Tools for a microscopic description of fission

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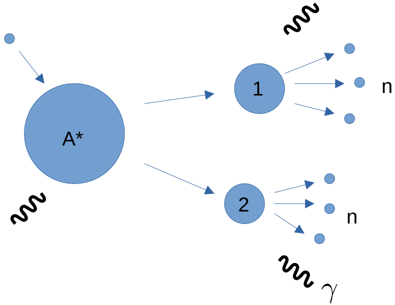
Nuclear Fission



Spontaneous

$$A^* \to F_1 + F_2 + n + p + e^{\pm} + \gamma$$

Induced

$$n+\gamma+\cdots+A \to F_1+F_2+n+p+e^{\pm}+\gamma$$

Observables

- Lifetime
  - Spontaneous
  - Induced (Fission cross section)
- Fragments' properties
  - N and Z
  - Mass distribution
  - Kinetic E
  - Angular momentum
  - Emitted p, n, γ, ...

Their values should be obtained by using the rules of quantum mechanics (QM)

Theoretical description

According to QM rules

$$\mathcal{P}_{i\to f} = |\langle\Psi_f|\hat{U}(\infty,-\infty)|\Psi_i\rangle|^2$$

- $|\Psi_i\rangle$ is the wave function of the initial system. Depends on intricate nuclear dynamics.
- $|\Psi_f\rangle$ wave function of fission channels

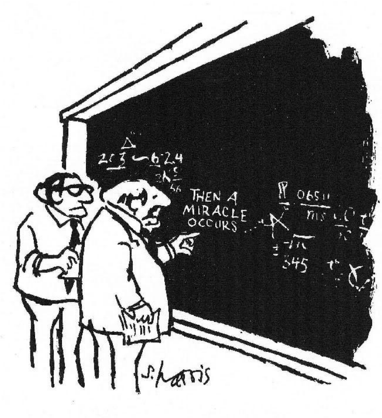
$$|\Psi_f\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle \otimes |n\rangle \otimes |\gamma\rangle \otimes \cdots$$

- $\hat{U}(\infty,-\infty)$ is the time evolution operator
  Time ordered exponential of the Hamiltonian including
  - Nuclear interaction
  - Electromagnetic interaction
  - Weak interaction

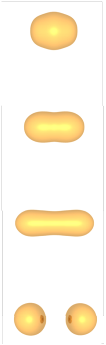
In addition: Protons and neutrons are fermions. Symmetrization principle

Simplifications

Daunting problem because the exact wave functions are not easily accessible, not to mention the evolution operator . . .



"I think you should be more explicit here in step two."



Liquid-drop picture comes to the rescue

First principle calculations are replaced by models incorporating the relevant physics/degrees of freedom

a bit of history

Letter | Published: 11 February 1939

Disintegration of Uranium by Neutrons: a New Type of Nuclear Reaction

Lise Meitner & O. R. Frisch

Nature **143**, 239–240 (1939) | Cite this article

SEPTEMBER 1, 1939 PHYSICAL REVIEW VOLUME 56

The Mechanism of Nuclear Fission

NIELS BOHR
University of Copenhagen, Copenhagen, Denmark, and The Institute for Advanced Study, Princeton, New Jersey

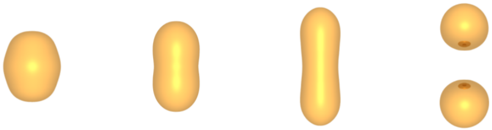
AND

JOHN ARCHIBALD WHEELER
Princeton University, Princeton, New Jersey

(Received June 28, 1939)

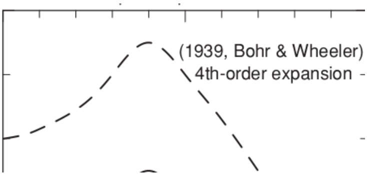
On the basis of the liquid drop model of atomic nuclei, an account is given of the mechanism of nuclear fission. In particular, conclusions are drawn regarding the variation from nucleus to nucleus of the critical energy required for fission, and regarding the dependence of fission cross section for a given nucleus on energy of the exciting agency. A detailed discussion of the observations is presented on the basis of the theoretical considerations. Theory and experiment fit together in a reasonable way to give a satisfactory picture of nuclear fission.

Basic concept



Requires the introduction of deformation parameters α
Competition between surface energy and Coulomb repulsion

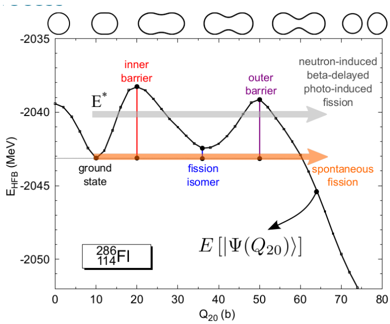
$$\Delta E(\alpha) = E_s^{(0)} \left(\frac{2}{5}(1-x)\alpha^2 - \frac{4}{105}(1+2x)\alpha^3 \right) \quad x = \frac{E_c}{2E_s^{(0)}}$$



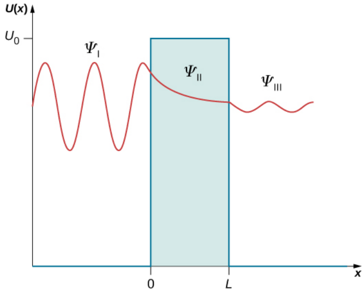
Concepts

- Potential energy surface
- Quantum tunnelling through the barrier

Tunnelling



Courtesy of S. Giuliani



Define $\beta^2 = \frac{2m}{\hbar^2}(U_0 - E)$ and $\gamma = \beta/k - k/\beta$

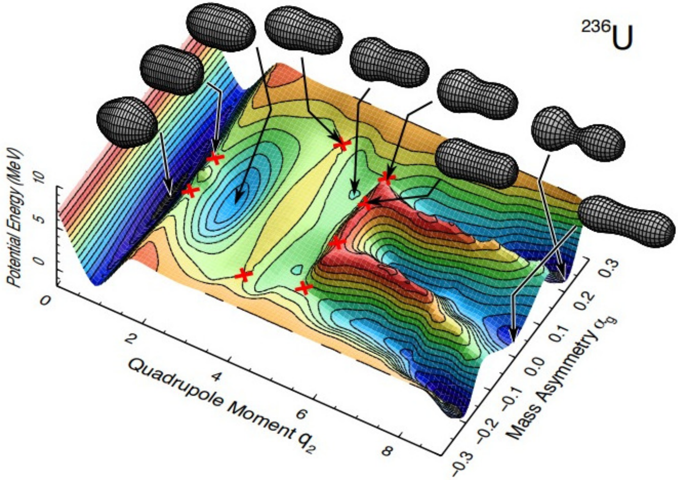
$$T(L, E) = \frac{1}{\cosh^2(\beta L) + (\gamma/2)^2 \sinh^2(\beta L)}$$

Penetrability depends upon

- Barrier height U_0
- Barrier width L
- Collective inertia m

Multiple deformation parameters

Several degrees of freedom are often required



From Ichikawa et al PRC 86 024610

Microscopic description

Based on Bohr's ideas requires

- Identifying the right degrees of freedom
  - Quadrupole, Octupole, Hexadecapole, Neck, ...
  - Pairing
- Perform constrained mean field calculations based on Hartree- Fock-Bogoliubov to obtain the PES
  Should correlation energies from symmetry restoration and quantum fluctuations be included ? Variation after projection (VAP) ?
- Compute collective inertias in the ATDHFB or GCM framework
  Avoid perturbative approximations. Are collective dof adiabatic ?
- Use WKB to obtain t_{F}
  Least energy or least action ?
- Use Time Dependent theories to obtain fragment mass distribution and properties
  - Exact TDHFB or TDGCM

$$i\hbar\partial/\partial t\mathcal{R} = [\mathcal{H}, \mathcal{R}]$$

  - Collective Schrodinger equation obtained with GOA

Extend the above methods to odd-A systems, finite temperature, etc

The standard computational framework involves

- Constrained HFB calculations on a huge basis to deal with the large variety of shapes involved in fission
  (Harmonic Oscillator basis, Lagrange Mesh, DVR, etc)
- Approximate formulas to compute
  - Correlation energies from symmetry restoration
    Rotational formula
    Lipkin-Nogami (VAP)
  - Correlation energies from quantum fluctuations
    Multipole (Quadrupole) zero point energy
  - Collective inertias both from ATDHFB or GCM
    Perturbative or non perturbative
- Assumptions about the validity of the GOA
  To reduce the TDHFB or TDGCM methods to a TD-Collective Schrodinger Equation on a few collective variables
- Assumptions how to extract physical quantities from the intrinsic wave function of the fragments
  Rotational model, among others

Beyond HFB

To move forward one needs to replace approximations by exact expressions and remove assumptions

- Restore symmetries exactly using projection techniques
  - Angular momentum and parity (SU(2))
  - Particle number (U(1))
- Restore symmetries in the fragments' wave functions using projection techniques in the domain
- Compute "zero point energies" from full fledged GCM or other alternative theories
- Solve TDHFB exactly to get rid of TD-CSE and GOA
- Solve TDGCM exactly to get rid of TD-CSE and GOA
- Use exact collective inertias in the calculation of the action

Beyond mean field

In most of techniques in the previous list one needs to compute overlaps of operators between HFB states

- The HFB states may correspond to different values of the collective degrees of freedom and/or HFB states obtained by applying symmetry operators (rotations in space, etc)

$$\langle \Psi(q) | \hat{O} | \Psi(q') \rangle \quad \langle \Psi(q) | \hat{O} \hat{R}(\Omega) | \Psi(q') \rangle$$

- The operator overlaps can be easily computed by using the Generalized Wick's theorem and modern formulas (no sign ambiguity) for the overlaps
- But standard GWT and pfaffian formulas require that bases used in the HFB states (or the rotated ones) span the same subspace of the Hilbert space
  Different bases must be connected by unitary transformations

Fission peculiarities

Practical fission calculations require specific bases

- Finite dimensional bases
- More states in the direction of elongation (typically z)
  Breaks rotational invariance
- Different oscillator lengths along three spatial directions b_x, b_y, and b_z
  Breaks rotational invariance
- Oscillator lengths adjusted to each deformation q

$$e^{-x^2/b^2} = e^{-x^2/b'^2} e^{-x^2[1/b^2 - 1/b'^2]} = e^{-x^2/b'^2} \sum_{n=0}^{\infty} \frac{(-x^2/B^2)^n}{n!}$$

Last three requirements involve non-unitarily connected bases

They can be overcome if a sufficiently large HO basis is used: only feasible with contact forces

Fission fragments

The two fragments resulting from fission are entangled
If fragments' properties are required one can

- Wait until fragments are very far appart
- Use restoration of symmetries on a domain*

Example: particle number on a domain $\mathcal{D}$ (Fragment's mass distribution)

$$P_{\mathcal{D}}^{N} = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{i\varphi(\hat{N}_{\mathcal{D}}-N_0)}$$

$\hat{N}_{\mathcal{D}}$ number of particles operator on the domain $\mathcal{D}$

$$e^{i\varphi\hat{N}_{\mathcal{D}}}\phi_a(\vec{r}) = \begin{cases} e^{i\varphi}\phi_a(\vec{r}) & \vec{r}\subset\mathcal{D} \\ \phi_a(\vec{r}) & \text{otherwise} \end{cases}$$

It is evident that the matrix connecting the original basis and the "rotated" one

$$\mathcal{R}_{ab} = \int d\vec{r}\phi_a^*(\vec{r})e^{i\varphi\hat{N}_{\mathcal{D}}}\phi_b(\vec{r}) = \delta_{ab} + (e^{i\varphi}-1)\mathcal{O}_{ab}$$

is not unitary (eigenvalues of $\mathcal{O}_{ab} = \int_{\mathcal{D}} d\vec{r}\phi_a^*(\vec{r})\phi_b(\vec{r})$ differ from 1 or 0) **

* Simenel, Phys. Rev. Lett. 105, 192701 ** Robledo, arXiv:2503.02696

Fission fragments

Example: Assume a 1D HO basis and $\mathcal{D} = \theta(z)$ then

$$\mathcal{O}_{nm} = \int_0^\infty dx \phi_n^*(x)\phi_m(x) = \sqrt{\frac{2^{n+m} n! m!}{4\pi}} \sum_{pq} \frac{(-)^{p+q}\Gamma((n+m-2p-2q)/2)}{2^{2p+2q} p! q! (n-2p)! (m-2q)!}.$$

If the basis only contains $n = 0$ and $n = 1$ states $\mathcal{O}_{11} = \mathcal{O}_{22} = 1/2$ and $\mathcal{O}_{12} = \mathcal{O}_{21} = 1/\sqrt{2\pi}$. The eigenvalues of $\mathcal{O}$ are $\theta_0 = 0.1010$ and $\theta_1 = 0.8989$ and therefore the eigenvalues of $\mathcal{R}_{ab} = \delta_{ab} + (e^{i\varphi} - 1)\mathcal{O}_{ab}$ given by $r_l = 1 + (e^{i\varphi} - 1)\theta_l$ are not phases as is the case for an unitary matrix.

How it comes ?

In QM spatial properties often require infinite dimensional Hilbert spaces

Example: Commutation relation $[\hat{X}, \hat{P}_x] = i\hbar$ can never be fulfilled if $\hat{X}$ and $\hat{P}_x$ are restricted to a finite dimension Hilbert space ($\mathrm{tr}[A, B] = 0$ by construction)

GWT non equivalent bases

- The GWT for non-equivalent bases was formulated in a series of papers * and applied to the use of HO bases with different oscillator lengths **.
- In Robledo, arXiv:2503.02696 it has been applied to particle number projection of HFB states on a domain

The differences with the standard formulation are in the overlaps of HFB wave functions

$$\langle \Psi_0 | e^{i\varphi \hat{N}_{\mathcal{D}}} | \Psi_1 \rangle = \sqrt{\det A \det \mathcal{R}}$$

and in the matrix A entering the contractions

$$A = \bar{U}_0^T \left(\mathcal{R}^T\right)^{-1} \bar{U}_1^* + \bar{V}_0^T \mathcal{R} \bar{V}_1^*$$

In the standard formulation $\left(\mathcal{R}^T\right)^{-1}$ is replaced by $\mathcal{R}^*$ and $\det \mathcal{R}$ is just a phase. Both formulations are equivalent if $\mathcal{R}$ is unitary !

* Robledo, PRC C50, 2874 (1994), PRC105, L021307 (2022), PL B866, 139550 (2025)

** Robledo, PRC105, 044317 (2022)

GWT non equivalent bases: some considerations

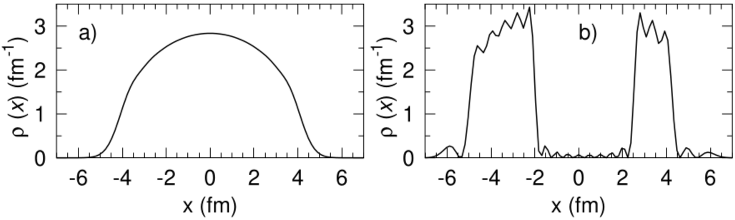
- The zero pairing limit of the GWT-NEB coincides with Simenel's result for HF states. This is not the case if $\left(\mathcal{R}^T\right)^{-1}$ is replaced by $\mathcal{R}^*$
- One can work out a pfaffian formula for the overlap of HFB states expressed in different bases[1]. The result is equivalent[2] to the formula in[3].
- Pfaffian formulas for operator overlaps[3] are only defined for equivalent bases. A generalization is still missing.
- For a reinterpretation in terms of quantum information and entanglement, see arXiv:2503.02696
- **Warning:** One can find in the literature several papers where the standard formalism, not justified in this case, is used.

[1] L. M. Robledo, Phys. Rev. C 84, 014307 (2011)
[2] L. Robledo, Physics Letters B 866, 139550 (2025)
[3] G. F. Bertsch and L. M. Robledo, Phys. Rev. Lett. 108, 042505 (2012)

Application in a toy model

- Basis of $N = 40$ 1D-HO states with oscillator length $b = 1$ fm
- Occupancies $v_n^2 = 1/(1 + \exp(n + 1 - n_0)/\sigma)$ where $n_0 = 10.5$ and $\sigma = 1$
- Average number of particles: 20
- To obtain a 2 fragment solution a transformation to a DVR basis is performed
- Occupancies for most of the DVR basis states zero, but $v_k^2 = 0.9$ for those with mesh points in between -4.6 fm and -2.25 fm (larger fragment) and in between 2.78 fm and 3.94 fm (smaller fragment)

Matter density corresponding to the two cases studed

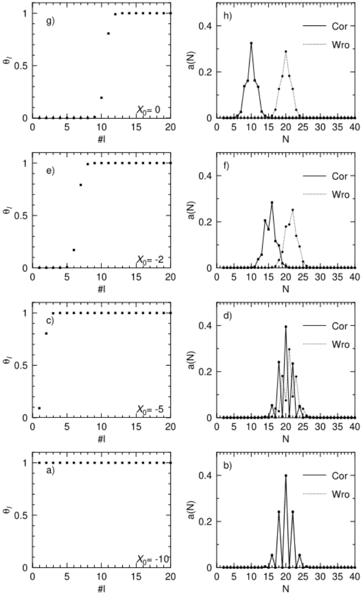


Application in a toy model (one fragment)

- Domain $\mathcal{D}$ given by $\theta(x - x_0)$ with $x_0 =$ -10, -5, -2 and 0. fm
- θ_l are the eigenvalues of the overlap matrix $\mathcal{O}$
- $a(N) = \langle \Psi | \Psi_{\mathcal{D}}^N \rangle$

$$a(N) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \langle \Psi | e^{i\varphi(\hat{N}_{\mathcal{D}} - N)} | \Psi \rangle$$

- Cor stands for present formalist, Wro for the one incorrectly assuming the standard GWT
- Both coincide for $x_0 = -10$ fm
- Have the same sum rule value $\langle N \rangle = \sum_N a(N) \times N$
- Sum rule differs for other x_0 values

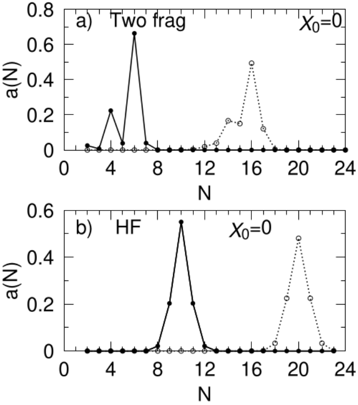


Application in a toy model (two fragments case)

- Domain $\mathcal{D}$ given by $\theta(x - x_0)$ with $x_0 = 0$ fm
- Average number of particles on the right fragment 5.4
- $a(N) = \langle \Psi | \Psi^N_{\mathcal{D}} \rangle$

$$a(N) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \langle \Psi | e^{i\varphi(\hat{N}_{\mathcal{D}} - N)} | \Psi \rangle$$

- Full lines stand for present formalist, dotted ones for the one incorrectly assuming the standard GWT
- In the HF limit the $a(N)$ computed with Simenel's formula is also plotted. It lies on top of the full line obtained with the present formalism



Realistic applications

- The formalism presented here is used by Marevic and Schunck in their fission calculations restoring angular momentum both in the whole nucleus and in the fragments

MICROSCOPIC THEORY OF ANGULAR MOMENTUM ... PHYSICAL REVIEW C **113**, 014612 (2026)

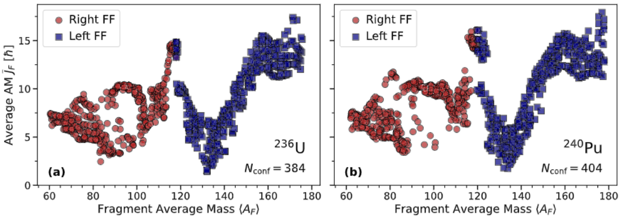


FIG. 3. Average angular momentum magnitude [Eq. (32)] of left FFs (blue squares) and right FFs (red circles) in all scission configurations for ^{236}U [panel (a)] and ^{240}Pu [panel (b)], as a function of the average FF mass [Eq. (36a)]. A sawtooth pattern is apparent in both nuclei.

- Scamps and Lacroix use the pfaffian formula of Bertsch and Robledo to compute $a(N)$. As mentioned before, the formula for the overlap is equivalent to the present formalism but not in the case of computing operator overlaps.

Concluding remarks

- It is essential to pay attention to potential problems associated with the use of finite bases, as they are the only alternative to numeric calculations
- The GWT for non equivalent bases (or alternative formulations) must be used, as the alternative of using bases unitarily equivalent is not an option in fission
- The formalism can be easily extended to angular momentum projection (see Marevic and Schunck)
- Clarification: The formalism for particle number projection on a domain presented here is discussed in the paper arXiv:2503.02696. For reasons unknown to the author, the paper is still in APS limbo

Backup: Contractions

Use GWT to write overlaps in terms of the contractions

$$\rho^{01}_{lk} = \frac{\langle \phi_0 | c^\dagger_{0,k} c_{1,l} | \phi_1 \rangle}{\langle \phi_0 | \phi_1 \rangle} = \begin{cases} \left[\bar{V}_1^* A^{-1} \bar{V}_0^T \right]_{lk} & l \subset \mathcal{B}_0, k \subset \mathcal{B}_1 \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

$$\bar{\kappa}^{01}_{k_1 k_2} = \frac{\langle \phi_0 | c^\dagger_{0,k_1} c^\dagger_{0,k_2} | \phi_1 \rangle}{\langle \phi_0 | \phi_1 \rangle} = \begin{cases} - \left[\left(\mathcal{R}^T \right)^{-1} \bar{U}_1^* A^{-1} \bar{V}_0^T \right]_{k_1 k_2} & k_1 \subset \mathcal{B}_0, k_2 \subset \mathcal{B}_0 \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

$$\kappa^{10}_{l_1 l_2} = \frac{\langle \phi_0 | c_{1,l_1} c_{1,l_2} | \phi_1 \rangle}{\langle \phi_0 | \phi_1 \rangle} = \begin{cases} \left[\bar{V}_1^* A^{-1} \bar{U}_0^T \left(\mathcal{R}^T \right)^{-1} \right]_{l_1 l_2} & l_1 \subset \mathcal{B}_1, l_2 \subset \mathcal{B}_1 \\ 0 & \text{otherwise} \end{cases} \tag{3}$$