Nuclear Density Functional Theory and Extensions

Input

- NN+NNN interactions
- Density Matrix Expansion
- Density dependent interactions
- Fit-observables
  - experiment
  - pseudo data

Optimization

- Energy Density Functional
  - DFT variational principle
    - HF, HFB (self-consistency)
    - Symmetry breaking

Observables

- Symmetry restoration
  - Multi-reference DFT (GCM)
  - Time dependent DFT (TDHFB)

Technology to calculate observables

- Global properties
- Spectroscopy
- DFT Solvers
- Functional form
- Functional optimization
- Estimation of theoretical errors

- Direct comparison with experiment
- Pseudo-data for reactions and astrophysics

- two fermi liquids
- self-bound
- superfluid (ph and pp channels)
- self-consistent mean-fields
- broken-symmetry generalized product states
Mean-Field Theory $\Rightarrow$ Density Functional Theory

Degrees of freedom: nucleonic densities

A broken-symmetry generalized product state does surprisingly good job for nuclei.

Nuclear DFT
- two fermi liquids
- self-bound
- superfluid
- mean-field $\Rightarrow$ one-body densities
- zero-range $\Rightarrow$ local densities
- finite-range $\Rightarrow$ gradient terms
- particle-hole and pairing channels
- Has been extremely successful.
Nuclear Energy Density Functional

- Constrained by microscopic theory: ab-initio functionals provide quasi-data!
- Not all terms are equally important. Usually \( \sim 12 \) terms considered
- Some terms probe specific experimental data
- Pairing functional poorly determined. Usually 1-2 terms active.
- Becomes very simple in limiting cases (e.g., unitary limit)
- Can be extended into multi-reference DFT (GCM) and projected DFT

**isoscalar (T=0) density** \( \left( \rho_0 = \rho_n + \rho_p \right) \) + isoscalar and isovector densities: spin, current, spin-current tensor, kinetic, and kinetic-spin + pairing densities

\[
\rho_0 = \rho_n + \rho_p
\]

**isovector (T=1) density** \( \left( \rho_1 = \rho_n - \rho_p \right) \)

\[
E = \int \mathcal{H}(r) \, d^3r
\]

\[
\mathcal{H}(r) = \frac{\hbar^2}{2m} \tau_0(r) + \sum_{t=0,1} \left( \chi_t(r) + \tilde{\chi}_t(r) \right)
\]

- p-h density
- p-p density (pairing functional)

Expansion in densities and their derivatives
Examples: Nuclear Density Functional Theory

Mass table

$\delta m = 0.581$ MeV

Traditional (limited) functionals provide quantitative description

BE differences

Goriely, Chamel, Pearson: HFB-17
Phys. Rev. Lett. 102, 152503 (2009)

How many protons and neutrons can be bound in a nucleus?


Literature: 5,000-12,000

Skyrme-DFT: $6,900 \pm 500_{\text{syst}}$
Small and Large-Amplitude Collective Motion

- New-generation computational frameworks developed
  - Time-dependent DFT and its extensions
  - Collective Schrödinger Equation
  - Quasi-particle RPA
  - Projection techniques
- Applied to HI fusion, fission, coexistence phenomena

Shape coexistence

Hinohara et al. PRC 84, 061302(R) (2011)

also: Tsunoda et al. Phys. Rev. C 89, 031301(R) (2014); HPCI

Fusion cross section

R. Keser et al., PRC 85, 044606 (2012)
Nuclear Fission

\[ T_{1/2} = \ln \frac{2}{(nP)} \quad P = \frac{1}{1 + e^{2S}} \]

\[ S(L) = \int_{s_{in}}^{s_{out}} \frac{1}{\hbar} \sqrt{2M_{\text{eff}}(s)(V(s) - E_0)} \, ds \]

Spontaneous fission yields


http://science.energy.gov/ascr/highlights/2015/ascr-2015-08-a/
Quest for understanding the neutron-rich matter on Earth and in the Cosmos

Crustal structures in neutron stars

The covariance ellipsoid for the neutron skin $R_{\text{skin}}$ in $^{208}\text{Pb}$ and the radius of a $1.4M_\odot$ neutron star. The mean values are: $R(1.4M_\odot)=10$ km and $R_{\text{skin}}=0.17$ fm.
ISNET: Enhancing the interaction between nuclear experiment and theory through information and statistics

JPG Focus Issue: [http://iopscience.iop.org/0954-3899/page/ISNET](http://iopscience.iop.org/0954-3899/page/ISNET)

Around 35 papers (including nuclear structure, reactions, nuclear astrophysics, medium energy physics, statistical methods... and fission...)

“Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful” (E.P. Box)

Error estimates of theoretical models: a guide
Information Content of New Measurements

- Developed a Bayesian framework to quantify and propagate statistical uncertainties of EDFs.
- Showed that new precise mass measurements do not impose sufficient constraints to lead to significant changes in the current DFT models (models are not precise enough).

Bivariate marginal estimates of the posterior distribution for the 12-dimensional DFT UNEDF$_1$ parameterization.
1 teraflop = $10^{12}$ flops
1 peta = $10^{15}$ flops (today)
1 exa = $10^{18}$ flops (next 10 years)

Tremendous opportunities for nuclear theory!

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**Table: Top 500 Supercomputers**

<table>
<thead>
<tr>
<th>Rank</th>
<th>Name</th>
<th>CPU Type</th>
<th>Site</th>
<th>Year</th>
<th>Cores</th>
<th>理論 pFLOPS</th>
<th>Power (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Tianhe-2 (Milkyway-2)</td>
<td>Intel Ivy Bridge (12C 2.2 GHz) &amp; Xeon Phi (57C 1.1 GHz), Custom interconnect</td>
<td>NUDT, China</td>
<td>2015</td>
<td>3,120,000</td>
<td>33.9</td>
<td>17.8</td>
</tr>
<tr>
<td>2</td>
<td>Titan</td>
<td>Cray XK7, Opteron 6274 (16C 2.2 GHz) + Nvidia Kepler GPU, Custom interconnect</td>
<td>DOE/SC/ORNL, USA</td>
<td>2015</td>
<td>560,640</td>
<td>17.6</td>
<td>8.2</td>
</tr>
<tr>
<td>3</td>
<td>Sequoia</td>
<td>IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect</td>
<td>DOE/NNSA/LLNL, USA</td>
<td>2015</td>
<td>1,572,864</td>
<td>17.2</td>
<td>7.9</td>
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<tr>
<td>4</td>
<td>K computer</td>
<td>Fujitsu SPARC64 VIII fx (8C 2.0 GHz), Custom interconnect</td>
<td>RIKEN AICS, Japan</td>
<td>2015</td>
<td>705,024</td>
<td>10.5</td>
<td>12.7</td>
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<tr>
<td>5</td>
<td>Mira</td>
<td>IBM BlueGene/Q, Power BQC (16C 1.60 GHz), Custom interconnect</td>
<td>DOE/SC/ANL, USA</td>
<td>2015</td>
<td>786,432</td>
<td>8.59</td>
<td>3.95</td>
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**Graph: Performance Development**

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http://top500.org
Future: large multi-institutional efforts involving strong coupling between physics, computer science, and applied math

“High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes a third leg supporting the field of nuclear physics.” (NAC Decadal Study Report)