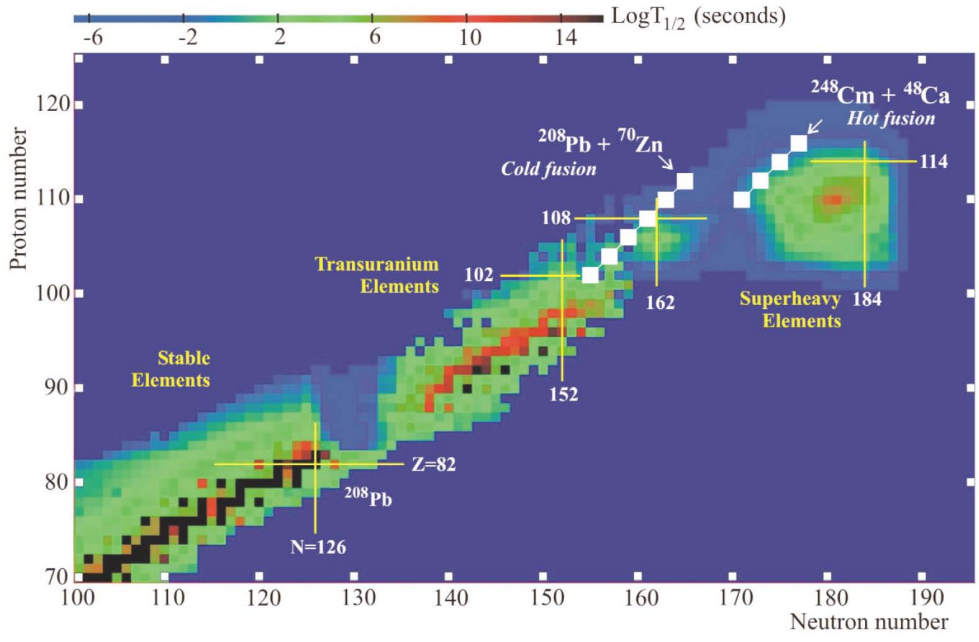
   733(2000).

2. hot-fusion in **Dubna**
   $(^{48}\mathrm{Ca}+^{244}\mathrm{Pu})^{292}114 \rightarrow ^{288}114+4n$

   Y. Oganessian, Pure Appl. Chem. 78, 889(2006).

3. highly-hot fusion experiment
   $^{312}124^{*}(^{74}\mathrm{Ge}+^{238}\mathrm{U}) > 10^{-18}$ s

   M. Morjean, et al., Phys. Rev. Lett. **101**, *072701(2008).*



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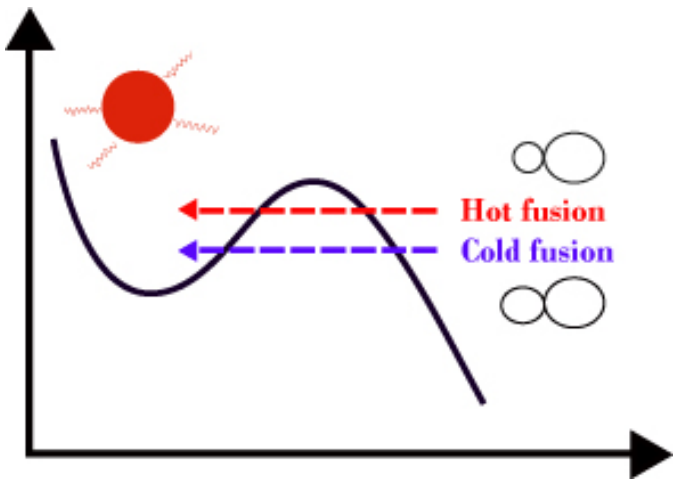

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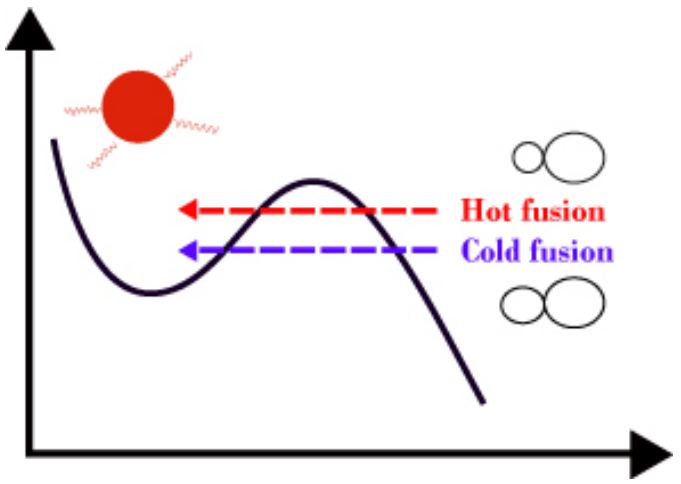

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What's the secrets here?

FT-HFBAX

In the case of Finite Temperature, the HFB density matrix ρ and pairing tensor κ is

$$\rho(\mathbf{r}) = \sum_i [f_i |U_i(\mathbf{r})|^2 + (1 - f_i)|V_i(\mathbf{r})|^2]$$

$$\tilde{\rho}(\mathbf{r}) = -\sum_i (1 - 2f_i) V_i(\mathbf{r}) U_i^*(\mathbf{r})$$

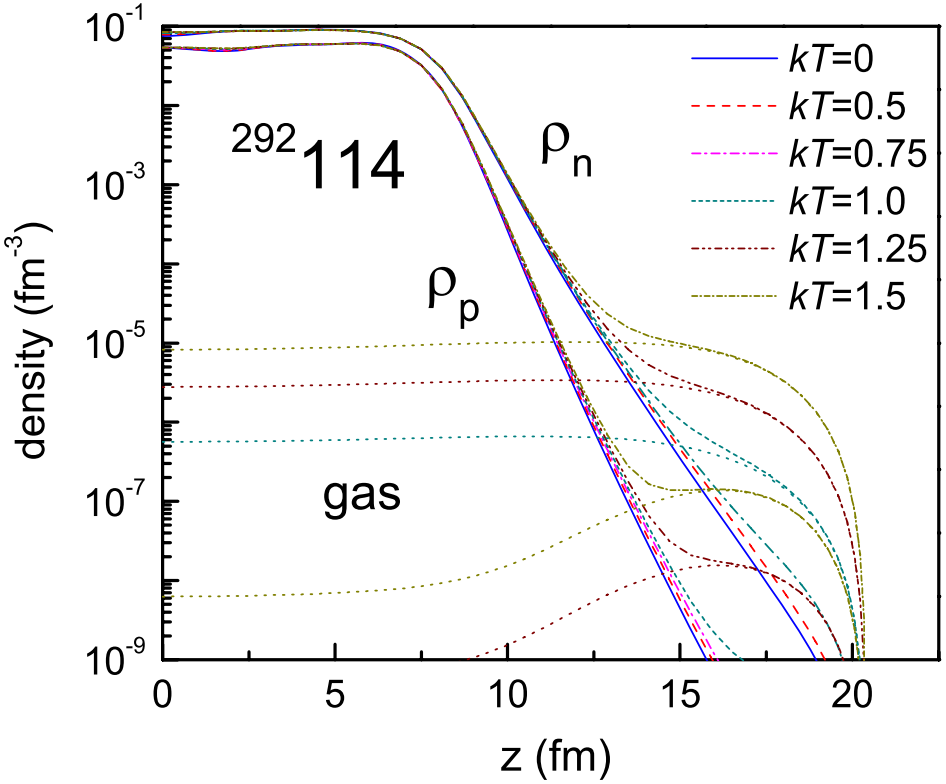
$$f_i = \frac{1}{1 + e^{(E_i/kT)}}$$

Also we should modify the kinetic densities τ, the spin currents $\nabla \cdot \mathbf{J}(r)$. Conventionally the potential energy is obtained by free energy $F = E - TS$, S is the entropy. The SkM* force is chosen for fission barrier calculations.

J. Pei, W. Nazarewicz, J.A. Sheikh , A.K. Kerman, to be appear.

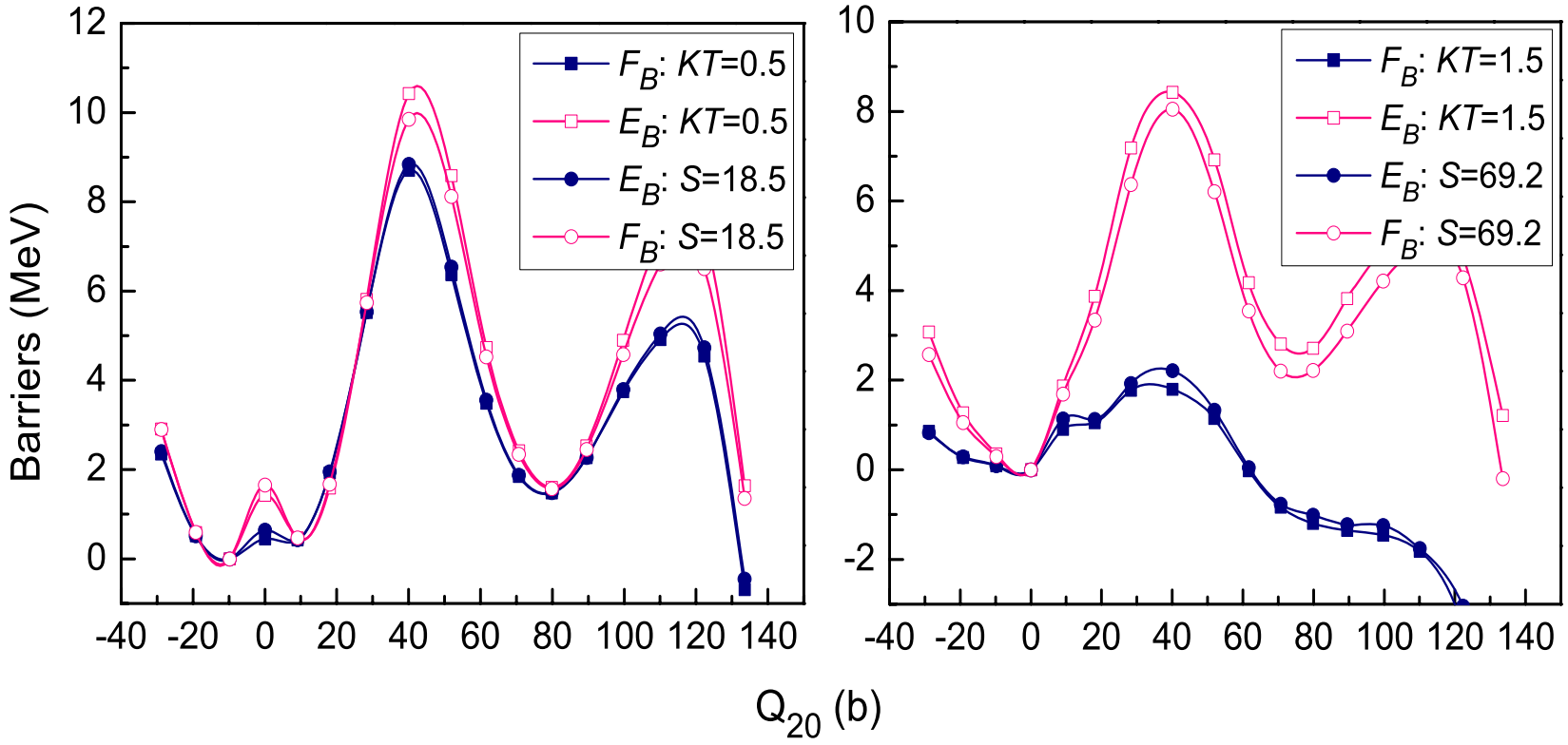
Gas solutions in box

unphysical gas is obatained by solving the Hartree-Fock equation without potential. *T. Vertse, A.T. Kruppa, W. Nazarewicz, PRC, 2000*



Fortunately the gas wouldn't change the fission barrier calculations.

Isothermal or isentropic fission

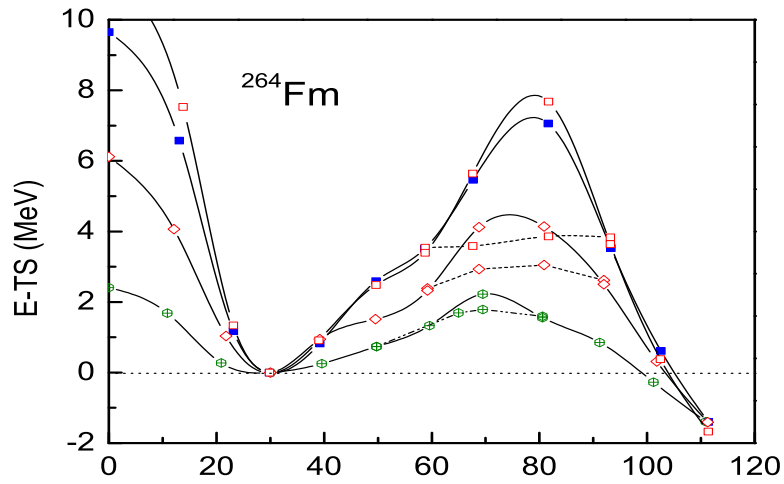


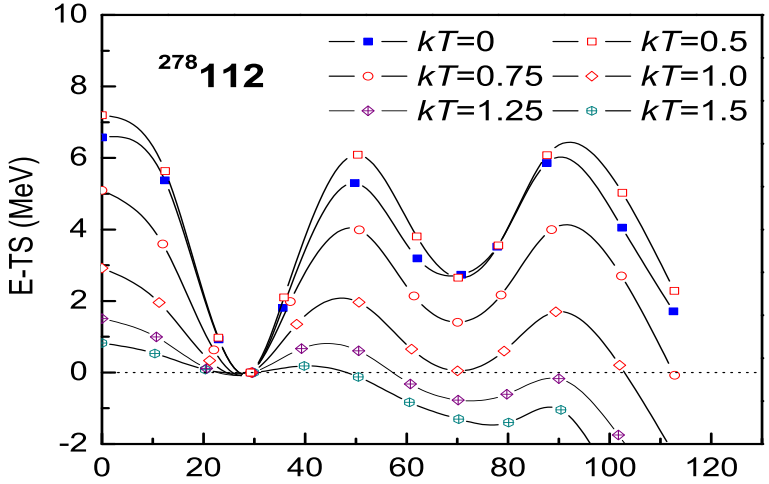
Equivalent at low temperatures in self-consistent calculations: consistent with the relation: $-P = (\frac{\partial U}{\partial V})_S = (\frac{\partial F}{\partial V})_T$

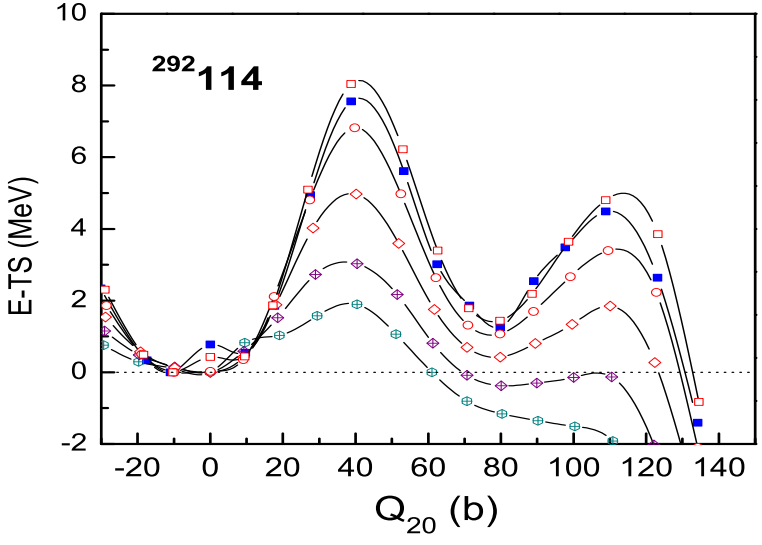
But they are very different in Maro-microscopic calculations:

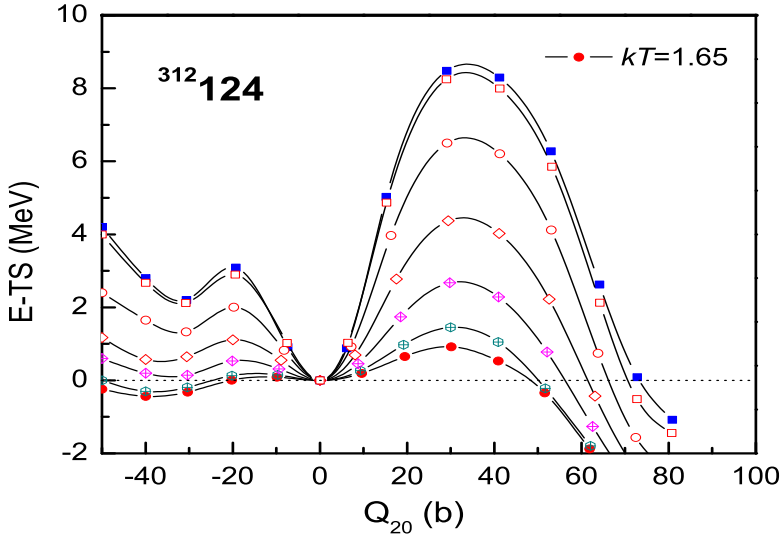
M. Diebel, K. Albrecht and R.W. Hasse, Nucl. Phys. **A355**, *66(1981).*

results

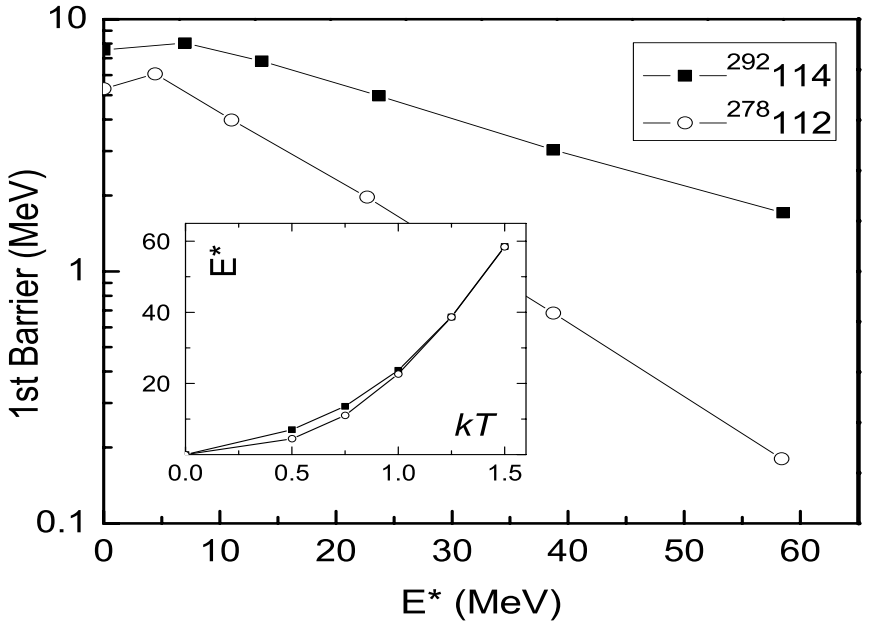

^{264}Fm
E-TS (MeV)


^{278}112
kT=0
kT=0.5
kT=0.75
kT=1.0
kT=1.25
kT=1.5
E-TS (MeV)


^{292}114
E-TS (MeV)
Q$_{20}$ (b)


^{312}124
kT=1.65
E-TS (MeV)
Q$_{20}$ (b)

results



In experimental analysis, usually we using a damping factor γ_D:

$$B_f = B_{LD} - \delta W e^{-\gamma_D E^*}$$

M.G. Itkis, Yu. Ts. Oganessian and V.I. Zagrebaev, Phys. Rev. C **65**, *044602(2002).*

We can fit that after $kT > 0.5$, $7.6e^{-E^*/16}$ for $^{278}112$ and $9.6e^{-E^*/34}$ for $^{292}114$.

Summary

- A 2D HFB-AX has been developed, it is very accurate, reasonable fast, very useful for describing weakly bound nuclei and elongated nuclear shapes.
- It can easily be extended to describe atomic system by SLDA.
- Interesting results have been obtained using the finite-temperature calculations of SHE fission barriers