Physics

The Fission Process (I)

EBSS 2014 Summer School

W. Younes

Physical and Life Sciences

Lawrence Livermore National Laboratory

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

"*it is conceivable that the nucleus breaks up into several large fragments, which would of course be isotopes of known elements but would not be neighbors of the irradiated element.*" – **Ida Noddak (1934)**

Fission is everywhere!

From the earth…

nature geoscience

nature.com ▸ journal home ▸ archive ▸ issue ▸ article ▸ abstract

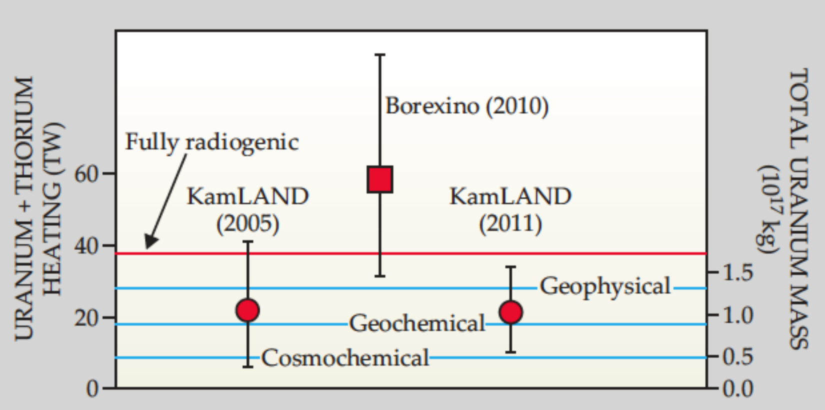
NATURE GEOSCIENCE | ARTICLE

Partial radiogenic heat model for Earth revealed by geoneutrino measurements

The KamLAND Collaboration

Affiliations | Contributions | Corresponding author

Nature Geoscience **4**, 647–651 (2011) | doi:10.1038/ngeo1205
Received 05 November 2010 | Accepted 14 June 2011 | Published online 17 July 2011



Physics Today 65, 46 (2012)

Nuclear fission confirmed as source of more than half of earth's heat

…To the stars

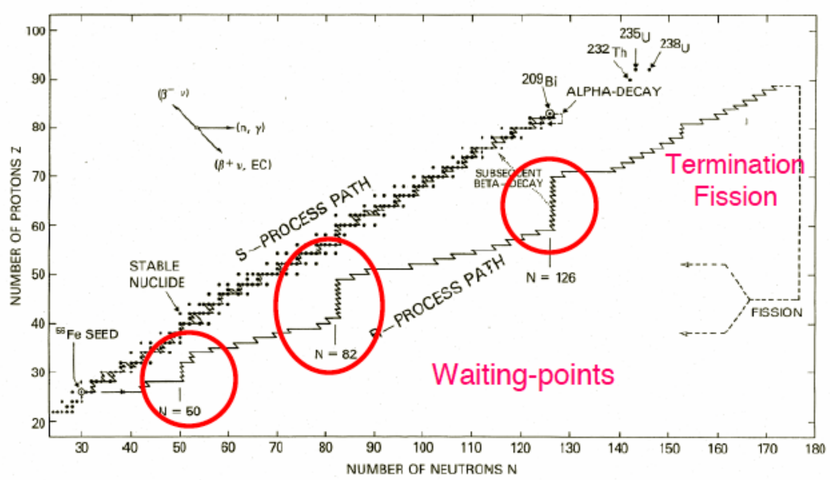
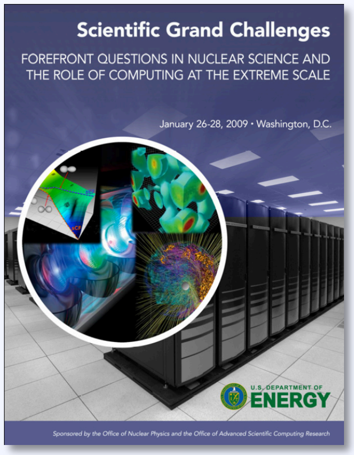


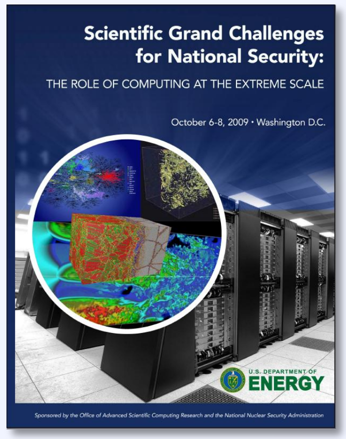
FIGURE 9.13. Neutron-capture paths for the *s*-process and the *r*-process are shown in the (*N*, *Z*)-plane. Both paths start with the iron-peak nuclei as seeds (mainly ^{56}Fe). The *s*-process follows a path along the stability line and terminates finally above ^{209}Bi via α-decay (Cla67). The *r*-process drives the nuclear matter far to the neutron-rich side of the stability line, and the neutron capture flows upward in the (*N*, *Z*)-plane until β-delayed fission and neutron-induced fission occur (Thi83). The *r*-process path shown was computed (See65) for the conditions $T_9 = 1.0$ and $N_n = 10^{24}$ neutrons cm^{-3}.

Fission limits heaviest element production & re-seeds r process

Isn’t fission a closed topic after 80 years?

- No! Tremendous conceptual and technical challenges remain





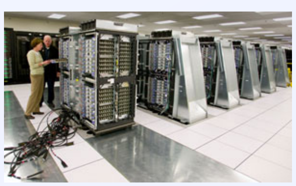
The microscopic description of nuclear fission is one of four Priority Research Directions for both basic <u>and</u> applied science

- The problem must be attacked on all fronts

Theory

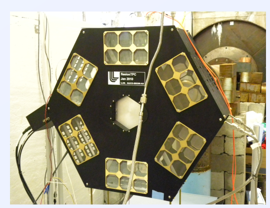
↕

HPC ⟷ Understanding Fission ⟷ Data Evaluation



↕

Experiments (TPC,…)



“Problems worthy of attack prove their worth by hitting back” – Piet Hein

What are some of the open questions?

- How is energy distributed in fission (kinetic vs. excitation, heavy vs. light fragment)?
- What is the interplay between collective and single-particle d.o.f.?
- What are the relevant d.o.f. as the nucleus approaches scission?
- What is scission in a quantum-mechanical context?
- How does fission behave in exotic environments (e.g. supernovae, crusts of neutron stars)
- …

A complex problem that has spawned different lines of attack

Liquid-drop model (1939-)

Statistical scission-point models (1970's-)

Microscopic models (1980's-)

I will focus on the microscopic approach for these lectures

But you should be aware of interesting recent work being done in other approaches as well

Work based on the liquid-drop model:

PRL **106,** 132503 (2011) PHYSICAL REVIEW LETTERS week ending 1 APRIL 2011

Brownian Shape Motion on Five-Dimensional Potential-Energy Surfaces: Nuclear Fission-Fragment Mass Distributions

Jørgen Randrup[1] and Peter Möller[2]

[1]*Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
[2]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

(Received 1 December 2010; published 30 March 2011)

Work based on a statistical scission-point model:

PRL **111,** 242502 (2013) PHYSICAL REVIEW LETTERS week ending 13 DECEMBER 2013

New Fission Fragment Distributions and *r*-Process Origin of the Rare-Earth Elements

S. Goriely,[1] J.-L. Sida,[2] J.-F. Lemaître,[2] S. Panebianco,[2] N. Dubray,[3] S. Hilaire,[3] A. Bauswein,[4,5] and H.-T. Janka[5]

[1]*Institut d'Astronomie et d'Astrophysique, CP-226, Université Libre de Bruxelles, 1050 Brussels, Belgium*
[2]*C.E.A. Saclay, Irfu/Service de Physique Nucléaire, 91191 Gif-sur-Yvette, France*
[3]*CEA, DAM, DIF, F-91297 Arpajon, France*
[4]*Department of Physics, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece*
[5]*Max-Planck-Institut für Astrophysik, Postfach 1317, 85741 Garching, Germany*

(Received 10 September 2013; revised manuscript received 26 October 2013; published 9 December 2013)

What is the microscopic approach?

Idea of microscopic approach:

Effective nucleon interaction (parameters) → **Hamiltonian** →

- **Particle densities**
- **Potential energy surface**
- **Inertia tensor**
- **Spectrum of states**
- **…**

Effective interaction is the only phenomenological input

The hierarchy of the microscopic approach

- Starting point is effective interaction between nucleons
  - Finite-range, fit a-priori, to very few nuclear data
- Simplest treatment of nucleon correlations is Mean Field
  - Valid if nearby excitations $\gg$ residual interaction (e.g., magic nuclei)
  - Otherwise true wave function mixes with nearby excitations
- Introduce correlations into Hamiltonian via successive improvements
  1. $H_{true} \approx H_{MF}$ (Hartree-Fock)
  2. $H_{true} \approx H_{MF} + V_{pair}$ (Hartree-Fock-Bogoliubov)
  3. $H_{true} \approx H_{MF} + V_{pair} + V_{coll}$ (Generator-coordinate method)
  4. $H_{true} \approx H_{MF} + V_{pair} + V_{coll} + V_{coll\text{-}intr}$ (GCM + qp excitations)
  5. …

Tractable approach to a microscopic treatment of fission

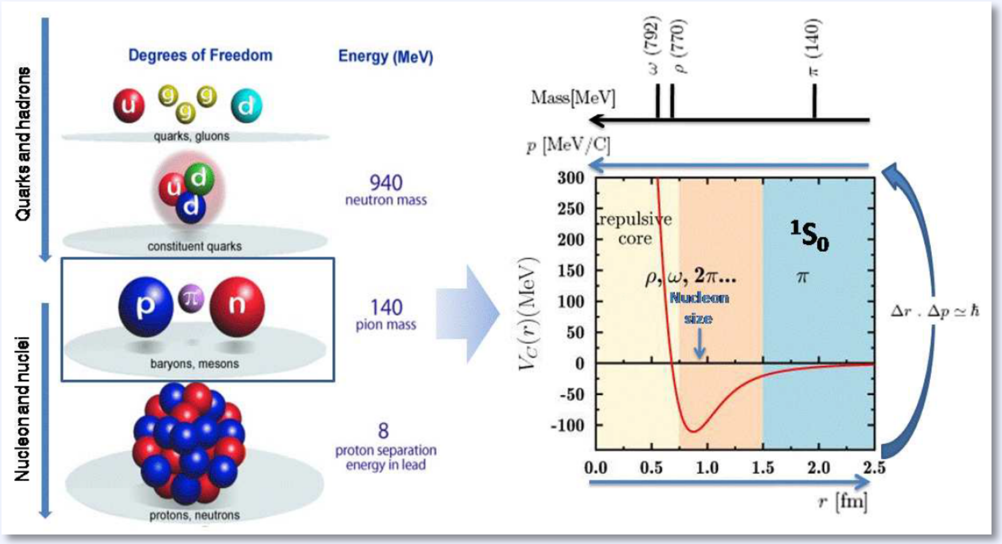
Some features of the microscopic approach

- Ingredients: protons, neutrons, and an effective interaction between them
- The spatial distribution of nucleons is a result, not an input
  - Found by minimizing the energy
  - In a fully microscopic approach, no parameters depending on A, Z, or the configuration of the nucleus
  - Important in fission since the system explores very exotic "shapes"
- Unified description of both single-particle and collective dof
  - Mean field constructed from nucleon dof
  - Residual interactions between nucleons can then cause this mean field to oscillate , generating a spectrum of collective states
- Starting point is Hamiltonian of A interacting nucleons
  - Quantum mechanics is built in from the start

But there are major challenges…

Challenge 1: we don't yet have a fundamental theory of the nucleon-nucleon interaction

We do not yet have a nuclear interaction completely derived from QCD



Although important progress is being made in that direction
(see, e.g., http://www.cenbg.in2p3.fr/heberge/EcoleJoliotCurie/coursannee/cours/D_lacroix.pdf)

For now, we use an <u>effective</u> interaction, with parameters adjusted to data

Effective interactions 101

- The N-N interaction is modified by its presence inside a nucleus
- Can be approximated by simple functional forms
  - Delta function ⇒ zero range

T.H.R. Skyrme, Phil. Mag. 1, 1043 (1956)

$$V\left(\vec{r}_1,\vec{r}_2\right) \sim \delta\left(\vec{r}_1 - \vec{r}_2\right)$$

  - Gaussian ⇒ finite range

D. Gogny, in “Nuclear self-consistent fields”, p. 333 (1975)

$$V\left(\vec{r}_1,\vec{r}_2\right) \sim e^{-\left(\vec{r}_1-\vec{r}_2\right)^2/\mu^2}$$

    - More computationally demanding than delta
    - Avoids mathematical pathologies of delta
    - This is what I will use for the rest of this lecture

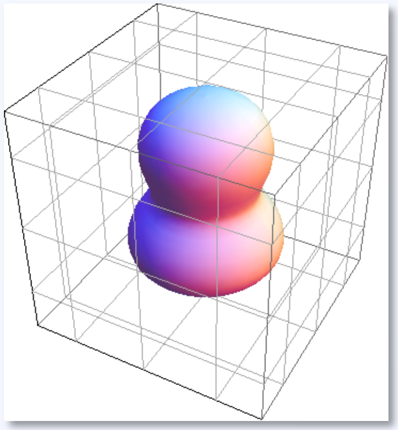
For simplicity, I have not written all the terms.
There are a dozen free parameters from those terms

Fixing the parameters of the interaction

- Parameters adjusted to a small number of quantities
  - Infinite nuclear matter
    - Saturation properties (E/A and k_F)
    - Incompressibility K_∞
    - Asymmetry parameter
  - Semi-infinite nuclear matter
    - Surface coefficient
  - Finite nuclei
    - Binding energies of ^{18}O and ^{90}Zr
    - Energy difference $1p_{1/2} - 1p_{3/2}$ in ^{16}O
    - Odd-even mass differences in a few Sn isotopes
    - Barrier height in ^{240}Pu

Important: not tuned to fission observables!

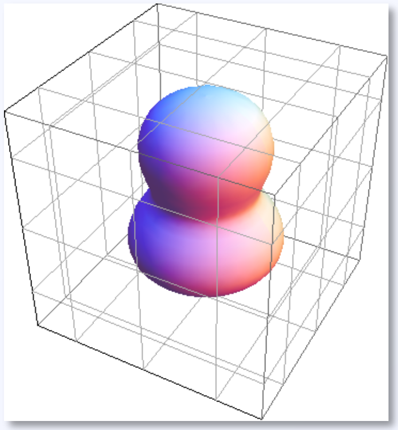
Challenge 2: Fission is a difficult quantum many body problem



Sizing up the problem with a simplistic calculation:

For ^{240}Pu fission: distribute 94 protons & 146 neutrons on 3D spatial lattice + spin, 20 fm to the side, 1 fm spacing $\Rightarrow 20^3 \times 2 = 16000$ lattice points:

Challenge 2: Fission is a difficult quantum many body problem

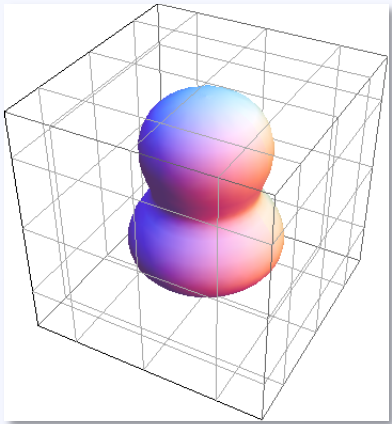


Sizing up the problem with a simplistic calculation:

For ^{240}Pu fission: distribute 94 protons & 146 neutrons on 3D spatial lattice + spin, 20 fm to the side, 1 fm spacing ⇒ $20^3 \times 2$ = 16000 lattice points:

$$\binom{16000}{94} \times \binom{16000}{146} \approx 10^{608} \text{ configurations!!!}$$

Challenge 2: Fission is a difficult quantum many body problem



Sizing up the problem with a simplistic calculation:

For ^{240}Pu fission: distribute 94 protons & 146 neutrons on 3D spatial lattice + spin, 20 fm to the side, 1 fm spacing ⇒ $20^3 \times 2 = 16000$ lattice points:

$$\binom{16000}{94} \times \binom{16000}{146} \approx 10^{608} \text{ configurations!!!}$$

- Too complicated to describe with full many-body wave function

⇒ Start with simplified picture, restore complexity in order of importance

⇒ Need High Performance Computing

⇒ Need to solve some tough conceptual problems
  - What are the relevant degrees of freedom? (collective vs. intrinsic)
  - How does the coupling between them affect fission?
  - What is scission? How do we separate pre- and post-scission?
  - …

The Hartree-Fock approximation

- The full many-body wave function has too many terms

$$\Psi = \sum_{\text{all configs}} c_{\text{config}} \left|\text{config}\right\rangle \qquad \text{number of terms} \sim \begin{pmatrix} \text{states} \\ \text{nucleons} \end{pmatrix}$$

- There are two commonly used solutions
  - The shell model: reduce the number of terms by restricting the number of states and nucleons to a few outside a closed shell
  - The Hartree-Fock approximation: replace Ψ with a simpler form:
    - Single Slater determinant, choose ~~the~~ one that minimizes the energy
    - e.g., for a system of 2 nucleons:

$$\Psi(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}} \begin{bmatrix} \varphi_a(\vec{r}_1) & \varphi_a(\vec{r}_2) \\ \varphi_b(\vec{r}_1) & \varphi_b(\vec{r}_2) \end{bmatrix} = \frac{1}{\sqrt{2}} \left[\varphi_a(\vec{r}_1)\varphi_b(\vec{r}_2) - \varphi_b(\vec{r}_1)\varphi_a(\vec{r}_2) \right]$$

This is not the most general form for Ψ(1,2,….): we are sacrificing some particle correlations for the sake of tractability

Solving the Hartree-Fock equations

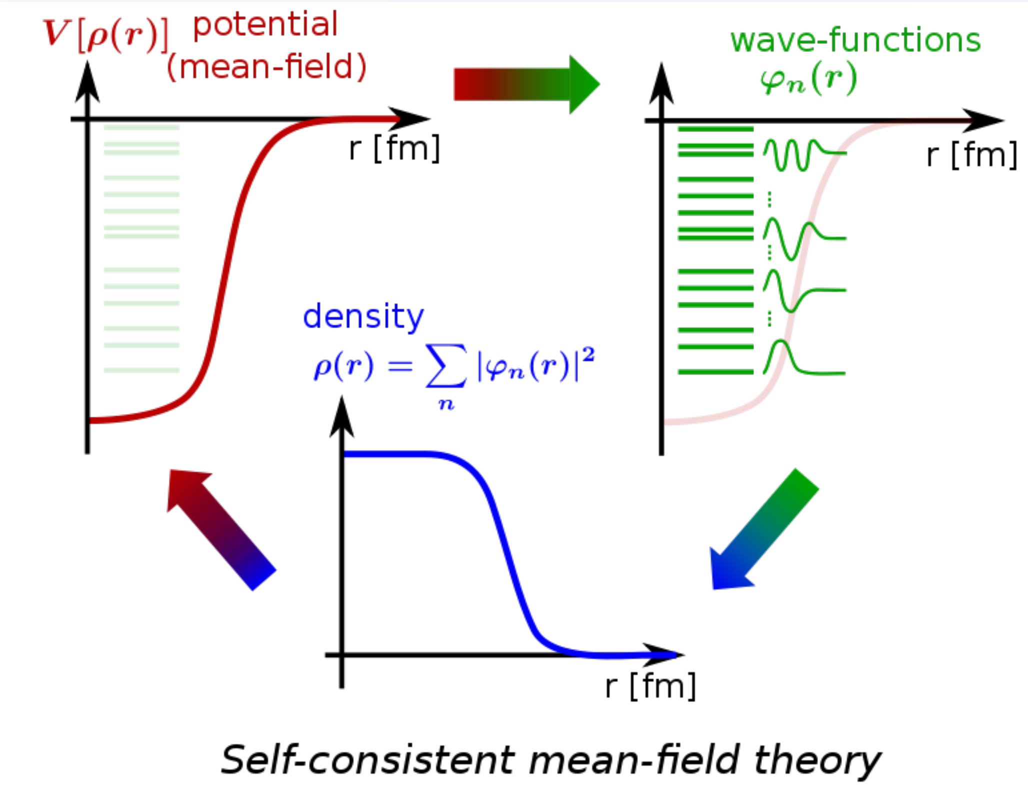


Image from commons.wikimedia.org

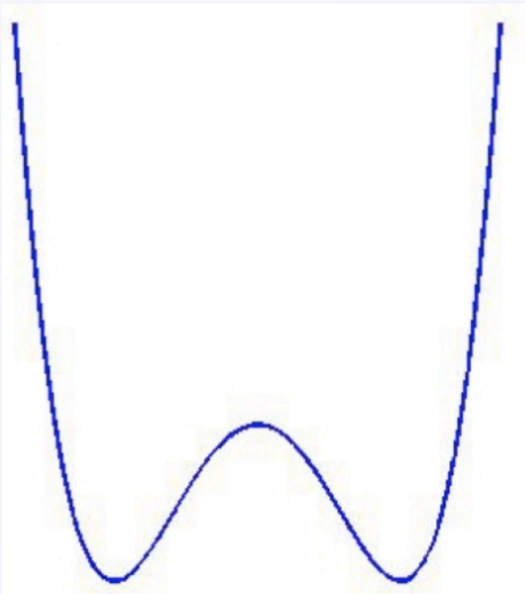
- From the Slater determinant, we calculate a one-particle density ρ
- From ρ we calculate a potential energy
- From the potential energy we get single-particle states $\varphi_n \Rightarrow$ Slater determinant

$\Rightarrow$ Hartree-Fock eqs are derived by a variational method and solved by an iterative process

$\Rightarrow$ Independent particles in a mean field, system in its lowest-energy state

Constrained Hartree Fock

Example:



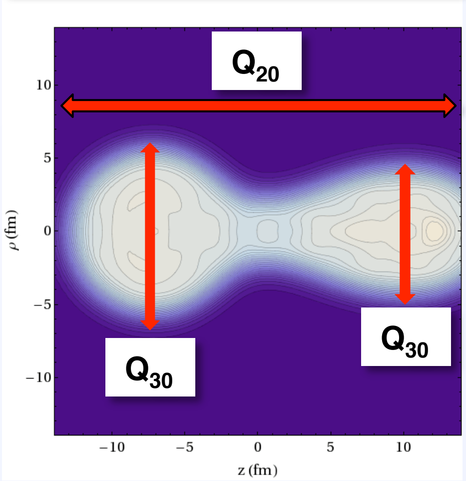
- Two minima in potential
- How do we reach both minima with Hartree Fock?
- Add a constraint to the minimization process via the method of Lagrange multipliers:

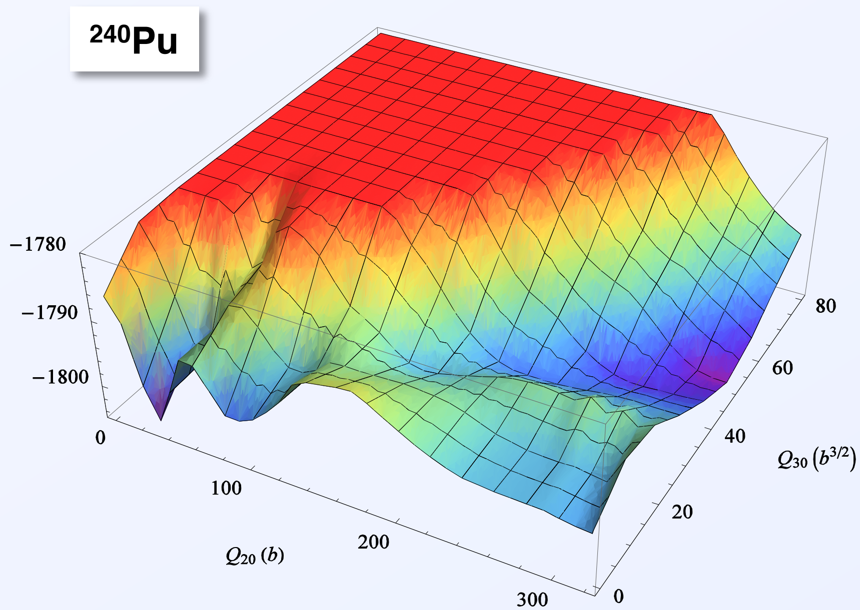
$$\delta\left\langle \mathrm{HF}\middle|\hat{H}-\lambda\hat{Q}\middle|\mathrm{HF}\right\rangle = 0$$

In fact, with constraints we can explore the entire potential energy curve (and not just the minima)

Example of constraints: quadrupole and octupole moments

$|\Phi(q)\rangle$ = mean-field solution at $q = \{Q_{20}, Q_{30}\}$





$$\left\langle \hat{Q}_{\ell m} \right\rangle = \int Y^*_{\ell m}(\theta,\phi) r^\ell \rho(\vec{x}) d^3x$$

Q_{20} controls "stretching" of nucleus
Q_{30} controls mass asymmetry

Beyond Hartree Fock: Hartree-Fock Bogoliubov

- HF generalized to HFB by: M. Baranger, Phys. Rev. 122, 992 (1961)
- Energy gap in even-even nuclei suggests independent-particle picture is incomplete
  - need to include pairing correlations!
  - This means going beyond mean field approximation
- Therefore the goal is:

Generalize Hartree Fock to describe independent pairs of correlated nucleons

Preserves the spirit of the mean-field approximation

Introduces pairing

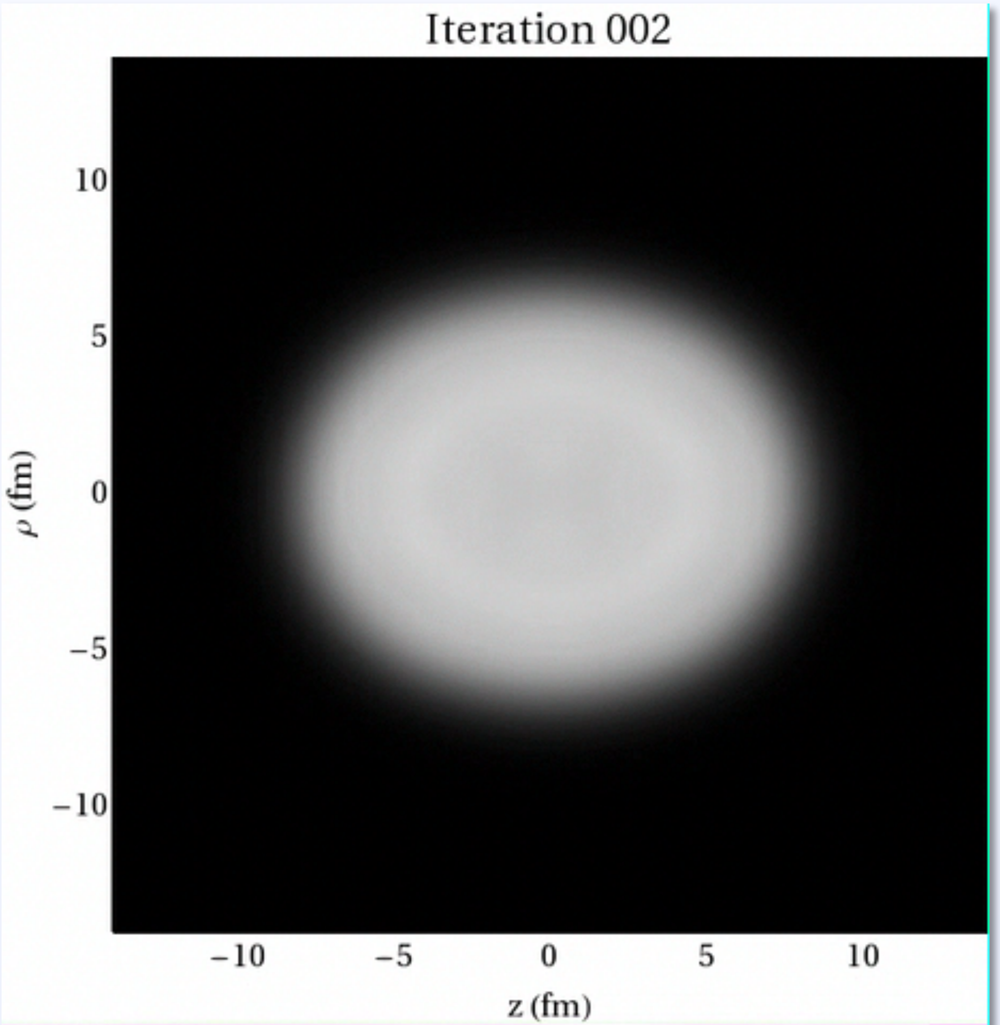
How do we do this?

Beyond Hartree Fock: Hartree-Fock Bogoliubov (cont)

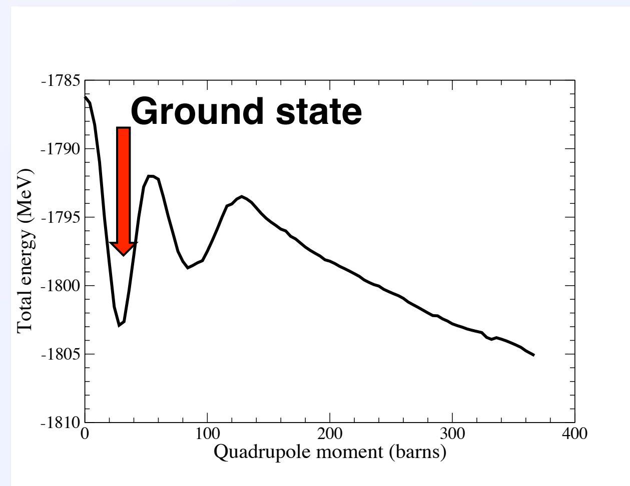
- Remember, we want independent pairs of <u>correlated</u> nucleons
- For example:
  - $\hat{a}_i^\dagger \hat{a}_j^\dagger$ creates a pair of <u>independent</u> nucleons
  - $P^\dagger \equiv \sum_{i>0} p_i \hat{a}_i^\dagger \hat{a}_{\bar{i}}^\dagger$ creates pairs of <u>correlated</u> nucleons
    - But the wave function $|\Psi\rangle \equiv \left(P^\dagger\right)^{N/2} |\mathrm{vacuum}\rangle$ is too complicated
- Instead, we use (Cooper pairs): $P_i^\dagger \equiv u_i + v_i \hat{a}_i^\dagger \hat{a}_{\bar{i}}^\dagger$
- And the ground state is: $|\Psi\rangle = P_1^\dagger P_2^\dagger \ldots P_{N/2}^\dagger |\mathrm{vacuum}\rangle$
- We can introduce the quasiparticle destruction operator: $\hat{\eta}_i \equiv u_i \hat{a}_i - v_i \hat{a}_{\bar{i}}^\dagger$
- And then $|\Psi\rangle \propto \eta_1 \eta_{\bar{1}} \eta_2 \eta_{\bar{2}} \ldots |\mathrm{vacuum}\rangle$ (i.e., the G.S. is the state without qp excitations)

HFB is then a mean-field theory for this new type of ground state

Example: ground state of ^{240}Pu

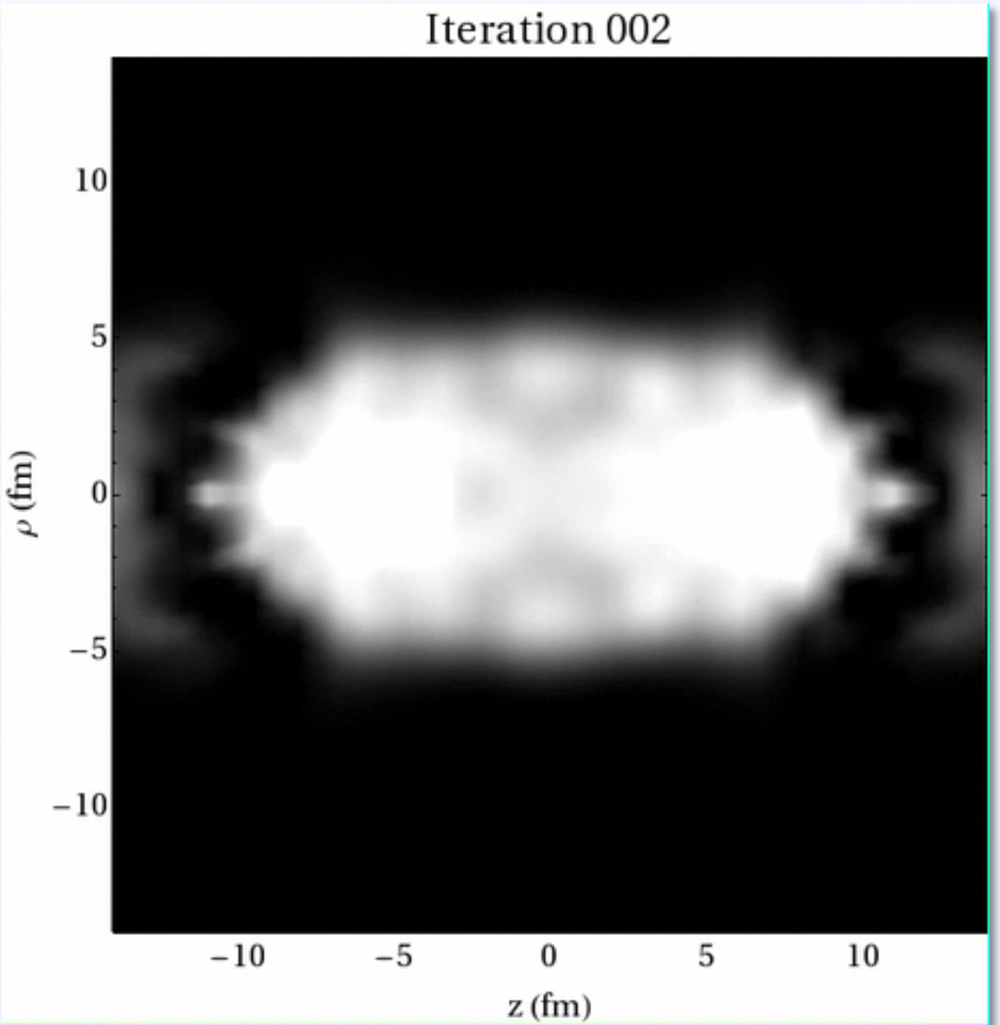


- Initial state = Slater determinant on deformed harmonic oscillator basis

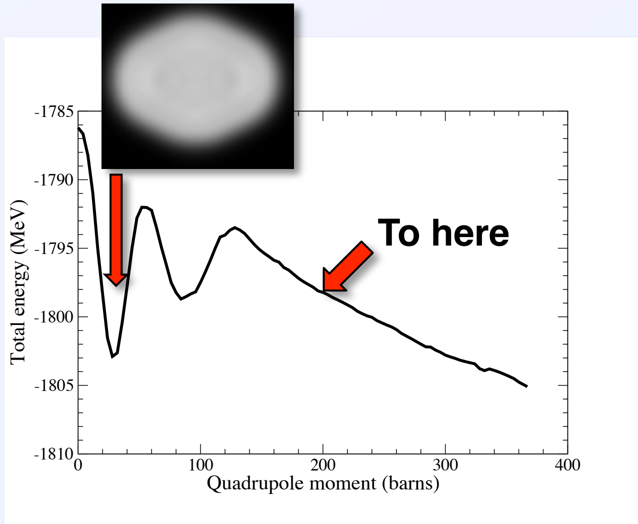


- Density settles rapidly into ground-state configuration (variational methods love minima!)

Example: deformed state of ^{240}Pu with Q_{20} = 200 b

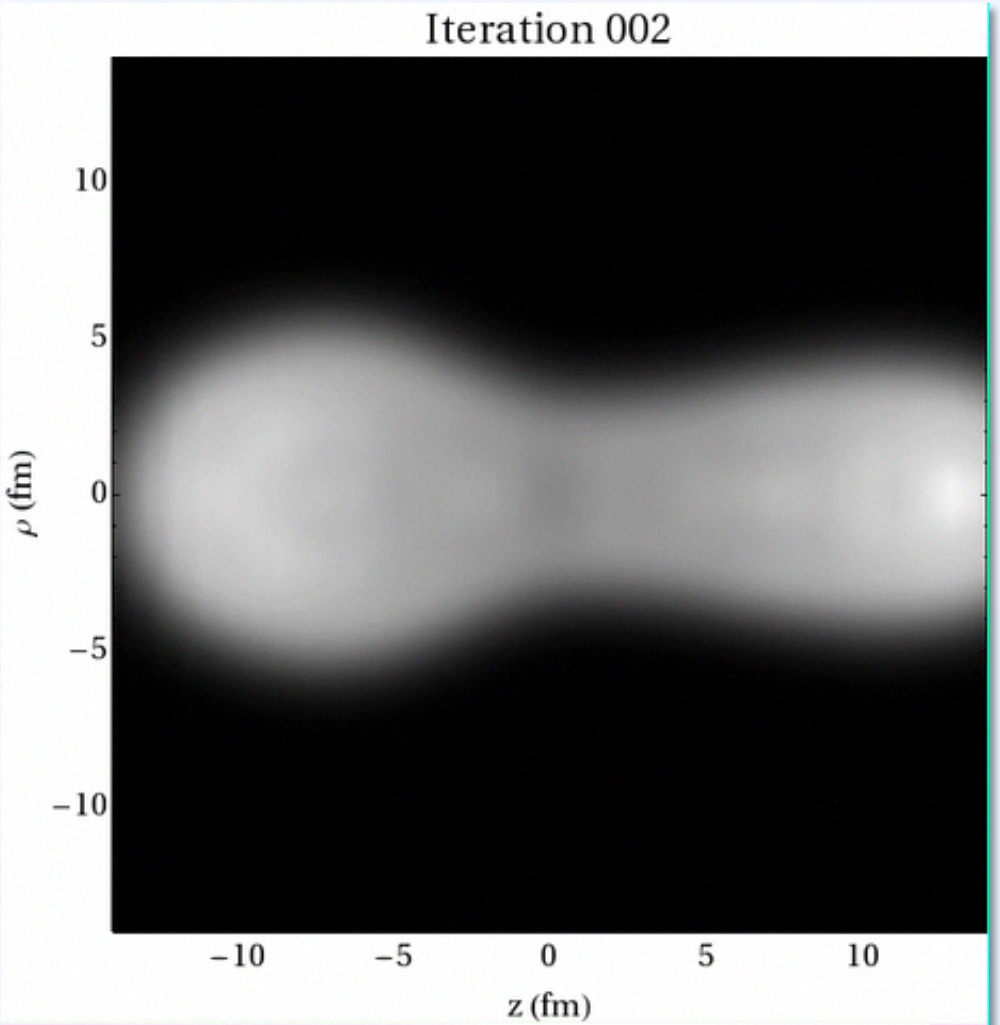


- Starting point is ground state solution:

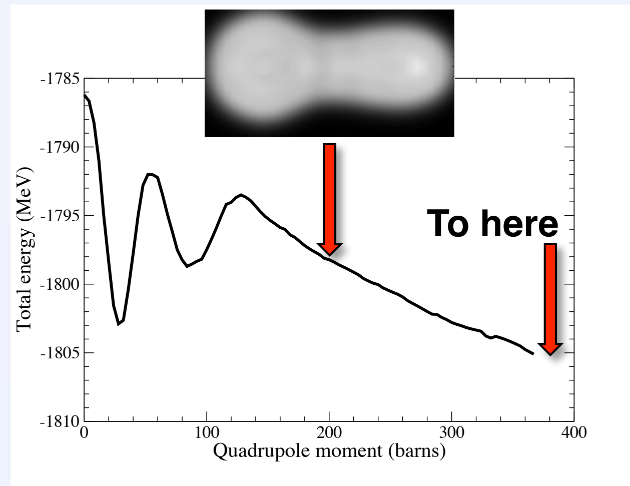


- Need constraint on Q_{20}
- Converges much more slowly
- Note mass asymmetry

Example: deformed state of ^{240}Pu with Q_{20} = 380 b



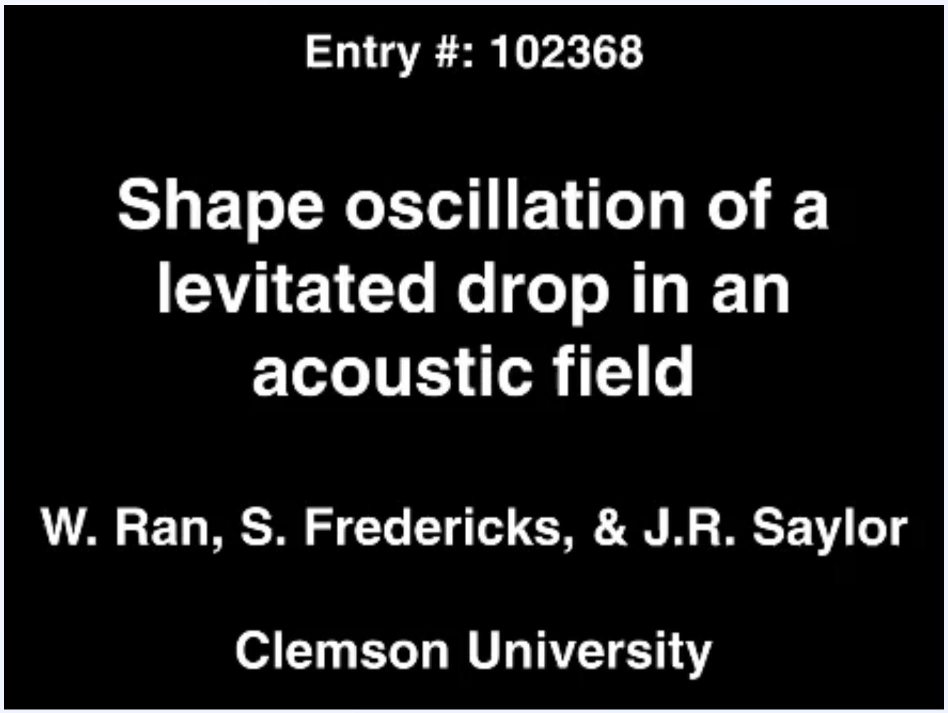
- Starting point is Q_{20} = 200 b solution:



- Need constraint on Q_{20}
- Converges very slowly
- Note that we have reached scission!

Collective and single-particle motion

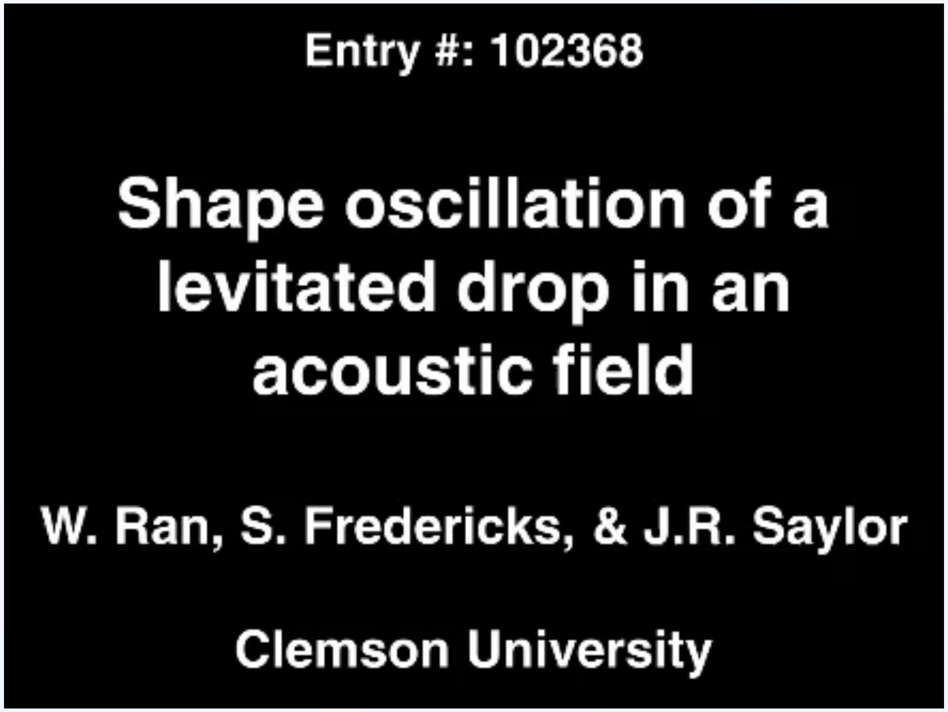
An example of collective motion:



From: W. Ran et al., arXiv:1310.2967v2 (2013)

Collective and single-particle motion

An example of collective motion:

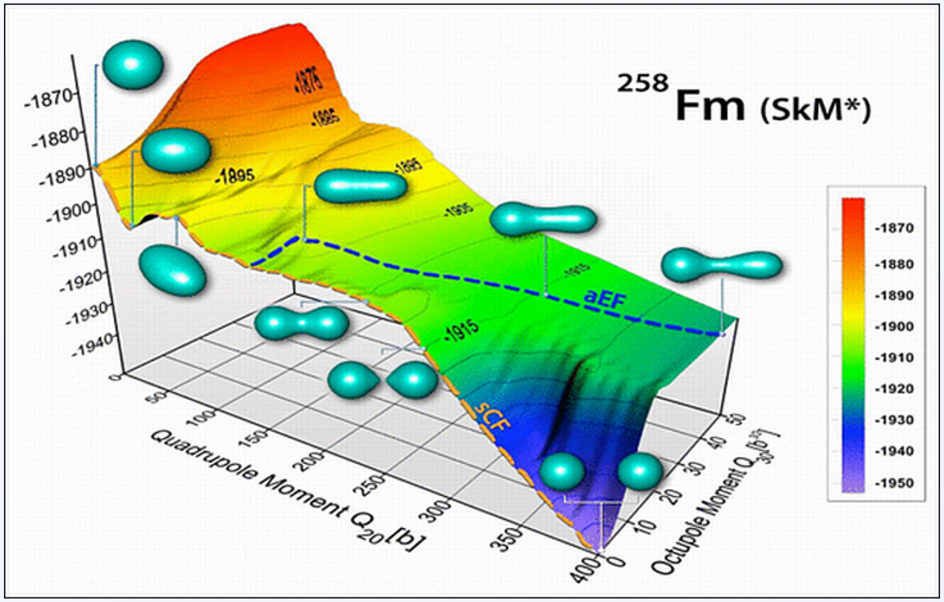


From: W. Ran et al., [arXiv:1310.2967v2] (2013)

Building collective motion from single-particle d.o.f.

How do we do this for nuclei?

Building collective motion from single particles: the nucleus



From ascr-discovery.science.doe.gov
Credit: *A. Staszczak et al., ORNL*

- Each point on map is a single-particle configuration: HFB ⇒ $\Phi(q)$
- The nucleus explores many such configurations ⇒ form linear superposition of $\Phi(q)$:

$$|\Psi\rangle = \int dq\, f(q) |\Phi(q)\rangle$$

- Use variational procedure to determine the weights $f(q)$

- This is the Generator Coordinate Method (GCM) first proposed by Hill & Wheeler in Phys. Rev. 89, 1106 (1953)
- A truly quantum-mechanical description of collectivity built from single-particle degrees of freedom

Calculations using the GCM

GCM wave function: $|\Psi\rangle = \int dq\, f(q)|\Phi(q)\rangle$

&

Variational principle: $\delta E = \delta \dfrac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 0$

Hill-Wheeler equation: $\int dq' \left[\langle\Phi(q)|H|\Phi(q')\rangle - E\langle\Phi(q)|\Phi(q')\rangle\right] f(q') = 0$

Integro-differential, non-local, non-linear equation = a nightmare in all but the simplest cases!

Non-orthogonal wf ⇒ overlap

Calculations using the GCM

GCM wave function: $|\Psi\rangle = \int dq\, f(q) |\Phi(q)\rangle$

&

Variational principle: $\delta E = \delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$

Hill-Wheeler equation: $\int dq' \left[\langle \Phi(q) | H | \Phi(q') \rangle - E \langle \Phi(q) | \Phi(q') \rangle \right] f(q') = 0$

Integro-differential, non-local, non-linear equation = a nightmare in all but the simplest cases!

Expand to 2nd order in non-locality s ≡ *q-q'*

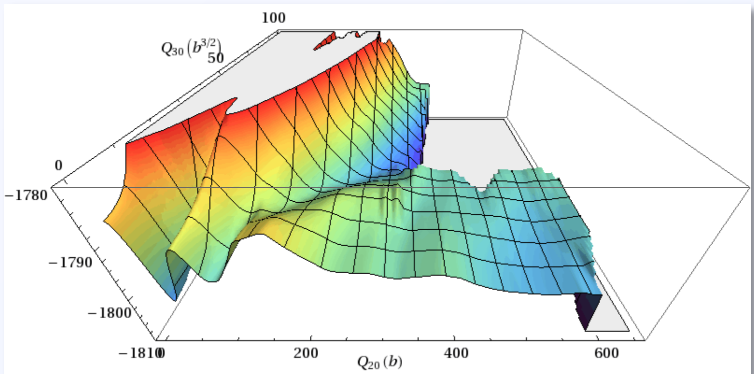
$\bar{q} \equiv \frac{q+q'}{2}$

$$\left[\overbrace{-\frac{1}{2} \frac{\partial}{\partial \bar{q}} \underbrace{B(\bar{q})}_{\text{inertia tensor}} \frac{\partial}{\partial \bar{q}}}^{\text{kinetic}} + \overbrace{\underbrace{\langle \Phi(\bar{q}) | H | \Phi(\bar{q}) \rangle}_{\text{HFB energy}} - \underbrace{\varepsilon_0(\bar{q})}_{\text{zero-point energy}}}^{\text{potential}} \right] g(\bar{q}) = E g(\bar{q})$$

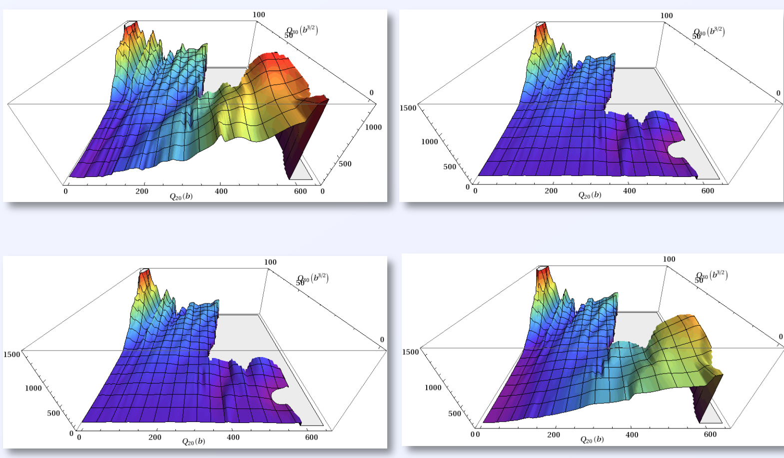
- **Collective Hamiltonian from single particles!**
- **Schrödinger-like equation in the collective coordinates**

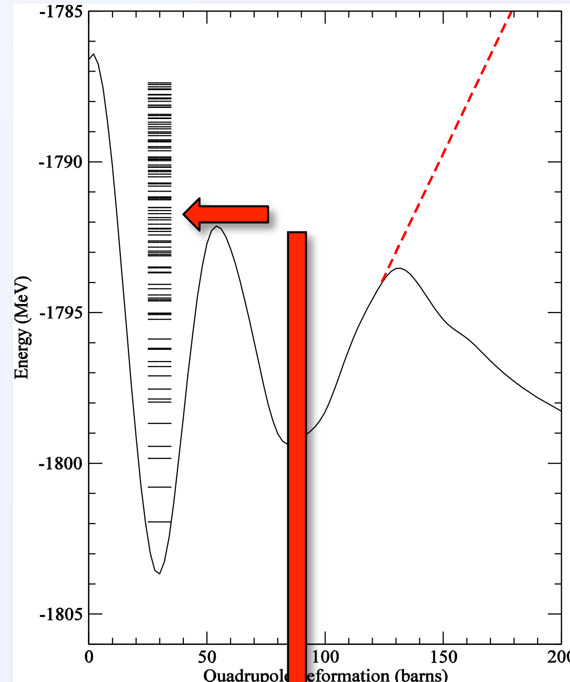
Application of the GCM: collective spectrum of ^{240}Pu

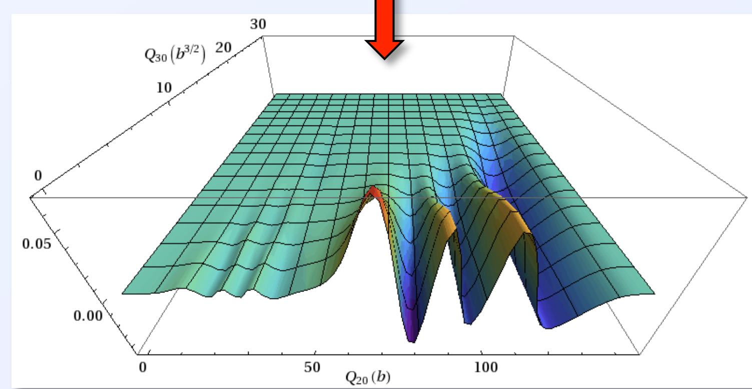
$$V\left(Q_{20},Q_{30}\right)=$$



$$B\left(Q_{20},Q_{30}\right)=$$







What have we learned so far? What's next?

- Fission is an old, but topical problem in nuclear physics
- Several approaches have been developed to tackle this difficult problem
- In the microscopic approach, the nucleus is built up from protons, neutrons, and an effective interaction
  - Effective interaction is the only phenomenological input
  - Starting point is mean field = independent particle model
  - Missing correlations are restored in a hierarchical approach
- The generator-coordinate method builds a collective Hamiltonian from the underlying single-particle degrees of freedom
- Next lecture:
  - Dynamics
  - Scission
  - Calculation of fission-fragment properties