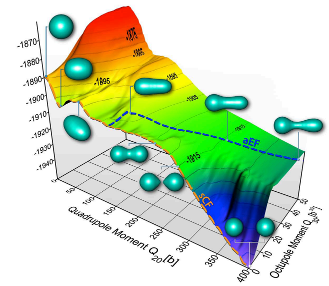
Program announcement:

Quantitative Large Amplitude Shape Dynamics: fission and heavy ion fusion

Institute for Nuclear Theory, Seattle

September 23 – November 15, 2013



http://www.int.washington.edu/PROGRAMS/13-3/

Main topics:

- Reevaluation of basic concepts
- Microscopic theory and phenomenological approaches
- Nuclear interactions and energy density functionals
- Time-dependent many-body dynamics
- Key experimental tests
- Experimental data needs
- Spectroscopic implications
- Computational methodologies for dynamics

1939: Bohr and Wheeler

N. Bohr, letter to Nature **143** 330

These circumstances find their straightforward explanation in the fact, stressed by Meitner and Frisch, that the mutual repulsion between the electric charges in a nucleus will for highly charged nuclei counteract to a large extent the effect of the short-range forces between the nuclear particles in opposing a deformation of the nucleus. The nuclear problem concerned reminds us indeed in several ways of the question of the stability of a charged liquid drop, and in particular, any deformation of a nucleus, sufficiently large for its fission, may be treated approximately as a classical mechanical problem,

The continuation of the experiments on the new type of nuclear disintegrations, and above all the closer examination of the conditions for their occurrence, should certainly yield most valuable information as regards the mechanism of nuclear excitation.

Bohr and Wheeler, Phys. Rev. **86** 426

WKB

$$\lambda_f(=\Gamma_f/\hbar)=5(\omega_f/2\pi)$$
$$\times\exp -2\int_{P_1}^{P_2}\{2(V-E)\sum_i m_i(dx_i/d\alpha)^2\}^{\frac{1}{2}}d\alpha/\hbar. \quad (28)$$

Transition state theory

$$\Gamma_f=(d/2\pi)\sum_i 1 \quad (36)$$

Goals of the Program

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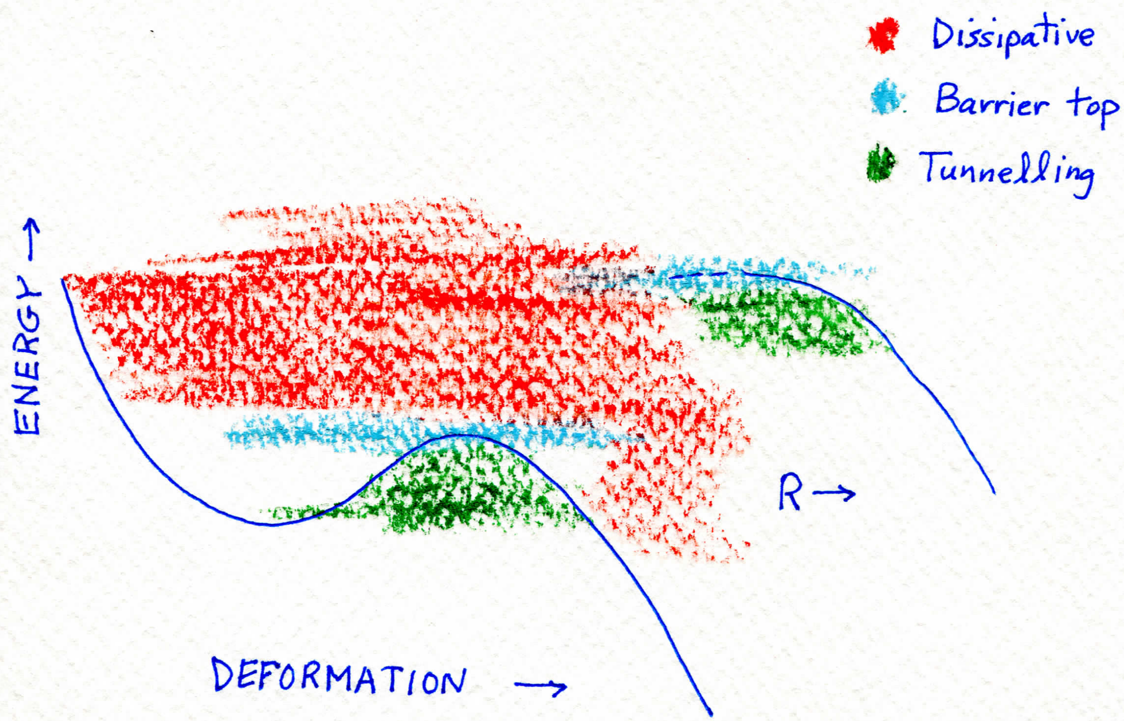
University of Washington

INT
Sept. 23, 2013

1. Reassessment of fundamental concepts
2. The potential energy surface (PES)
3. Dynamics
4. My personal goal
5. Outside world
6. Experimental needs
7. Cultural aspects

The three regions of shape dynamics



scission

Dynamics

	Inertial reversible		Dissipative Irreversible; needs T
Macroscopic		Fokker-Planck	Smoluchowski
		Transition State Theory Bohr-Wheeler	
Microscopic	ATDHFB TD-Schrödinger TD-HF TD-HFB		Wall formula 2B dissipation

Reassessment of fundamental concepts

Ground rule:

Constrained HFB with its quasiparticle excitations provides the basis for a controllable theory of LASD.

1) What the barrier? How precise is its experimental definition?

2) How reliable is transition state theory?

The Potential Energy Surface I

The paradox of the FRLDM:

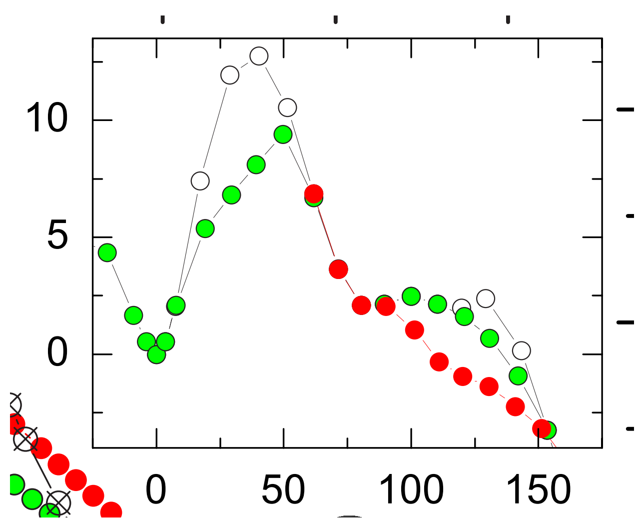
Phenomenologically defined one-body theories are justified by the HFB approximation, but seem to do better than the HFB itself.

The Potential Energy Surface II

How many degrees of freedom are needed to specify it?

FRLDM: five

Triaxial degrees of freedom can be important for spontaneous fission. PRC87 024320

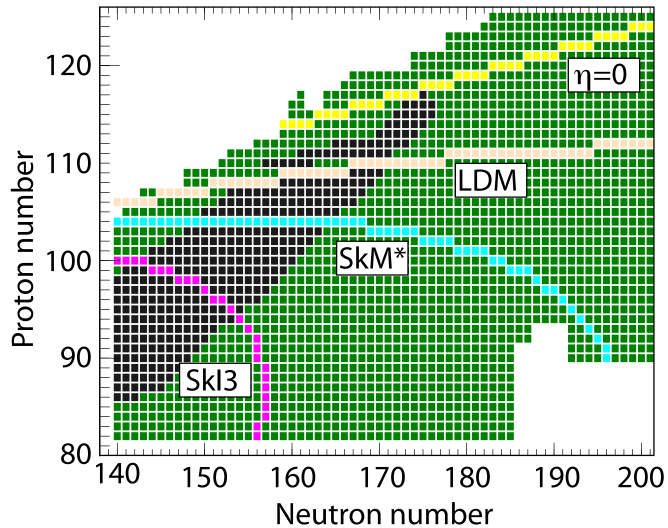


Is there a third barrier?

Potential energy surface III

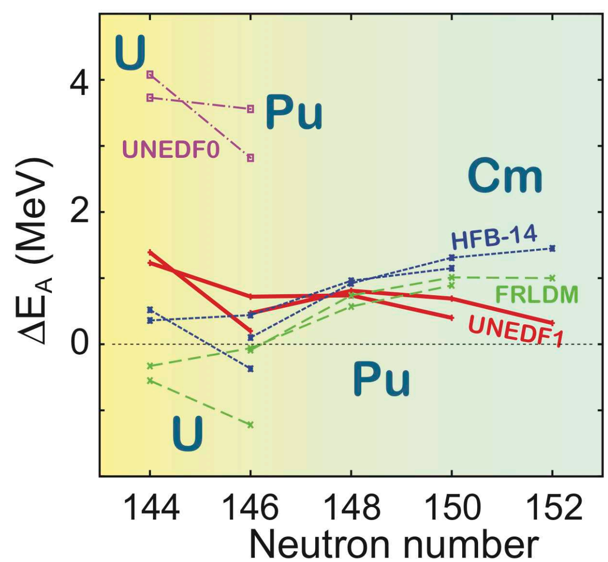
How well do we know it?

Fissility boundary for heavy neutron-rich nuclei



Phys. Rev. C 83 034305

Fission barriers



Phys. Rev. C 85 024304

The energy region above the PES:

We have no useful microscopic theory of the statistical mechanics of nuclear excitations.

Observed levels densities are incompatible with HF effective masses.

Weisskopf, Nucl. Phys. **3** 423

THE PROBLEM OF AN EFFECTIVE MASS IN NUCLEAR MATTER

VICTOR F. WEISSKOPF
Department of Physics and Laboratory of Nuclear Science
Massachusetts Institute of Technology, Cambridge, Massachusetts

Received 26 January 1957

Abstract: It is shown that the existence of nuclear matter and the independent particle description of its properties implies by itself that the average potential energy is momentum dependent. If this momentum dependence is expressed in terms of an effective mass m^*, one gets $m/m^* = 3/2+(5/2)(P/T_f)$, where P is the packing fraction and T_f the

Dynamics I: subbarrier

1. Standard approximation: WKB+HFB+cranking
2. Comment I: Inertia is dominated by pairing
3. Comment II: Better theory is needed for path determination.

From abstract of arXiv:1305.0293:

> "The experimental trend [of spontaneous fission lifetimes] with mass number is reasonably well reproduced over a range of 27 orders of magnitude. However, the theoretical predictions suffer from large uncertainties... Modifications of a few percent in the pairing correlation strengths strongly modify the collective inertias with a large impact in the spontaneous fission lifetimes in all the nuclei considered."

Analytic on the role of pairing in the dynamics:

HFB+cranking

$$B_{\beta\beta} \approx \tfrac{1}{16}\hbar^2 \,|\langle \partial\mathcal{H}/\partial\beta\rangle_{\mathrm{Av}}|^2 (g^{\mathrm{sp}}/\Delta^2). \qquad \text{(IX.48)}$$

Brack, et al., RMP **44** 320 (1972)

GCM/GOA

$$I_q = \frac{\pi^2}{32\Delta^2}\frac{dn}{d\epsilon}\left|\frac{\partial\epsilon}{\partial q}\right|^2 .$$

Bertsch and Flocard, Phys. Rev. C **43** 2200 (1991)

Dynamics at the barrier

1. Transition state approximation
2. Showcase examples
3. Nuclear barrier is very complicated
4. A challenge problem for theory

A short history of the transition state approximation

Bohr and Wheeler, Phys. Rev. **56**, 426 (1939)

$$\Gamma_f = N^*/2\pi\rho(E) = (d/2\pi)N^* \qquad (32)$$

Prehistory

RRKM chemical reaction theory 1927-1952
Polanyi and Wigner 1928
Weisskopf 1937

Posthistory

$$\Gamma = \frac{1}{2\pi\rho(E)}\sum_c T_c$$

Hauser-Feshbach 1952

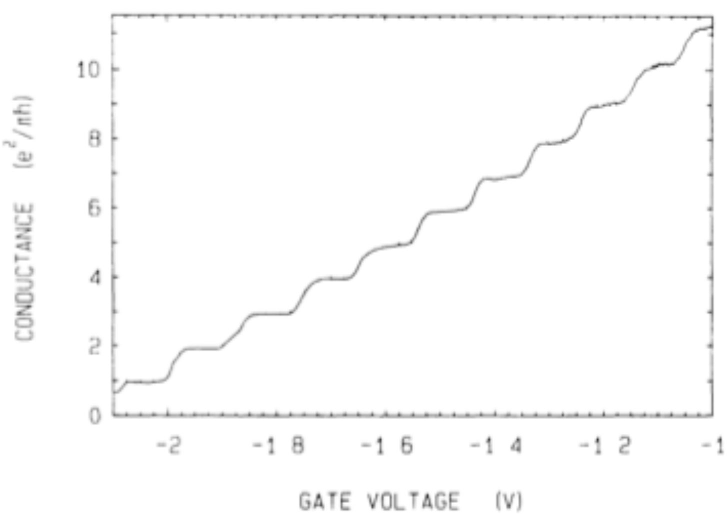
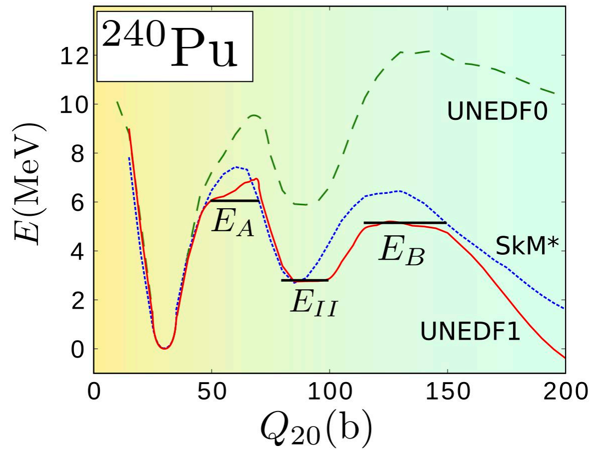
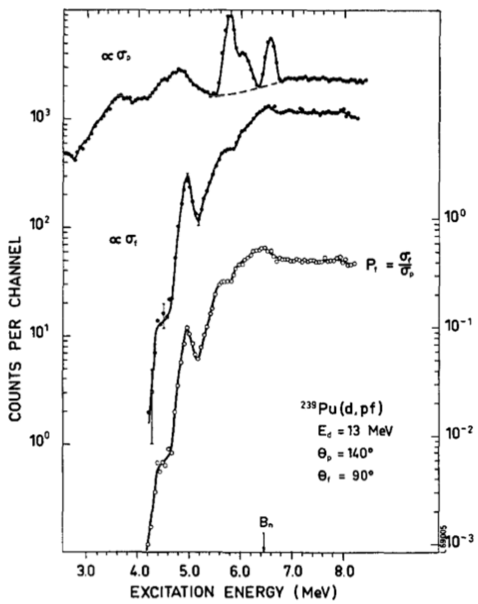


FIG. 2. Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/\pi\hbar$.

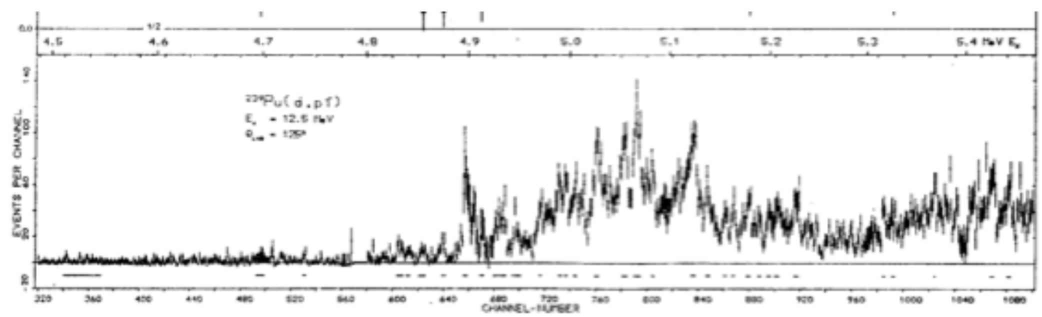
van Wees, et al.
Phys. Rev. Lett. **60** 848 (1988)

The nuclear barrier top is way more complicated.





Back, et al. Nucl. Phys. **A165 449** (1976)



Glaessel, et al. Nucl. Phys. **A256** 220 (1976)

Does the structure depend only on V(q) or does B(q) play a role as well?

Dissipative Dynamics

1. Standard approximation: Kramers' formula
2. Mechanisms of dissipation
    a. Wall formula
    b. 2-B dissipation
3. Fluctuations from multidimensional Schrodinger dynamics?

Kramers' formula

$$\Gamma = K\frac{\omega_0}{2\pi}e^{-E_B/T} \qquad K = \left(1+\left(\frac{T}{2I\omega_B D}\right)^2\right) - \frac{T}{2I\omega_B D}$$

where D is a diffusion coefficient and ω_B is the barrier frequency.

Dissipative limit (Smoluchowski Eq.):

Cha and Bertsch, Phys. Rev. C **46** 306 (1992)

$$\Gamma = D\frac{\sqrt{k_0 k_B}}{2\pi T}e^{-E_B/T}$$

k is curvature of PES

What is the temperature dependence of D?

One-body dissipation

The wall formula correctly describes the damping of ripples on the surface of a Fermi liquid, treated in the time-dependent Hartree-Fock approximation.

Not reliable

Bertsch and Esbensen, Phys. Lett. 161B 248 (1985).

But: wall formula is wrong for L=1 and L=2 modes of a spherical nucleus.

A microscopic theory for 2-body D:

Bush, Bertsch, and Brown, Phys. Rev. C **45** 1709 (1992)

$$D_\beta = \frac{2\pi}{\hbar}\sum_f (\beta_i - \beta_f)^2 \left|\langle i|v_{\text{residual}}|f\rangle\right|^2 \delta(E_f - E_i) \quad .$$

Predicts a very strong temperature dependence.

Comes out too small

A personal goal for LASD

Define and evaluate a test model for large-amplitude inertial dynamics. The model must be simple enough to be accurately solvable numerically. It must be rich enough to exhibit differences in approximate treatments of the dynamics. The leading approximate treatments:

cranking
GCM/GOA
GCM/DB
ATDHFB
and not forgetting Im(T)HF.

Comments:

0) The percent difference between exact and approximate could be taken as a contribution to the systematic error in applications of the approximate inertias.
1) I would welcome off-line discussion of the test model.
2) A corresponding model for dissipative dynamics would be even more interesting, but I believe it is beyond our computational resources.

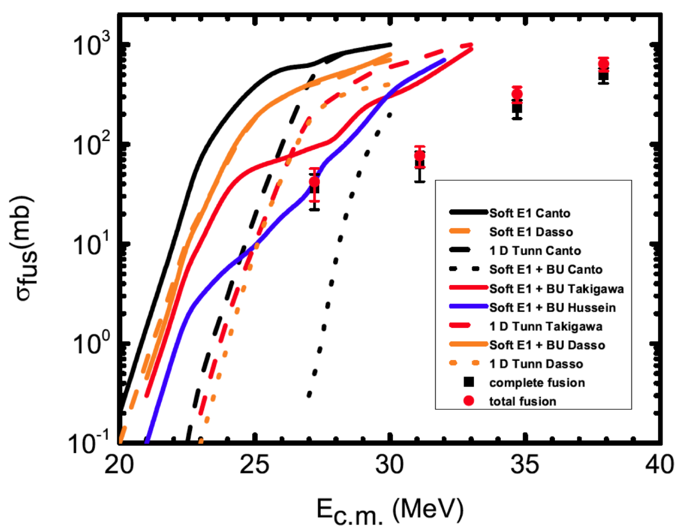
The outside world

Fission recycling: can we calculate fission properties reliably enough to be informative about the r-process environment? See Arcone's simulation on the home page.

How accurately do we know the neutrino spectrum from fission products of reactors? The "neutrino anomaly" is the subject of a workshop in week 7 of the program.

NNSA (National Nuclear Security Administration)

Experimental needs: Example I



The predictions of the best theory groups for the fusion excitation function for 11Li + 208Pb differ by up to four orders of magnitude AND bear no resemblance to the data. We apparently do not understand the fusion of halo nuclei.

A.M. Vinodkumar et al., Phys. Rev. C **87**, 044603 (2013)

Experimental Needs: Example II

Production of heavy elements in complete fusion reactions

$$\sigma_{\mathrm{EVR}}(E_{\mathrm{c.m.}}) = \sum_{J=0}^{J_{\max}} \sigma_{\mathrm{CN}}(E_{\mathrm{c.m.}}, J) W_{\mathrm{sur}}(E_{\mathrm{c.m.}}, J),$$

where

$$\sigma_{\mathrm{CN}}(E_{\mathrm{c.m.}}) = \sum_{J=0}^{J_{\max}} \sigma_{\mathrm{capture}}(E_{\mathrm{c.m.}}, J) P_{\mathrm{CN}}(E_{\mathrm{c.m.}}, J),$$

- We need to know three spin-dependent quantities: (a) the capture cross section, (b) the fusion probability and (c) the survival probability, and their isospin dependence. Our understanding of PCN, the fusion/quasifission competition, is extremely POOR. (no real clue)

W. Loveland, J. Phys. Conf. Series 420 012004 (2013).

Experimental Needs: Example III

“Scission” neutrons

- In spontaneous and thermal neutron induced fission, some investigators report that up to 30% of the prompt neutrons are emitted isotropically rather than being correlated with the direction of motion of the fission fragments. How can we understand these “scission” neutrons? Can they really be emitted isotropically?

N. Carjan, Phys. Rev. C82 014617 (2010).

Cultural

1. critical assessment (a.k.a. error bars)
2. computer codes
3. collaboration

An example of a theoretical calculation that includes an assessment of its reliability: equation of state of neutron matter.

PHYSICAL REVIEW C **88**, 025802 (2013)

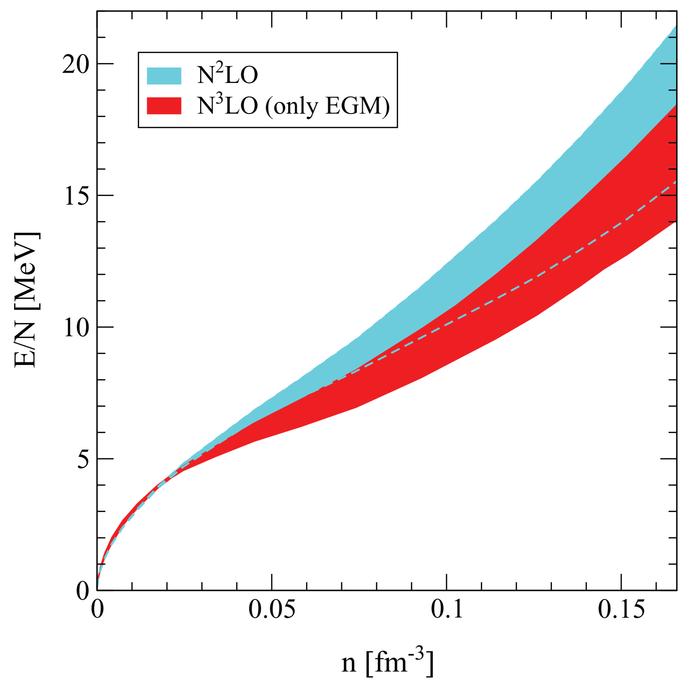


FIG. 8. (Color online) Neutron-matter energy per particle as a function of density at N^{2}LO (upper blue band that extends to the dashed line) and N^{3}LO (lower red band). The bands are based on the EGM NN potentials and include uncertainty estimates as in Fig. 7.

Computer codes

PERSPECTIVE

Nature 482 485 (2012).

doi:10.1038/nature10836

The case for open computer programs

Darrel C. Ince[1], Leslie Hatton[2] & John Graham-Cumming[3]

Scientific communication relies on evidence that cannot be entirely included in publications, but the rise of computational science has added a new layer of inaccessibility. Although it is now accepted that data should be made available on request, the current regulations regarding the availability of software are inconsistent. We argue that, with some exceptions, anything less than the release of source programs is intolerable for results that depend on computation. The vagaries of hardware, software and natural language will always ensure that exact reproducibility remains uncertain, but withholding code increases the chances that efforts to reproduce results will fail.

Examples:

Bonche, Flocard and Heenen, CPC 171
Dobaczewski, et al., CPC 102-183
Robledo & Bertsch, PR C84

Collaboration

An example:

PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

18 authors, 7 different calculational methods

TABLE I. The expectation values $\langle T\rangle$ and $\langle V\rangle$ of kinetic and potential energies, the binding energies E_b in MeV, and the radius in fm.

Method	$\langle T\rangle$	$\langle V\rangle$	E_b	$\sqrt{\langle r^2\rangle}$
FY	102.39(5)	−128.33(10)	−25.94(5)	1.485(3)
CRCGV	102.30	−128.20	−25.90	1.482
SVM	102.35	−128.27	−25.92	1.486
HH	102.44	−128.34	−25.90(1)	1.483
GFMC	102.3(1.0)	−128.25(1.0)	−25.93(2)	1.490(5)
NCSM	103.35	−129.45	−25.80(20)	1.485
EIHH	100.8(9)	−126.7(9)	−25.944(10)	1.486