Theoretical study of fission barriers in odd-A nuclei using the Gogny force

S. Pérez and L.M. Robledo

Departamento de Física Teórica
Universidad Autónoma de Madrid

Saclay, 9th May 2006

Workshop on the Theories of Fission and Related Phenomena
Outline

1. Introduction
   - Motivation

2. Theoretical Framework
   - Mean Field

3. Justification of this approximation
   - FT-HFB Theory

4. Calculation of Fission Barriers
   - Details of the calculation
   - Numerical Results
Introduction

Motivation

Theoretical Framework

Mean Field

Justification of this approximation

FT-HFB Theory

Calculation of Fission Barriers

Details of the calculation

Numerical Results
Introduction

Aims

We are interested in having a microscopic description of fission because we want to understand the phenomenon by itself.

Such description would be very helpful to make predictions for neutron rich nuclei, essential for stellar nucleosynthesis calculations, as well as for superheavies.
Introduction

Aims

We are interested in having a microscopic description of fission because we want to understand the phenomenon by itself.

Such description would be very helpful to make predictions for neutron rich nuclei, essential for stellar nucleosynthesis calculations, as well as for superheavies.
In general, we would like to have a microscopic description of fission in odd-A nuclei using a *mean field theory* with realistic interactions. The traditional procedure (blocked HFB) implies the breaking of time-reversal symmetry, which means a *high computational cost*, specially for the study of fission processes. The alternative is to use *Equal Filling Approximation*, which keeps the time-reversal symmetry (and also axiallity).
Introduction

Aims

- In general, we would like to have a microscopic description of fission in odd-A nuclei using a mean field theory with realistic interactions. The traditional procedure (blocked HFB) implies the breaking of time-reversal symmetry, which means a high computational cost, specially for the study of fission processes.

- The alternative is to use Equal Filling Approximation, which keeps the time-reversal symmetry (and also axiallity).
Introduction

Aims

- In general, we would like to have a microscopic description of fission in odd-A nuclei using a *mean field theory* with realistic interactions. The traditional procedure (blocked HFB) implies the breaking of time-reversal symmetry, which means a *high computational cost*, specially for the study of fission processes.

- The alternative is to use *Equal Filling Approximation*, which keeps the time-reversal symmetry (and also axiality).
**Introduction**

In general, we would like to have a microscopic description of fission in odd-A nuclei using a *mean field theory* with realistic interactions. The traditional procedure (blocked HFB) implies the breaking of time-reversal symmetry, which means a *high computational cost*, specially for the study of fission processes.

The alternative is to use *Equal Filling Approximation*, which keeps the time-reversal symmetry (and also axiallity).
Outline

1. Introduction
   - Motivation

2. Theoretical Framework
   - Mean Field

3. Justification of this approximation
   - FT-HFB Theory

4. Calculation of Fission Barriers
   - Details of the calculation
   - Numerical Results
HFB Theory

The Hartree-Fock-Bogoliubov theory has been used. The quasi-particle creation and annihilation operators are given by the most general linear transformation from the particle operators:

\[
\begin{pmatrix}
\alpha_k \\
\alpha_k^\dagger
\end{pmatrix} = \sum_l \begin{pmatrix} U^\dagger & V^\dagger \\ VT & UT \end{pmatrix}_{kl} \begin{pmatrix} c_l \\
c_l^\dagger \end{pmatrix}
\]

The matrices \( U \) and \( V \) will be the variational parameters which minimise the HFB energy:

\[
\langle H \rangle = \text{Tr} (t \rho) + \frac{1}{2} \text{Tr} (\Gamma \rho) - \frac{1}{2} \text{Tr} (\Delta \kappa^*)
\]

\[
\rho_{ij} = \langle c_j^\dagger c_i \rangle = (V^* V^T)_{ij} \; ; \; \kappa_{ij} = \langle c_j c_i \rangle = (V^* U^T)_{ij}
\]

\[
\Gamma_{ij} = \sum_{kl} \bar{v}_{ijkl} \rho_{lk} \; ; \; \Delta_{ij} = \frac{1}{2} \sum_{kl} \bar{v}_{ijkl} \kappa_{kl}
\]
The ground state of even-even nuclei is represented as the QP vacuum:

\[ |\phi\rangle = \prod_{k>0} \alpha_k \alpha_{\bar{k}} | - \rangle \Rightarrow \rho = V^* V^T \text{ and } \kappa = V^* U^T \]

However, the ground state of odd nuclei can be characterised by means of:

\[ |\phi_{1qp}\rangle = \alpha_i^+ |\phi\rangle \Rightarrow \rho_{kk'} = (V^* V^T)_{kk'} + \{ U_{ki} U_{k'i}^* - V_{ki}^* V_{k'i} \} \]
\[ \kappa_{kk'} = (V^* U^T)_{kk'} + \{ U_{ki} V_{k'i}^* - V_{ki}^* U_{k'i} \} \]

**Drawback**

With this ansatz the time-reversal symmetry is broken.
Time-reversal invariant description

To restore the time reversal symmetry, an intuitive solution comes in terms of the Equal Filling Approximation (EFA):

\[ \rho^{eфа}_{kk'} = (V^* V^T)_{kk'} + \frac{1}{2} \left\{ U_{ki} U_{k'i}^* - V_{ki}^* V_{k'i} + U_{ki}^* U_{k'i} - V_{ki} V_{k'i}^* \right\} \]

\[ \kappa^{eфа}_{kk'} = (V^* U^T)_{kk'} + \frac{1}{2} \left\{ U_{ki} V_{k'i}^* - V_{ki}^* U_{k'i} + U_{ki}^* V_{k'i} - V_{ki} V_{k'i}^* \right\} \]

Without any justification, and using it in the same way as in the ordinary HFB theory, the energy is computed as:

\[ E^{eфа} = Tr(t \rho^{eфа}) + \frac{1}{2} Tr(\Gamma^{eфа} \rho^{eфа}) - \frac{1}{2} Tr(\Delta^{eфа} \kappa^{eфа*}) \]

the \( U \) and \( V \) matrices are computed by solving the HFB equation

\[
\begin{pmatrix}
  t + \Gamma^{eфа} & \Delta^{eфа} \\
  - \Delta^{*eфа} & -t^* - \Gamma^{*eфа}
\end{pmatrix}
\begin{pmatrix}
  U_k \\
  V_k
\end{pmatrix}
= 
\begin{pmatrix}
  U_k \\
  V_k
\end{pmatrix} E_k
\]

again without any foundation
Outline

1. Introduction
   - Motivation

2. Theoretical Framework
   - Mean Field

3. Justification of this approximation
   - FT-HFB Theory

4. Calculation of Fission Barriers
   - Details of the calculation
   - Numerical Results

S. Pérez and L.M. Robledo
Theoretical study of fission barriers in odd-A nuclei using the Gogny force
Writing the density matrix and the pairing tensor in term of matrices:

$$\mathcal{R}_{efa} = \begin{pmatrix} \rho_{efa} & \kappa_{efa} \\ -\kappa_{efa}^* & 1 - \rho_{efa}^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} f & 0 \\ 0 & 1 - f \end{pmatrix} \begin{pmatrix} U^+ & V^+ \\ V^T & U^T \end{pmatrix}$$

where

$$f_k = \begin{cases} \frac{1}{2} & k = i \text{ or } k = \bar{i} \\ 0 & \text{otherwise} \end{cases}$$

which reminds us the Finite-Temperature HFB Theory!
From the self-consistent FT-HFB theory, the energy could be expanded through:

\[ E = \text{Tr}(D\hat{H}) = \frac{1}{Z} \sum_{\{|n\rangle\}} \langle \phi | \alpha_k^-, \ldots, \alpha_k^+, H\alpha_k^+, \ldots, \alpha_k^+ | \phi \rangle e^{-\beta(\sum E_k)} \]

Both expressions give the same results:

\[ E^{\text{efa}} = \frac{1}{4} \left\{ \langle \phi | H | \phi \rangle + \langle \phi | \alpha_i^+ H \alpha_i^- | \phi \rangle + \langle \phi | \alpha_i^- H \alpha_i^+ | \phi \rangle + \langle \phi | \alpha_i \alpha_i^+ H \alpha_i^- \alpha_i^- | \phi \rangle \right\} = \]

\[ = \text{Tr}(t\rho^{\text{efa}}) + \frac{1}{2} \text{Tr}(\Gamma^{\text{efa}} \rho^{\text{efa}}) - \frac{1}{2} \text{Tr}(\Delta^{\text{efa}} \kappa^{\text{efa}\ast}) \]

Therefore, we have, again, a theory based on the variational principle on the EFA energy given above.
Since the FT-HFB equations are nonlinear, they can be solved by iteration. The use of iterative diagonalization generates some problems about the convergence and has complications that arise in cases with one or more constraints. These facts drive us to employ the gradient method. The gradient method can be used because the EFA equations come from the variational principle on the EFA energy. This method is based on the Thouless parametrisation of the most general HFB wave function:

\[ |\phi_1(Z)\rangle = \mathcal{N} \exp\left[ \sum_{k<k'} Z_{kk'} \alpha_k^+ \alpha_{k'}^+ \right] |\phi_0\rangle \]
Advantages of having a justification

Thanks to this justification, we can extend the use of the EFA in more advanced frameworks, such as the time-dependent HFB theory, projection methods, etc. Specifically, the adiabatic approximation of the TD-HFB theory has been used to evaluate the collective masses involved in the Collective Hamiltonian.
Outline

1. Introduction
   - Motivation

2. Theoretical Framework
   - Mean Field

3. Justification of this approximation
   - FT-HFB Theory

4. Calculation of Fission Barriers
   - Details of the calculation
   - Numerical Results

S. Pérez and L.M. Robledo
Theoretical study of fission barriers in odd-A nuclei using the Gogny force
Effective Interaction

The Gogny density dependent effective force with the D1S parametrisation has been used:

\[
V_{12} = \sum_{i=1}^{2} \left( W_i + B_i \hat{P}_\sigma - H_i \hat{P}_\tau - M_i \hat{P}_\sigma \hat{P}_\tau \right) e^{-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\mu_i^2}} \\
+ i W_{LS} (\vec{\nabla}_1 - \vec{\nabla}_2) \times \delta(\vec{r}_1 - \vec{r}_2)(\vec{\nabla}_1 - \vec{\nabla}_2) \cdot (\vec{\sigma}_1 + \vec{\sigma}_2) \\
+ t_0 (1 + x_0 \hat{P}_\sigma) \delta(\vec{r}_1 - \vec{r}_2) \left[ \rho \left( \frac{\vec{r}_1 + \vec{r}_2}{2} \right) \right]^\gamma + V_{\text{Coul}}
\]
Approximations and Basis

We have used the Slater approximation to compute the Coulomb exchange term:

\[ E_{CE} = -\frac{3}{4} e^2 \left( \frac{3}{\pi} \right)^{1/3} \int \rho^p(\vec{r})^{3/4} d^3\vec{r} \]

The QP operators have been expanded into an axially symmetric harmonic oscillator basis including 17 shells. In order to have an accurate fission driving coordinate, we have used the \( Q_{20} \) degree of freedom. The three lowest QP states for each \( J_z \) value (\( J_z = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, and \frac{11}{2} \)) have been selected to be blocked.
The spontaneous fission half-life has been calculated using the traditional WKB approximation:

$$T_{sf}(s) = 2.86 \times 10^{-21} \left(1 + e^{2S}\right)$$

where $S$ is the action

$$S = \int_{a}^{b} dQ_{20} \sqrt{2B(Q_{20})(V(Q_{20}) - E_{0})}$$

where $B$ is the collective mass computed in the framework of the adiabatic TDHFB.

In the collective potential energy $V(Q_{20})$ the rotational energy correction has been taken into account.
Projection techniques

In order to better describe the odd-A nuclei we can implement the parity and number parity projection, and check when it is important to apply them.

Parity Projection
Since the reflexion symmetry is broken when octupole deformation appears, we will check how and when parity projection is important.

Number Parity Projection
Since we are describing an odd-A nuclei, only odd quasi-particles states should be considered. Therefore, in order to keep only one quasi-particle states, the number parity projection must be applied.

\[ E_{\text{PRO}}^{\text{efa}} = \frac{1}{2} \left( \langle \phi | \alpha_i H \alpha_i^+ | \phi \rangle + \langle \phi | \alpha_i H \alpha_i^+ | \phi \rangle \right) \]
Parity Projection

Interesting examples on which to apply parity projection should have octupole deformation in the ground state. We have chosen the 229 Radium isotope to make this study.

**Projection After Variation drawbacks:**

In order to be close to the Variation After Projection method, we shall study the Projection After Variation solution in terms of the octupolar degree of freedom, even if the mean field ground state doesn’t show octupolarity.
Therefore we can extract from these calculations that this projection is important when the octupolarity is in a certain range, $\beta \sim 0.01 - 0.1$, not more not less.
We have used the $^{235}$U fission barrier to see the effects of this projection.
It is easy to check that the modification is very small and of the order of 100keV. Therefore we can state that the Equal Filling Approximation is a very good way to describe odd-A nuclei, since to number parity correction is very small.
We have applied the EFA method to the calculation of two fission barriers, one for a nucleus blocking in the proton channel, that is $^{235}_{93}Np_{142}$, and other blocking in the neutron channel, $^{235}_{92}U_{143}$. We have restricted to a mean field like study (EFA) as we know that Parity and Number Parity projections produce very tiny changes on the energies of the configurations relevant to fission.
Introduction

Motivation

Theoretical Framework

Mean Field

Justification of this approximation

FT-HFB Theory

Calculation of Fission Barriers

Details of the calculation

Numerical Results

S. Pérez and L.M. Robledo

Theoretical study of fission barriers in odd-A nuclei using the Gogny force
The Selection of the even nuclei

We have two possibilities to select the even-even neighbour nucleus of the $^{235}U$, let’s say $^{234}U$ and $^{236}U$.

In order to check whether this selection is important or not, we have computed the PES for $^{235}U$ blocking the first state with $j_z = \frac{1}{2}$ and using the quasi-particle states of both even neighbour nuclei $^{234}U$ and $^{236}U$. 

![Graph showing the energy vs. Q20 for $^{235}U$.]
$^{234}U$ and $^{236}U$

It is easy to see that the results are exactly the same, so we can conclude that it doesn’t matter which even neighbour nucleus is selected.
Comparison

An average calculation has been performed, just to have a reference to compare with.

![Graph showing fission barriers comparison](graph.png)
Introduction

Theoretical Framework

Justification of this approximation

Calculation of Fission Barriers

Numerical Results

Energy

S. Pérez and L.M. Robledo

Theoretical study of fission barriers in odd-A nuclei using the Gogny force
Theoretical study of fission barriers in odd-A nuclei using the Gogny force

Ground state spectrum

Calculated

$^\text{235}U$

Measured

S. Pérez and L.M. Robledo
Theoretical study of fission barriers in odd-A nuclei using the Gogny force.

**Calculated Ground state spectrum**
- $1/2^+$
- $7/2^-$
- $5/2^+ (0.6)$
- $5/2^- (0.8)$

**Fission Isomer spectrum**
- $1/2^+ (0)$
- $3/2^- (1)$
- $9/2^- (0.8)$
- $11/2^+ (0.4)$
- $5/2^+ (1.2)$
Pairing energy

\[ 235\text{U} \]

\[
\begin{align*}
Q_{20} (\text{b}) & \quad E_{\text{pp}} (\text{MeV}) \\
\text{prot.} & \quad \text{neut.} & \quad \text{AVE} & \quad 235\text{U} \\
\end{align*}
\]
Collective masses

\[
Q^2(\beta) \quad B_{ATDFH} A^{4/3} (b^2)
\]

S. Pérez and L.M. Robledo

Theoretical study of fission barriers in odd-A nuclei using the Gogny force
The spontaneous fission half-lives are some orders of magnitude larger in odd-A nuclei than in even-A nuclei. This is because of:

1) The specialisation energy:
$^{235}U$ Spontaneous fission half-life

2) The larger inertia $B(Q_{20})$ due to the smaller pairing energy in odd-A nuclei.

\begin{center}
\begin{tabular}{c c c c}
\textbf{Measured} & \textbf{Calculated} \\
$^{234}U$ & $4.47 \times 10^{23}$ s & $1.9 \times 10^{19}$ s \\
$^{235}U$ & $3.24 \times 10^{26}$ s & $5.7 \times 10^{37}$ s \\
$^{236}U$ & $7.65 \times 10^{23}$ s & $3.34 \times 10^{23}$ s \\
\end{tabular}
\end{center}
Theoretical study of fission barriers in odd-A nuclei using the Gogny force

Energy

<table>
<thead>
<tr>
<th>235Np</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 20 40 60 80 100 120 140</td>
</tr>
<tr>
<td>Q_20 (b)</td>
</tr>
</tbody>
</table>

| E (MeV) |
| -1785 -1780 -1775 -1770 -1765 -1760 |
| 1/2 3/2 5/2 7/2 9/2 11/2 |

S. Pérez and L.M. Robledo
Ground state spectrum

**Calculated**
- $\frac{3}{2}^-$
- $\frac{3}{2}^+$
- $\frac{5}{2}^+$
- $\frac{5}{2}^-$

**Measured**
- $\frac{7}{2}^-$
- $\frac{3}{2}^-$
- $\frac{1}{2}^-$
- $\frac{5}{2}^-$
- $\frac{5}{2}^+$
Theoretical study of fission barriers in odd-A nuclei using the Gogny force
Theoretical study of fission barriers in odd-A nuclei using the Gogny force
Theoretical study of fission barriers in odd-A nuclei using the Gogny force.
We have calculated, in the same way as for $^{235}\text{Np}$ and $^{235}\text{U}$ the fission barrier of the $^{237}\text{Pu}$ and $^{237}\text{Am}$.
The experimental excitation energy of the fission isomer is 2.6 MeV. Our result for this value is 3.82 MeV.
**237 Americium Fission Study**

The experimental ground state of $^{237}Am$ is $\frac{5}{2}^-$.

Our result for the excitation energy of the fission isomer is 2.12 MeV.
We have justified the EFA in terms of the FT-HFB. Based on this justification, techniques beyond mean field can be used.

The small effect of the Number Parity Projection shows that EFA is a good approximation for odd-A nuclei.

Important results have been obtained when Parity projections have been applied, such as in the Radium isotopes.

A study of the fission barrier of $^{235}U$ and $^{235}Np$ has been carried out. Results regarding the spin, parity and energy of the ground and shape isomeric states are very satisfactory.

These promising results make us optimistic about the scope of the EFA.