Some Open Problems in Nuclear Large Amplitude Collective Motion (including fission)

Aurel Bulgac
University of Washington
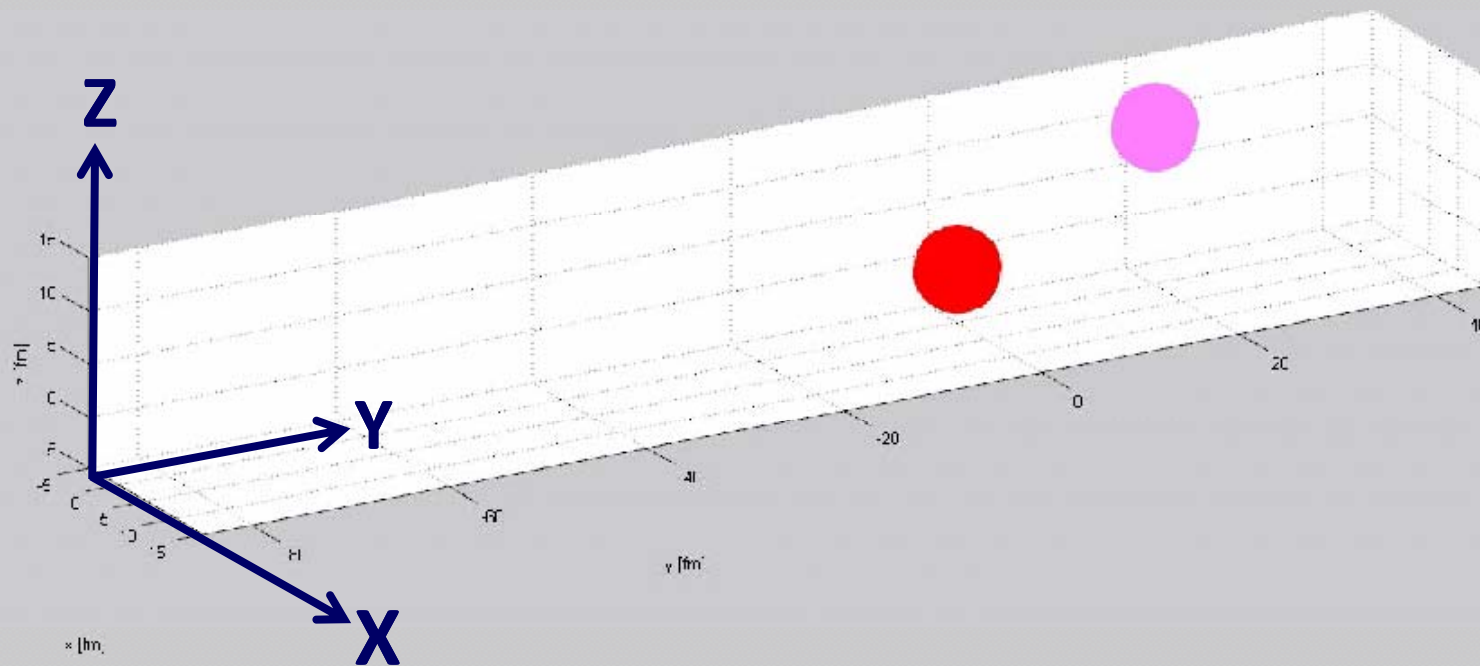
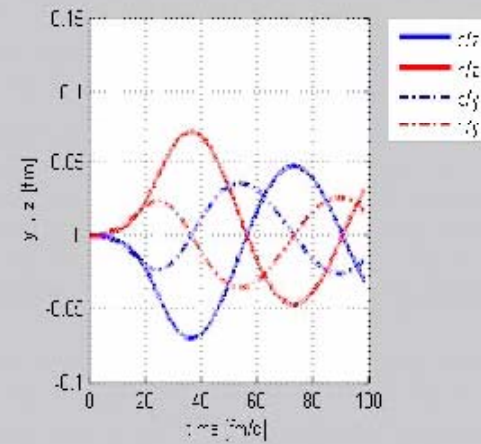**This will consist mostly a discussion of some issues with LACM and future possible approaches**
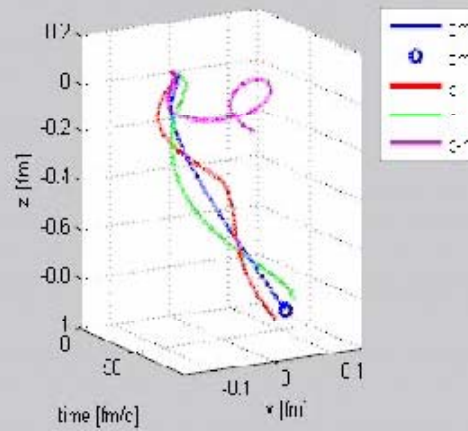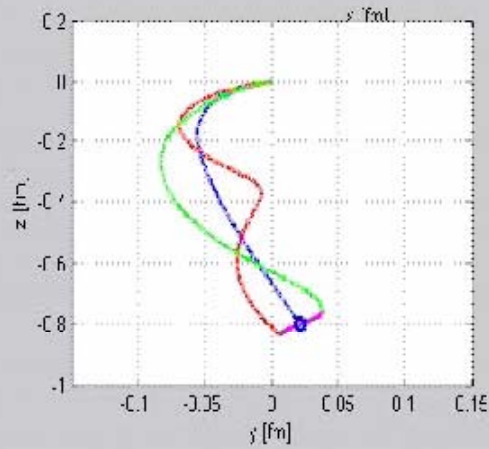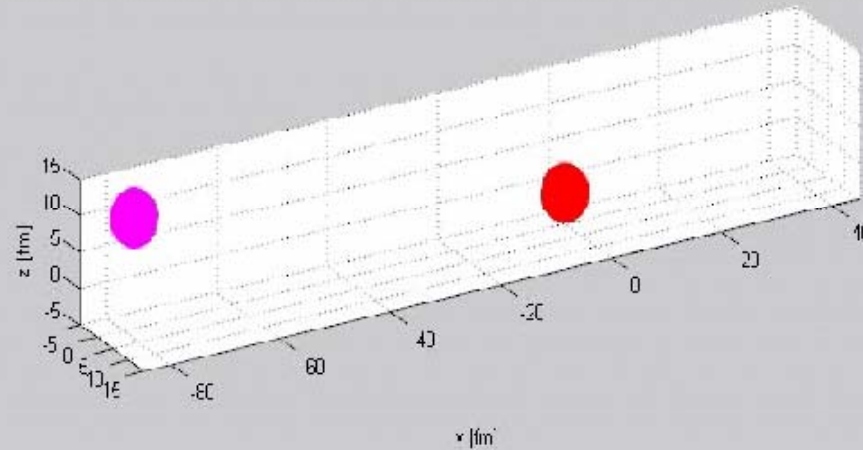
I will show some results due to my collaboration with:

Sukjin YOON   (UW)
Kenneth J. ROCHE   (PNNL-Seattle)

Yongle YU   (now at Wuhan Institute of Physics and Mathematics)
Yuan Lung LUO   (UW)
Piotr MAGIERSKI   (Warsaw and UW)
Ionel STETCU   (UW)

Coulomb excitation of ^{48}Cr by an ultra-relativistic heavy ion

Isoscalar transition density, X = 0

Isoscalar transition density, Z = 0

Isovector density, X = 0

Isovector density, Z = 0

Time [fm/c] = 0

mm.avi

http://www.phys.washington.edu/groups/qmbnt/nuclei_dynamics/movies/td_densities.mov
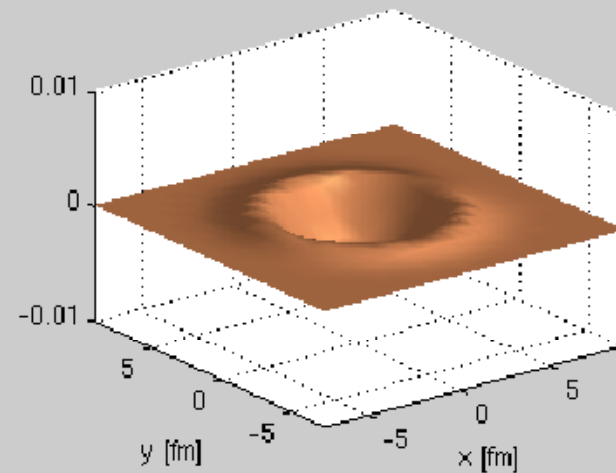
A few details of the calculation:

• **We solved the time-dependent 3D SLDA (HFB) equations for ^{48}Cr**
• **Only Coulomb interaction between the projectile and target**
(10 fm impact parameter)
• **We described ^{48}Cr with approximately 3,600 quasiparticle wave functions**
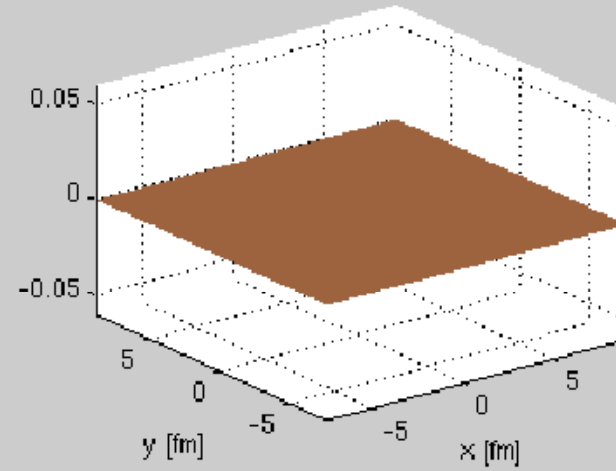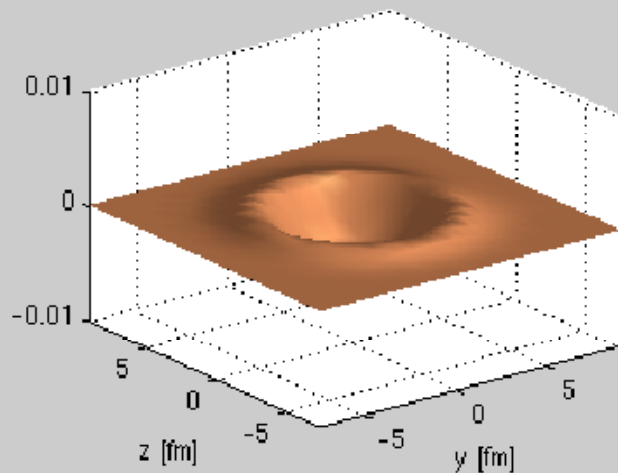*(this is already about an order of magnitude above all current TDHF calculations, and we still have about two or more orders of magnitude in store to expand easily)*
• **We used 3,600 processors on Franklin at NERSC for about 10 hours**
(both weak and strong scaling properties of the code are essentially perfect up to about 50,000 processors so far)

More movies of TD-SLDA simulations are available for viewing at

http://www.phys.washington.edu/groups/qmbnt/vortices_movies.html

Outline:

- **Where do we stand right now with the theory?**

  o **Open problems in (nuclear) LACM.**
  o **Current approaches and their limitations.**
  o **The computational tools we have developed so far for today's leadership class computers and beyond.**

- **Our long-range vision for the study of:**

  o **Nuclear dynamics - large and small amplitude collective motion (LACM), reactions and fission**
  o **Vortex creation and dynamics in neutron stars (pinning and de-pinning mechanism)**
  o **Cold atoms in static and dynamic traps and optical lattices and other condensed matter systems.**

From the point of view of numerical simulations we could say that the work of the founding fathers of statistical mechanics has been to transform a simple problem (B) into a terrible mess (A). Of course we have learned a lot in this process.

Statistical Field Theory, by Giorgio Parisi
Addison-Wesley, 1988

$$E = \langle H \rangle = \frac{\int dx dp \; \mathrm{H} \exp\left[-\beta H\right]}{\int dx dp \; \exp\left[-\beta H\right]}, \qquad \text{(A)}$$

$$\dot{x}_i(t) = p_i(t), \quad \dot{p}_i(t) = -\frac{\partial V(x_1(t),...,x_n(t))}{\partial x_i} \qquad \text{(B)}$$

SINGLE-ELECTRON INTERFERENCE AT HITACHI
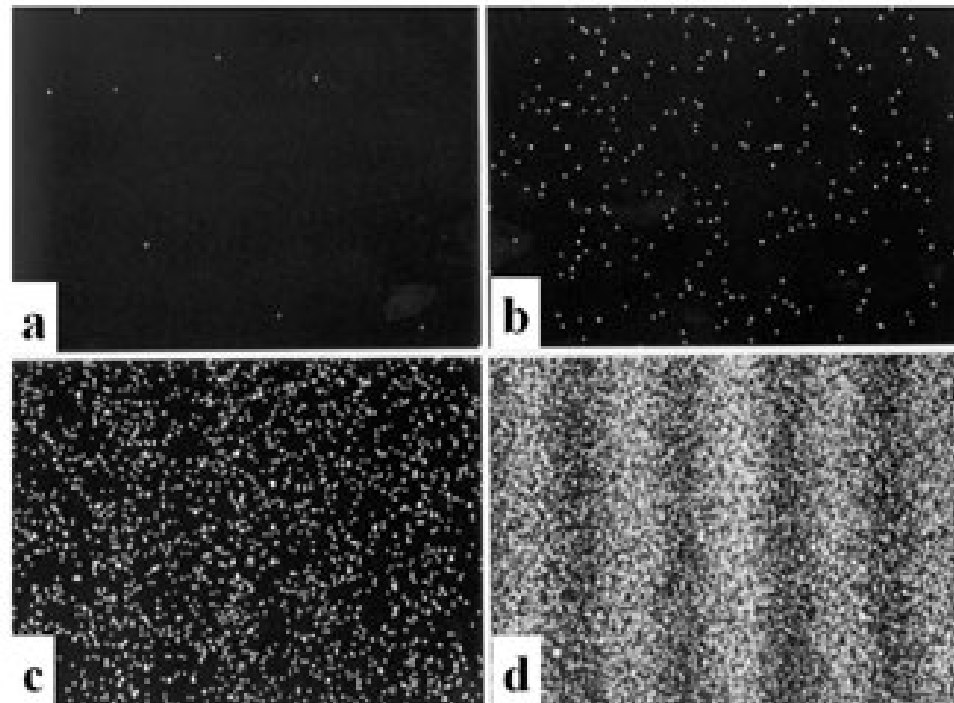
Single-electron Build-up of Interference Pattern

Single-electron events build up over a 20 minute exposure to form an interference pattern in this double-slit experiment by Akira Tonomura and co-workers. (a) 8 electrons; (b) 270 electrons; (c) 2000 electrons; (d) 60,000. A video of this experiment will soon be available on the web (www.hqrd.hitachi.co.jp/em/doubleslit.html).

Present theoretical approaches and phenomenology for LACM and fission studies:

o **Pure phenomenogical stochastic dynamics :**
    Langevin/Kramers equations
    Stochastic/Langevin TDHF

o **Adiabatic Time-Dependent Hartree-Fock-Bogoliubov (ATDHFB) theory**
    The basic assumption is that LACM/nuclear fission can be described with a many-body wave function with the GCM- structure:

$$\int \prod_{i=1}^{n} dq_i \Phi_{\text{Coll.}}\left(q_1,...,q_n\right) \Psi_{\text{Slater det.}}\left(x_1,...,x_A,\{q_1,...,q_n\}\right)$$

o **Microscopic-macroscopic <u>model</u>**
    not based on *ab intio* input
    no self-consistency
    physical intuition drives the definition of relevant degrees of freedom

3D-Langevin Eq.

$$M \frac{dv}{dt} = -\beta v + F(t) \qquad \langle F_i(t)F_j(t') \rangle = D^2 \delta_{ij} \delta(t-t')$$

$$D^2 = 2\beta T$$

$$m \frac{d^2 q}{dt^2} = -\frac{\partial V}{\partial q} - \beta m \frac{dq}{dt} + \sqrt{\beta T} f(t)$$

q_1 = deformation

q_2 = neck size

q_3 = mass asymmetry

Inertia Tensor

Friction Tensor

Karpov, Nadtochy et al. Phys.Rev. C63, 2001

May 13 – 16, 2009   Fission09, Château de Cadarache

Extended, … Stochastic TDHF approaches

Wong and Tang, Phys. Rev. Lett. 40, 1070 (1978)
Ayik, Z. Phys. A 298, 83 (1980)

...
Ayik Phys. Lett. B658, 174 (2008)

$$i\hbar \frac{\partial \psi_k(x,t)}{\partial t} = h[\rho(x,y,t)]\psi_k(x,t)$$

$$\rho(x,y,t) = \sum_{kl} \psi_k^*(x,t) n_{kl}(t) \psi_l(x,t)$$

$$\langle n_{kl}(t) \rangle = \delta_{kl} n_k$$

$$\langle \delta n_{kl}(t) \delta n_{ij}(t) \rangle = \frac{1}{2} \delta_{kj} \delta_{li} \left[n_i(1-n_j) + n_j(1-n_i) \right]$$

Gaussian random numbers defined a prescribed temperature in a Fermi-Dirac distribution

Subsequently these equations are *projected* on a collective subspace and a Langevin equation is introduced for the collective DoF

While ATDHFB approximation has a great number of positive aspects, it comes with a long series of great deficiencies:

- **The determination of the number of relevant degrees of freedom is as a rule determined by the practioner using intuition/prejudice or prevailing attitudes.**

There are knows methods on how to mechanize this process and eliminate arbitrariness, but they are extremely difficult to implement in practice.
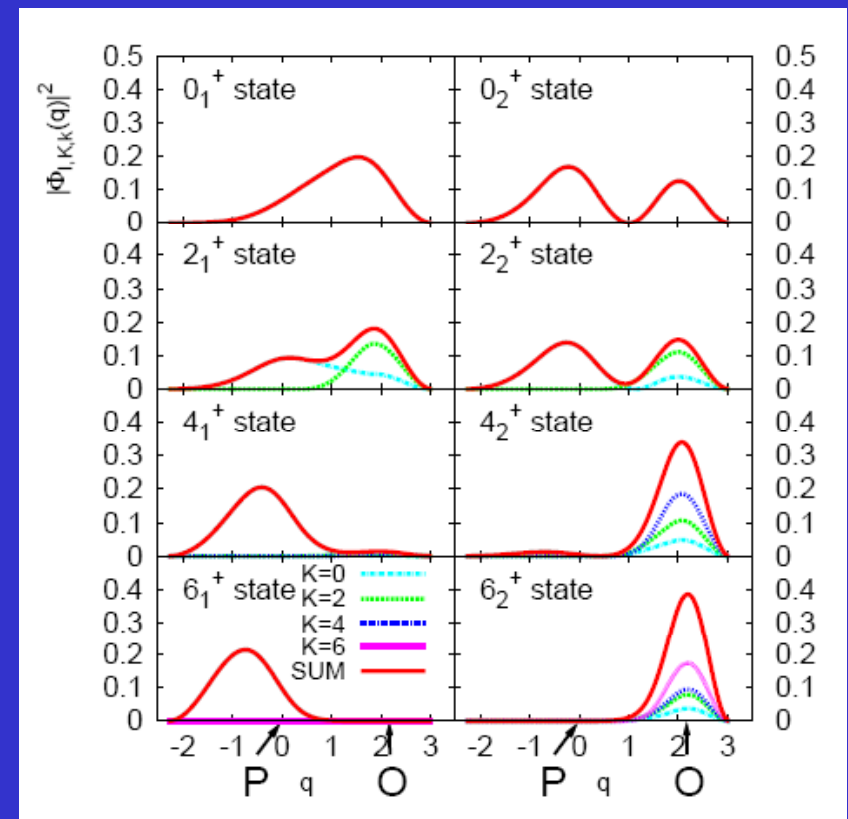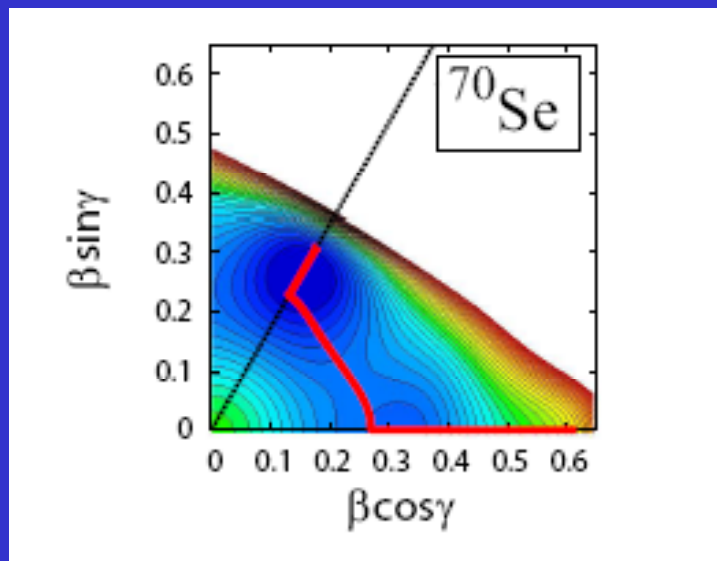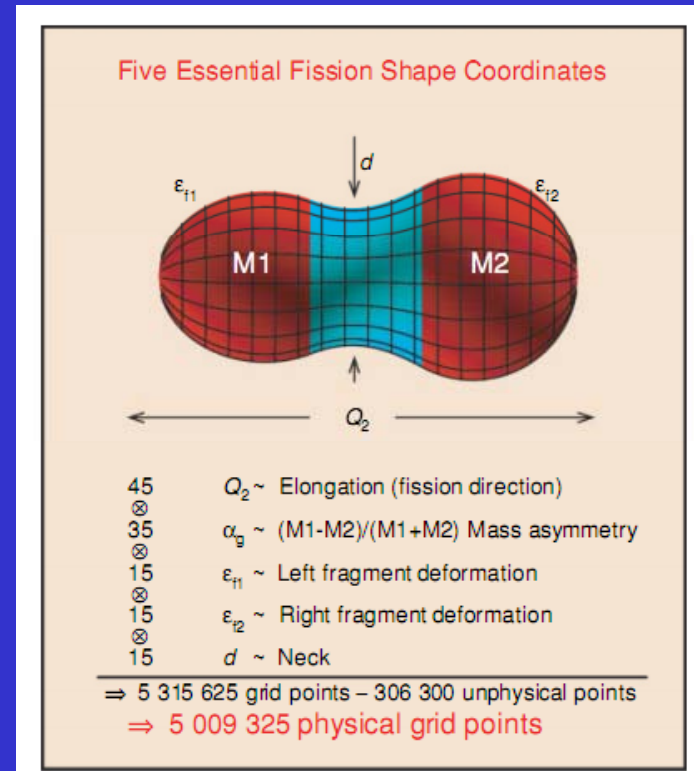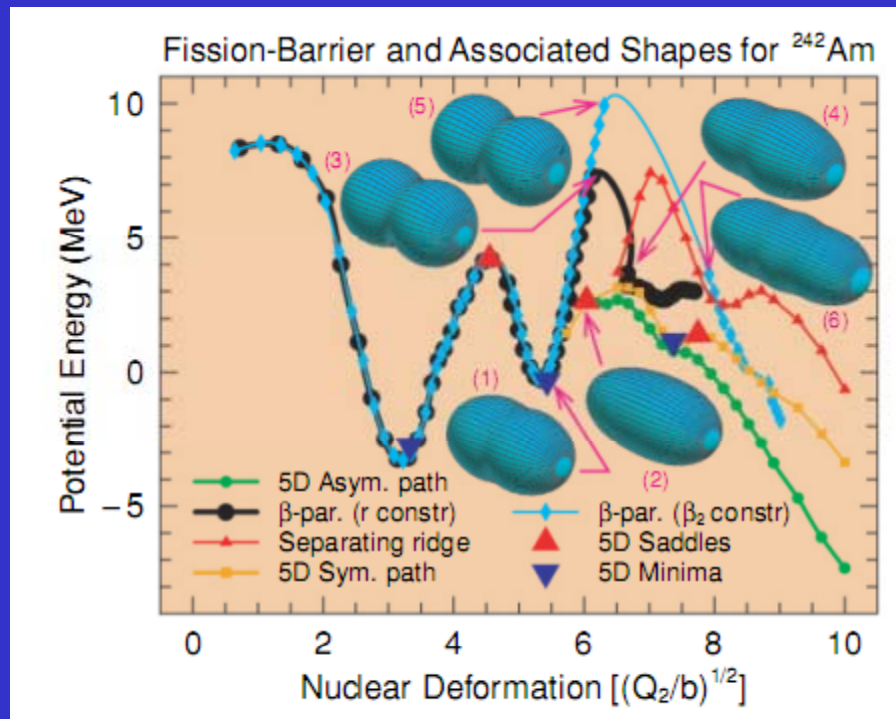

Hinohara, Nakatsukasa, Matsuo, and Matsuyanagi, Phys. Rev. C 80, 014305 (2009)

- **Computing the potential energy surface alone for only <u>3</u> collective degrees of freedom is equivalent to computing the entire nuclear mass table.**

P. Moller and collaborators need more than 5,000,000 shapes in a <u>five</u> dimensional space.

Is this the right and the entire complete set of collective coordinates?

Fission-Barrier and Associated Shapes for ^{242}Am

Potential Energy (MeV) vs Nuclear Deformation $[(Q_2/b)^{1/2}]$

- 5D Asym. path
- β-par. (r constr)
- Separating ridge
- 5D Sym. path
- β-par. (β$_2$ constr)
- 5D Saddles
- 5D Minima

Five Essential Fission Shape Coordinates

45	Q_2 ~ Elongation (fission direction)
⊗ 35	α_g ~ (M1-M2)/(M1+M2) Mass asymmetry
⊗ 15	ε_{f1} ~ Left fragment deformation
⊗ 15	ε_{f2} ~ Right fragment deformation
⊗ 15	d ~ Neck

⇒ 5 315 625 grid points – 306 300 unphysical points
⇒ 5 009 325 physical grid points

P.Moller *et al.* Phys. Rev. C <u>79</u>, 064304 (2009)

$$\int \prod_{i=1}^{n} dq_i \Phi_{\text{Coll.}}(q_1,...,q_n) \Psi_{\text{Slater det.}}(x_1,...,x_A,\{q_1,...,q_n\})$$

• **In order to determine the collective part of the wave function one needs to solve the Hill-Wheeler integral equation in the corresponding *n*-dimensional space.**

This is routinely (but not always) performed by invoking a further approximation (Gaussian Overlap Approximation) the accuracy of which is difficult to assess and one generates a Schrödinger equation in collective coordinates.

• **ATDHFB theory is based on the assumption that an expansion in velocities is accurate up to second order terms. However there are clear examples where this is wrong.**

• **The inertial tensor is usually hard to evaluate and often approximate methods are used.**

•It is obvious that a significantly larger number of degrees of freedom are necessary to describe LACM and fission in particular.

One would like to have as well: charge asymmetry, shapes of the fragments, excitation energy of the fragments, …

In this case the ATHFB approach becomes clearly unmanageable, even for computers envision in the next decade, and the veracity of the approximation is questionable .

``Spontaneous fission'' of ³²S
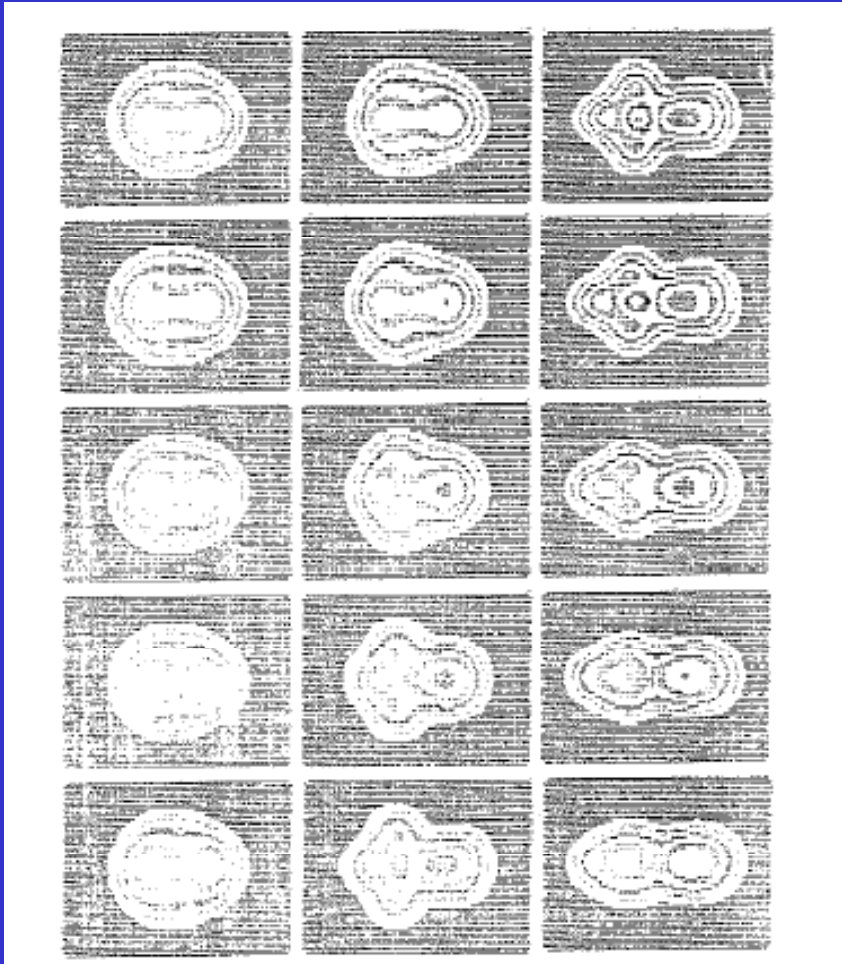
Even though the initial and final states have axial symmetry, along the fission path this symmetry is broken in order to rearrange occupation probabilities and avoid a diabolical point/level crossing, where a <u>Dirac monopole</u> resides.

J.W. Negele, Nucl. Phys. <u>A 502</u>, 371c (1989)
An unpublished calculation due to R. Wolff, G. Puddu and J.W. Negele

- **8 occupied orbitals evolved in 3D and imaginary time on a mesh $20^3 \times 1000$**
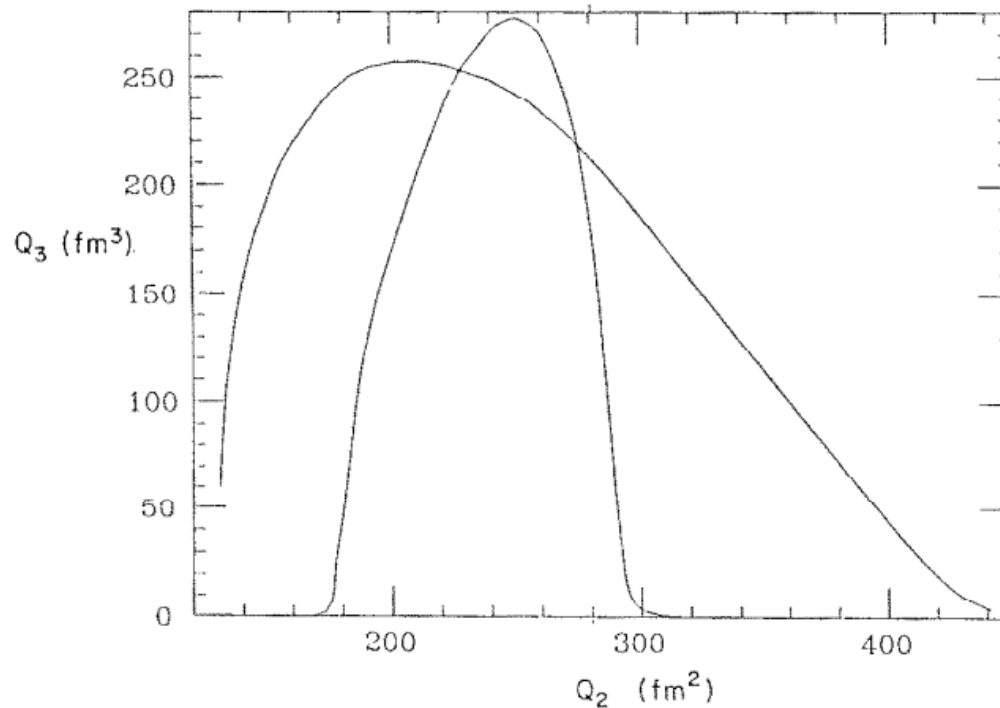- **no isospin dof, no pairing, simplified nuclear EDF**

Fig. 8: Collective motion path for the fission of ^{23}S in constrained mean-field theory (dashed line) and in imaginary-time mean-field theory (solid line).

J.W. Negele, Nucl. Phys. A 502, 371c (1989)
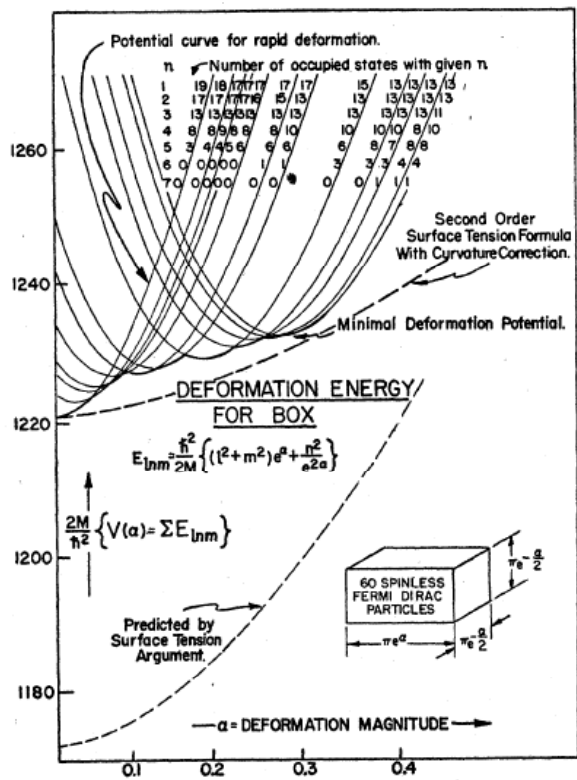
How do nuclei deform?

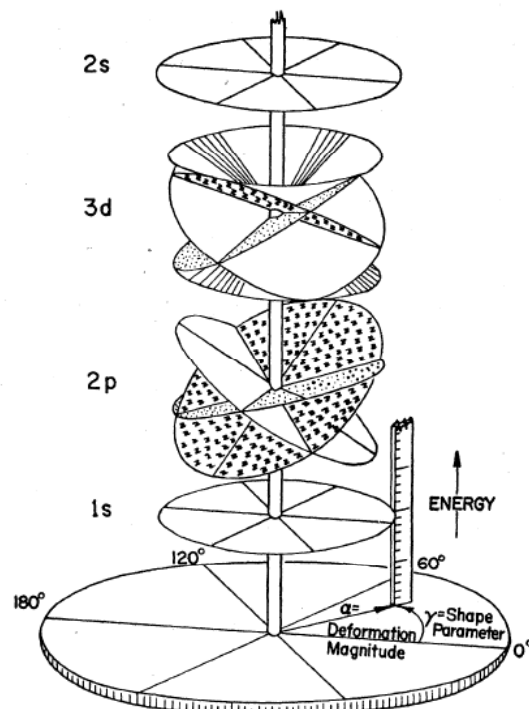FIG. 12. Potential curves for a deformable rectangular box.

FIG. 14. Qualitative effect of small ellipsoidal deviations from sphericity upon the first few energy levels of a single nucleon.
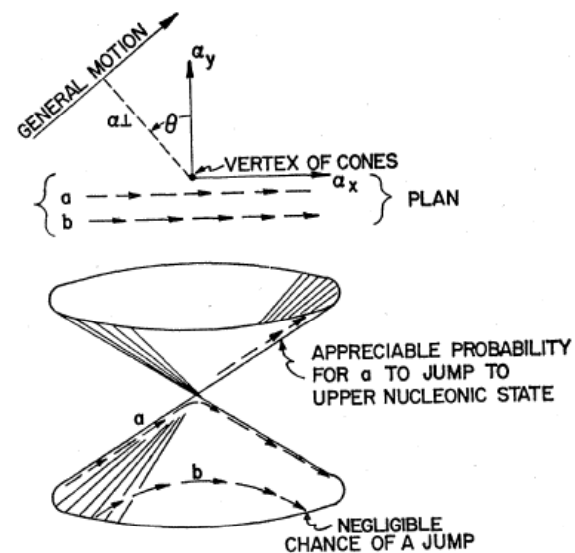

FIG. 35. Transition cross section for energy surfaces in conical contact.

D.L. Hill and J.A. Wheeler, Phys. Rev. 89, 1102 (1953)
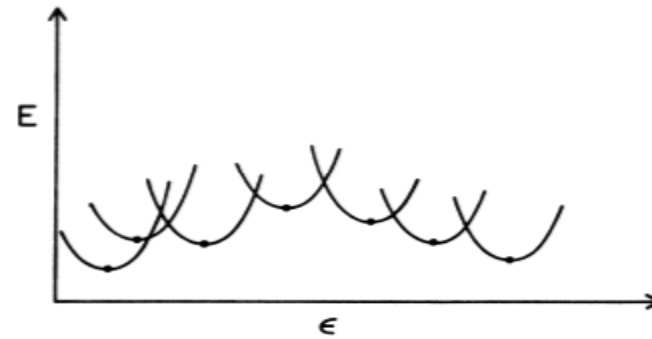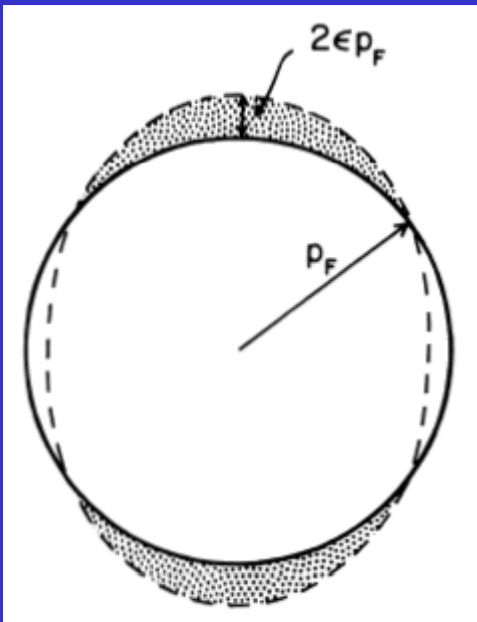*Nuclear Constitution and the Interpretation of Fission Phenomena*

Fig. 2. Schematic picture of Hartree–Fock states as a function of deformation. The states are shown as dots; the curves show their energy when distorted by the transformations (6).
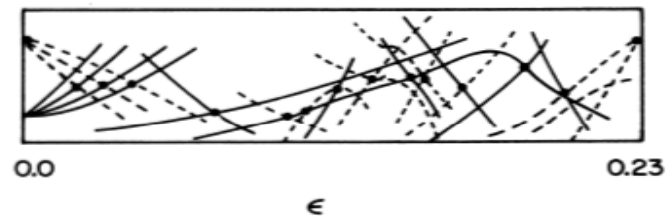
Fig. 3. Neutron single-particle levels at the Fermi surface in ^{240}Pu, taken from ref. [4]. Levels crossing the Fermi surface are shown as dots.
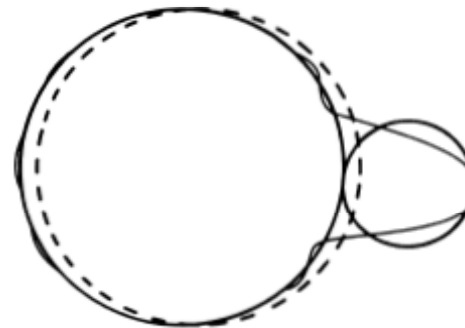
Fig. 4. Shape transitions for the decay ^{223}Ra $\rightarrow$ ^{209}Pb + ^{14}C. The original nucleus is shown dashed; the touching daughter nuclei as heavy solid lines. The transformation described in the text carries the initial shape to the one shown by the light solid line.

G.F. Bertsch, F. Barranco, and R.A. Broglia, *How Nuclei Change Shape*
in *Windsurfing the Fermi Sea*, eds. T.T.S. Kuo and J. Speth

• It is not obvious that the Slater determinant wave function should minimize the energy. Entropy production, level crossings, symmetry breaking.

Generic adiabatic large amplitude potential energy <u>SURFACES</u>
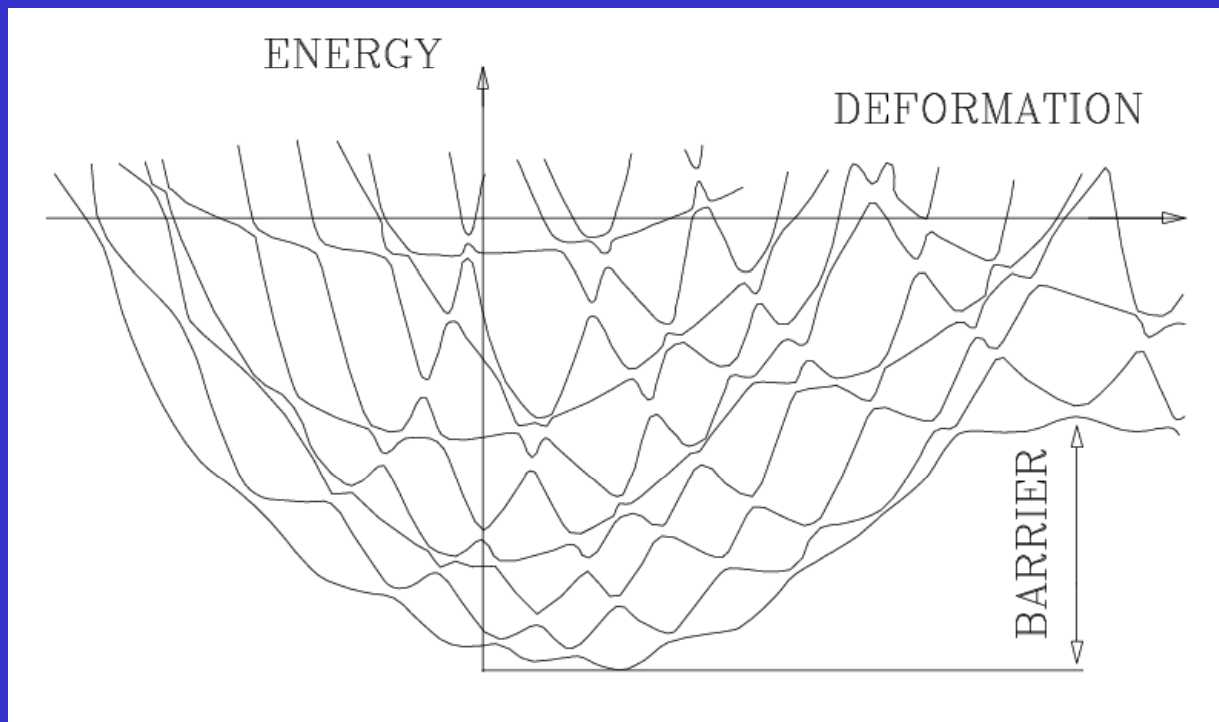
• In LACM adiabaticity/isentropic or isothermal behavior is not a guaranteed
• The most efficient mechanism for transitions at level crossing is due to pairing
• Level crossings are a great source of : entropy production (dissipation), dynamical symmetry breaking , non-abelian gauge fields (Dirac monopoles reside at level crossings)

Evolution operator of an interacting many-body system
(after a Trotter expansion and a Hubbard-Stratonovich transformation)

$$\exp\left[-iH(t_f-t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n)\exp\left[i\frac{\Delta t}{2}\sum_{abcd}\sigma_{ab}(n)V_{abcd}\sigma_{cd}(n)\right] \times$$

$$\exp\left[i\Delta t \sum_{ab}\left(T_{ab}+\sum_{cd}V_{abcd}\sigma_{cd}(n)\right)\alpha_a^\dagger\alpha_b\right]$$

This representation is not unique!

The one-body evolution operator is arbitrary!!!

Kerman, Levit, and Troudet, Ann. Phys. 148, 443 (1983)

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i\frac{\Delta t}{2} \sum_{abcd} \sigma_{ab}(n) V_{abcd} \sigma_{cd}(n)\right] \times$$

$$\exp\left[i\Delta t \sum_{ab} \left(T_{ab} + \sum_{cd} V_{abcd}\sigma_{cd}(n)\right)\alpha_a^\dagger \alpha_b\right]$$

What is the _best_ one-body propagator?

Stationary phase approximation leads to some form of Time-Dependent Meanfield

However, there is a bright spot if one is interested in one-body observables alone

Time-Dependent Density Functional Theory (TDDFT) asserts that there exists an __exact__ description, which formally looks like Time-Dependent Selfconsistent Meanfield.

A.K. Rajagopal and J. Callaway, Phys. Rev. B __7__, 1912 (1973)
V. Peuckert, J. Phys. C __11__, 4945 (1978)
E. Runge and E.K.U. Gross, Phys. Rev. Lett. __52__, 997 (1984)

http://www.tddft.org

There is a problem however!

Nobody knows how the true Time-Dependent (or not) Density Functional really looks like and there are no known exact algorithms for its generation.

But we know that it exits for sure.

So what is this DFT stuff?

Kohn-Sham theorem

$$H = \sum_i^N T(i) + \sum_{i<j}^N U(ij) + \sum_{i<j<k}^N U(ijk) + \ldots + \sum_i^N V_{ext}(i)$$

$$H\Psi_0(1,2,\ldots N) = E_0\Psi_0(1,2,\ldots N)$$

$$n(\vec{r}) = \left\langle \Psi_0 \left| \sum_i^N \delta(\vec{r}-\vec{r}_i) \right| \Psi_0 \right\rangle$$

Injective map (one-to-one)

$$\boxed{\Psi_0(1,2,\ldots N) \;\Leftrightarrow\; V_{ext}(\vec{r}) \;\Leftrightarrow\; n(\vec{r})}$$

$$E_0 = \min_{n(\vec{r})} \int d^3r \left\{ \frac{\hbar^2}{2m^*(\vec{r})}\tau(\vec{r}) + \varepsilon\big[n(\vec{r})\big] + V_{ext}(\vec{r})n(\vec{r}) \right\}$$

$$n(\vec{r}) = \sum_i^N \left|\varphi_i(\vec{r})\right|^2, \qquad \tau(\vec{r}) = \sum_i^N \left|\vec{\nabla}\varphi_i(\vec{r})\right|^2$$

Universal functional of particle density alone
Independent of external potential

Normal Fermi systems only!

However, not everyone is normal!

SLDA - Extension of Kohn-Sham approach to superfluid Fermi systems

$$E_{gs} = \int d^3r \; \varepsilon(n(\vec{r}), \tau(\vec{r}), \nu(\vec{r}))$$

$$n(\vec{r}) = 2\sum_k |v_k(\vec{r})|^2, \quad \tau(\vec{r}) = 2\sum_k |\vec{\nabla}v_k(\vec{r})|^2$$

$$\nu(\vec{r}) = \sum_k u_k(\vec{r})v_k^*(\vec{r})$$

$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix}$$

Mean-field and pairing field are both local fields!
(for sake of simplicity spin/isopsin degrees of freedom are not shown)

There is a little problem! The densities ν and τ diverges!
But all this can be fixed rather easily.

For time-dependent phenomena one has to add currents.

$$E(t) = \int d^3 r \left[\ \varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \vec{j}(\vec{r},t)) + V_{ext}(\vec{r},t)n(\vec{r},t) + ...\right]$$

$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]u_i(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)]v_i(\vec{r},t) = i\hbar \dfrac{\partial u_i(\vec{r},t)}{\partial t} \\[4mm] [\Delta^*(\vec{r},t) + \Delta_{ext}^*(\vec{r},t)]u_i(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]v_i(\vec{r},t) = i\hbar \dfrac{\partial v_i(\vec{r},t)}{\partial t} \end{cases}$$

DFT has however a serious restriction. One can not extract any information about two-body observables.

For example, if we were to study the fission of a nucleus, we will in principle determine the average masses of the daughters, but we will have no information about the width of the mass distribution.

There is a relatively simple solution in time-dependent meanfield theory due to Balian and Veneroni (late 1980's and early 1990's)
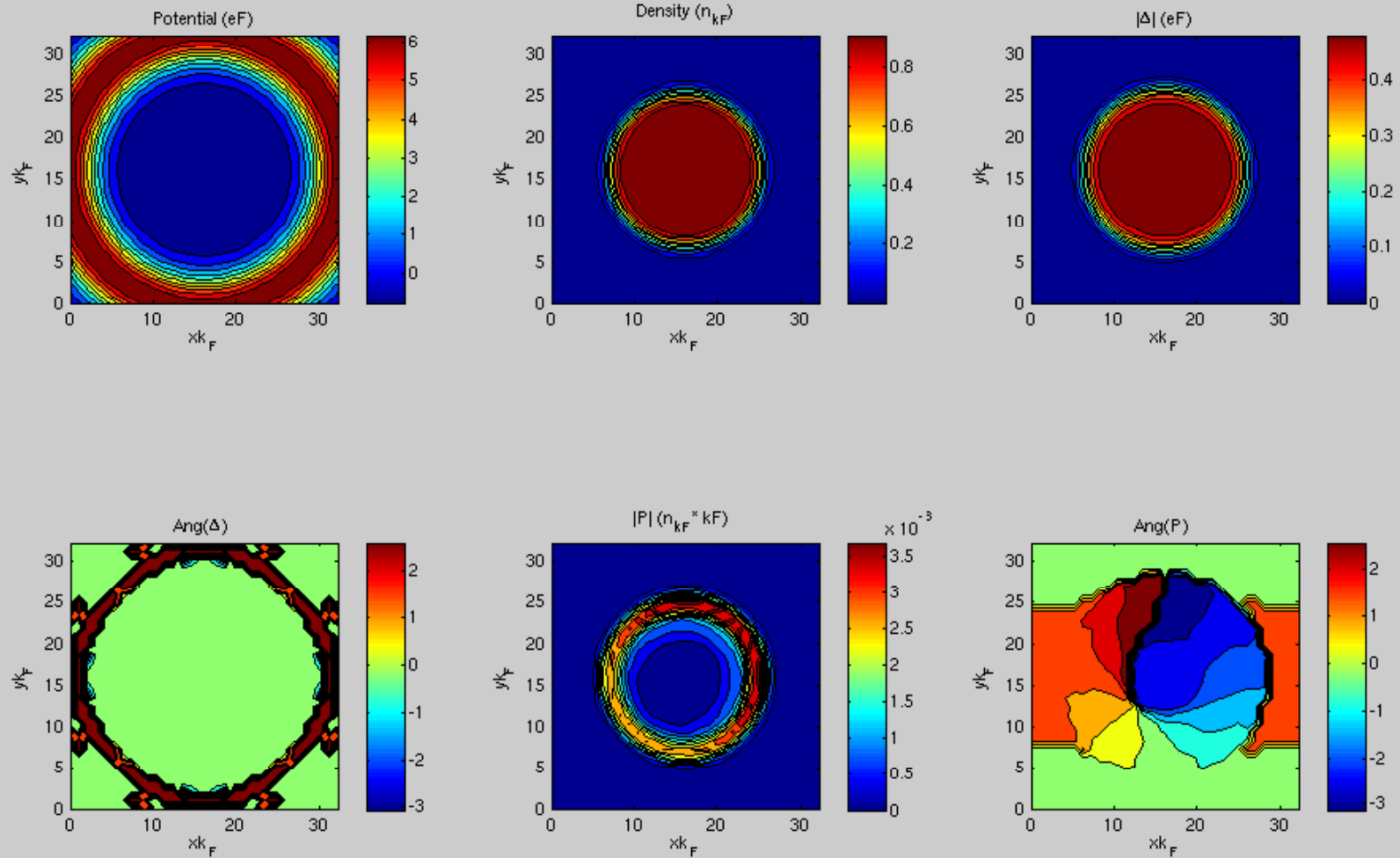
$$\rho(t_0) \quad \overset{TDHF}{\Rightarrow} \quad \rho(t_1)$$

$$\sigma(t_1, \varepsilon) = \exp\left(i\varepsilon\hat{Q}\right)\rho(t_1)\exp\left(-i\varepsilon\hat{Q}\right)$$

$$\sigma(t_0, \varepsilon) \quad \overset{TDHF}{\Leftarrow} \quad \sigma(t_1, \varepsilon)$$

$$\left(\Delta Q_{BV}\right)^2\Big|_{t_1} = \lim_{\varepsilon \to 0} \frac{1}{2\varepsilon^2}\text{Tr}\left[\rho(t_0) - \sigma(t_0, \varepsilon)\right]$$

This method allows in principle the evaluation of both averages and widths.

Time $\varepsilon_F = 0$ $T_{step} = 1$

7vortices.avi

The main problem however is that we have to consider the generic situation with multiple potential energy surfaces, and not only one self-consistent field.
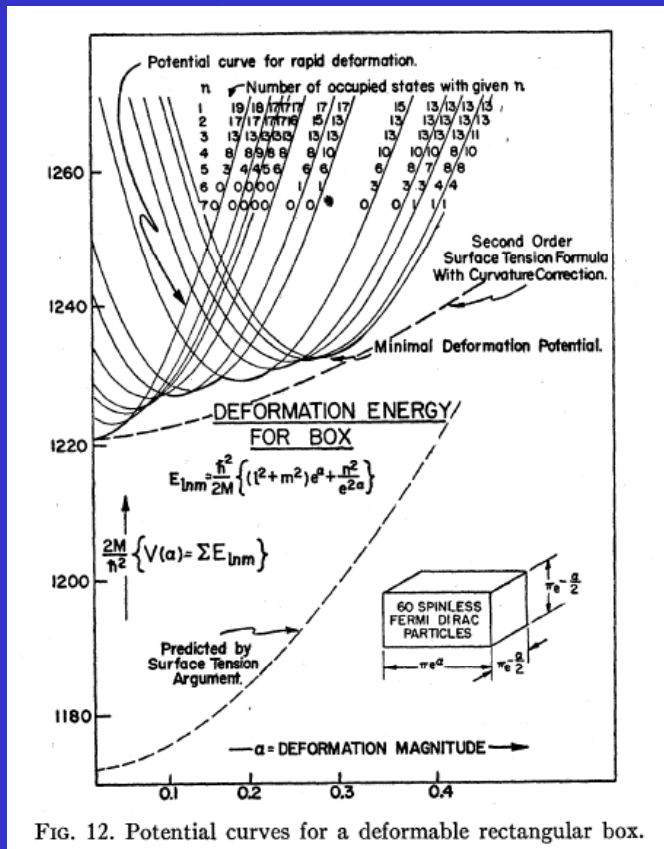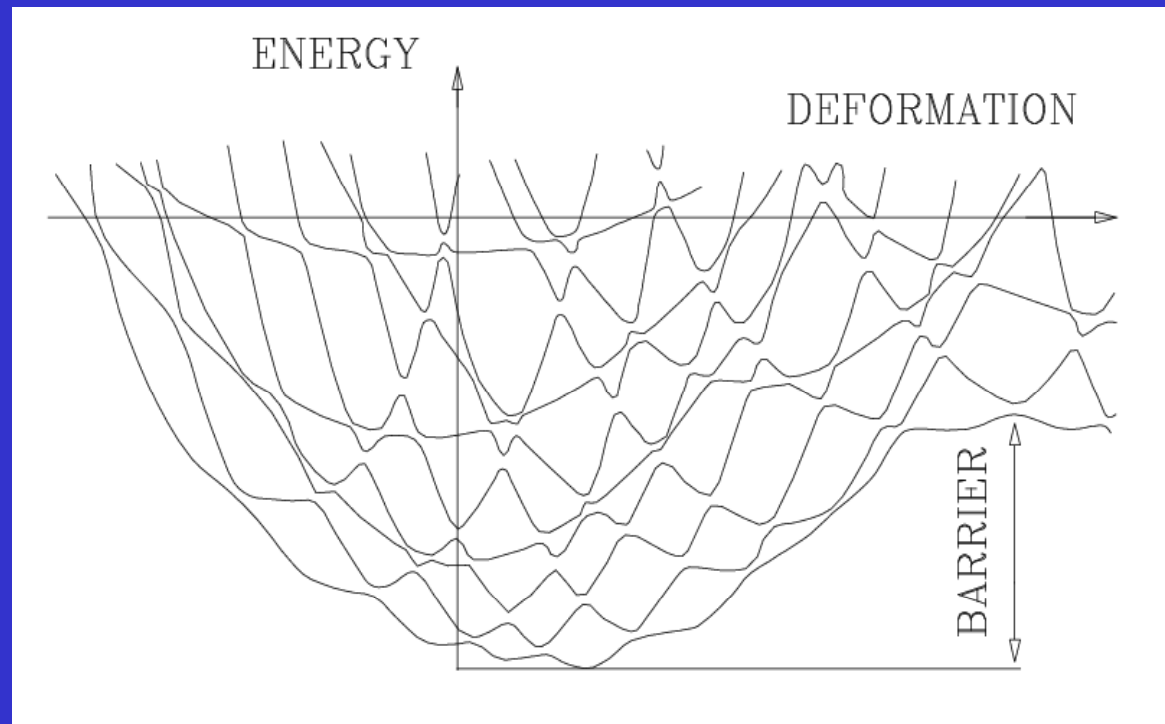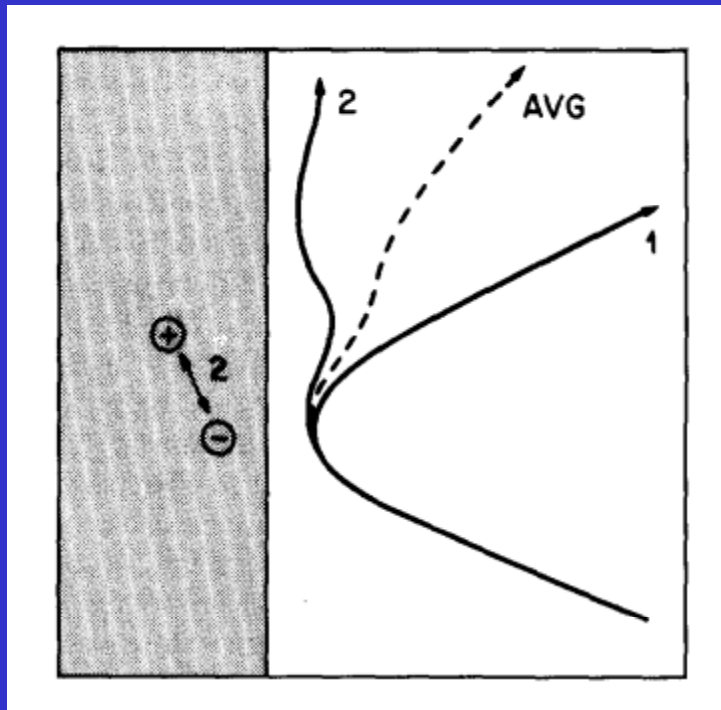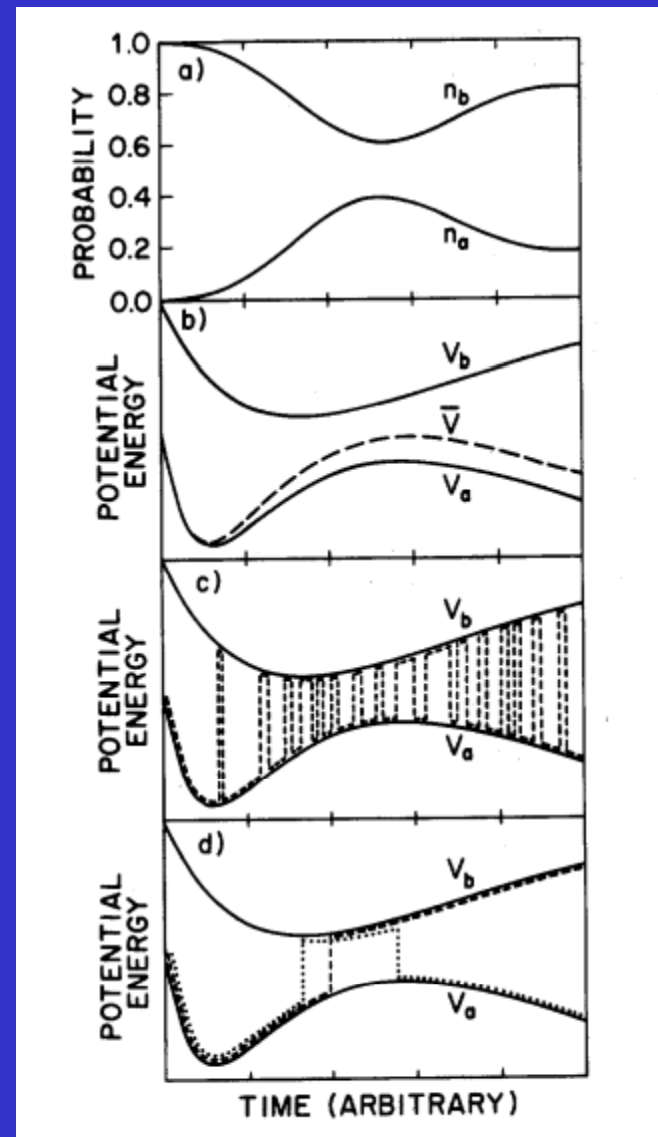

FIG. 12. Potential curves for a deformable rectangular box.

John C. Tully suggested the following recipe for condensed matter and chemistry applications
J. Chem. Phys. 93, 1061 (1990)

$$\psi(\vec{r}, \vec{R}, t) = \sum_i c_i(\vec{R}, t) \varphi_i(\vec{r} | \vec{R})$$

The best solution however is to implement and treat the auxiliary fields as stochastic ⟹ **Stochastic TD-SLDA**

$$\exp\left[-iH(t_f - t_i)\right] \propto \int \prod_n \prod_{ab} d\sigma_{ab}(n) \exp\left[i\frac{\Delta t}{2}\sum_{abcd}\sigma_{ab}(n)V_{abcd}\sigma_{cd}(n)\right] \times$$
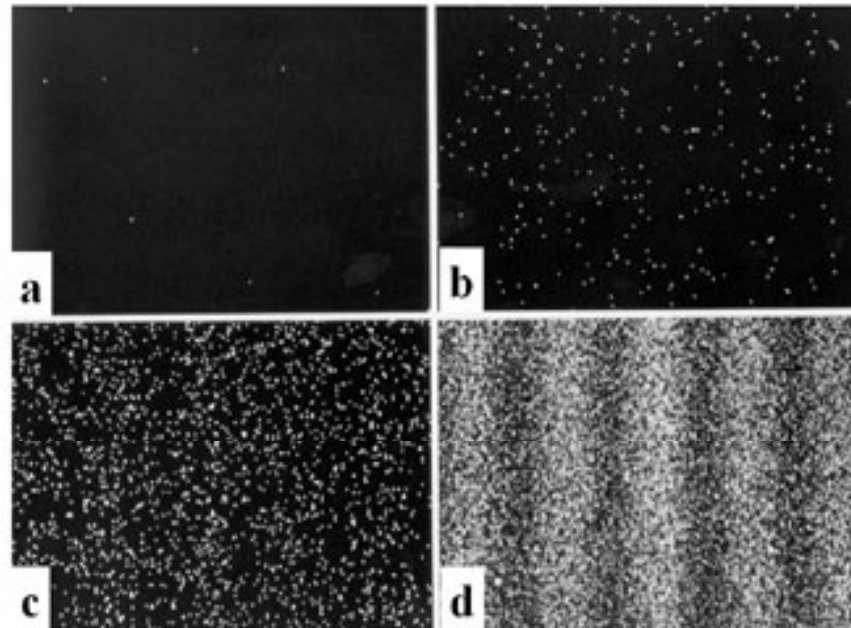
$$\exp\left[i\Delta t \sum_{ab}\left(T_{ab} + \sum_{cd}V_{abcd}\sigma_{cd}(n)\right)\alpha_a^\dagger\alpha_b\right]$$

In 3D this is a problem for the petaflop to exaflop supercomputers

What do we gain following this route?
We are going to solve the interacting quantum many-body problem in a manner similar to how this experimental result was obtained.

SINGLE-ELECTRON INTERFERENCE AT HITACHI

Single-electron Build-up of Interference Pattern

Single-electron events build up over a 20 minute exposure to form an interference pattern in this double-slit experiment by Akira Tonomura and co-workers. (a) 8 electrons; (b) 270 electrons; (c) 2000 electrons; (d) 60,000. A video of this experiment will soon be available on the web (www.hqrd.hitachi.co.jp/em/doubleslit.html).

We are going to get away from the terrible mess
and solve instead a simpler problem.

*From the point of view of numerical simulations we could say that
the work of the founding fathers of statistical mechanics has been
to transform a simple problem (B) into a terrible mess (A). Of
course we have learned a lot in this process.*

Statistical Field Theory, by Giorgio Parisi

Addison-Wesley, 1988

$$E = \langle H \rangle = \frac{\int dx\, dp\ H \exp[-\beta H]}{\int dx\, dp\ \exp[-\beta H]}, \qquad \text{(A)}$$

$$\dot{x}_i(t) = p_i(t), \quad \dot{p}_i(t) = -\frac{\partial V(x_1(t),\ldots,x_n(t))}{\partial x_i} \qquad \text{(B)}$$

For the sake of discussion let us see what we could in principle be able to calculate?

• We do not need to determine any collective coordinates, potential energy surfaces, inertia tensor, non-abelian gauge fields, etc. as the system will find naturally the right collective manifold

• We will not need to assume either isentropic, isothermal, … meanfield solutions. Instead the temperature and entropy of the collective subsystem will evolve according to the rules of QM. This will be the most natural framework to describe dissipation in collective nuclear motion.

• We should be able to compute directly the mass, charge distributions and the excitation energy distributions of each fragment

• We should be able to follow in real time a real experimental situation, such as induced fission or fusion

All this is naturally not limited to nuclear physics alone, this is a general approach to solve a large class of many-body problems numerically exactly, with quantifying errors, within the next decade … or sooner.