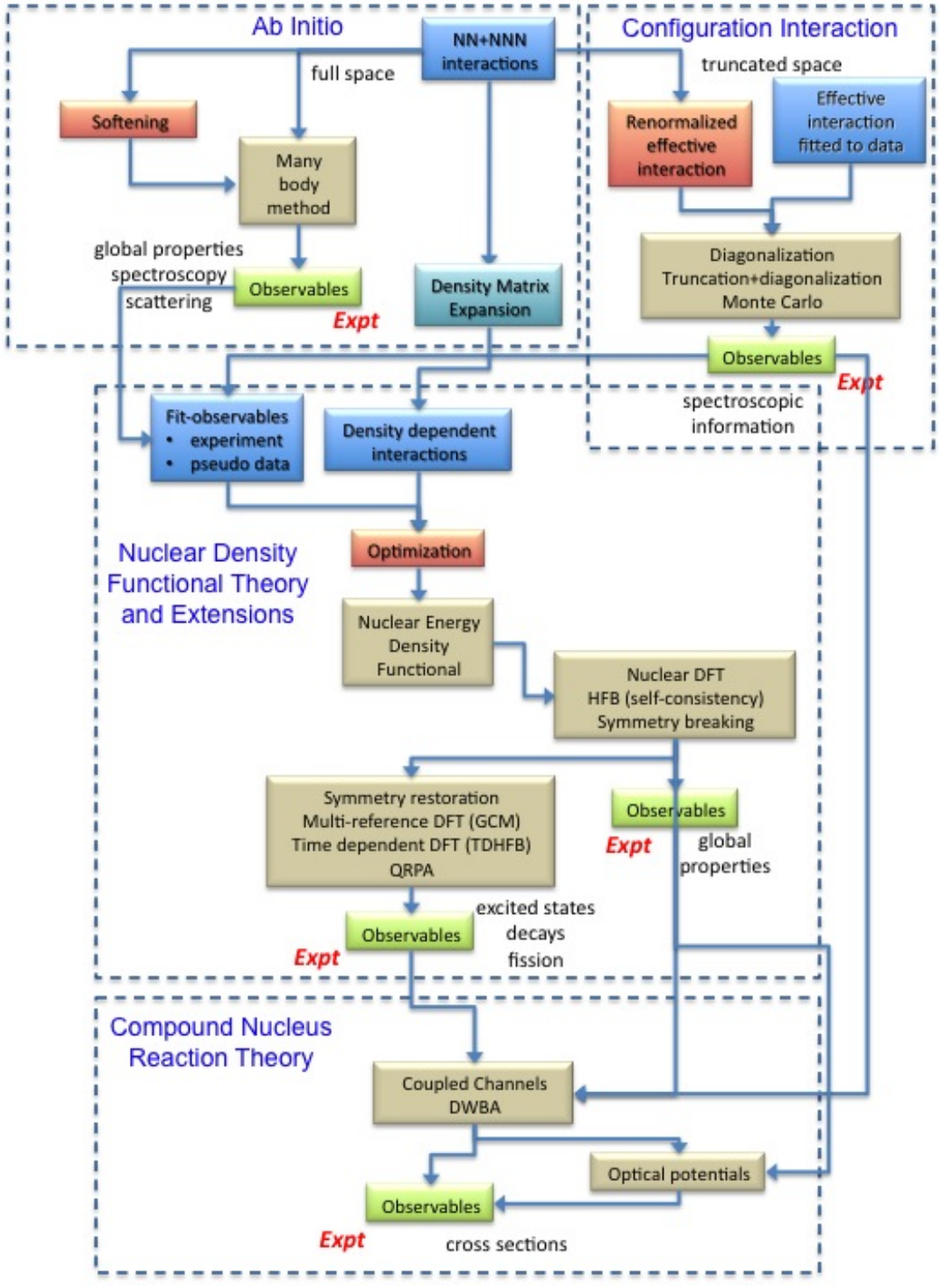
Ab Initio Functionals

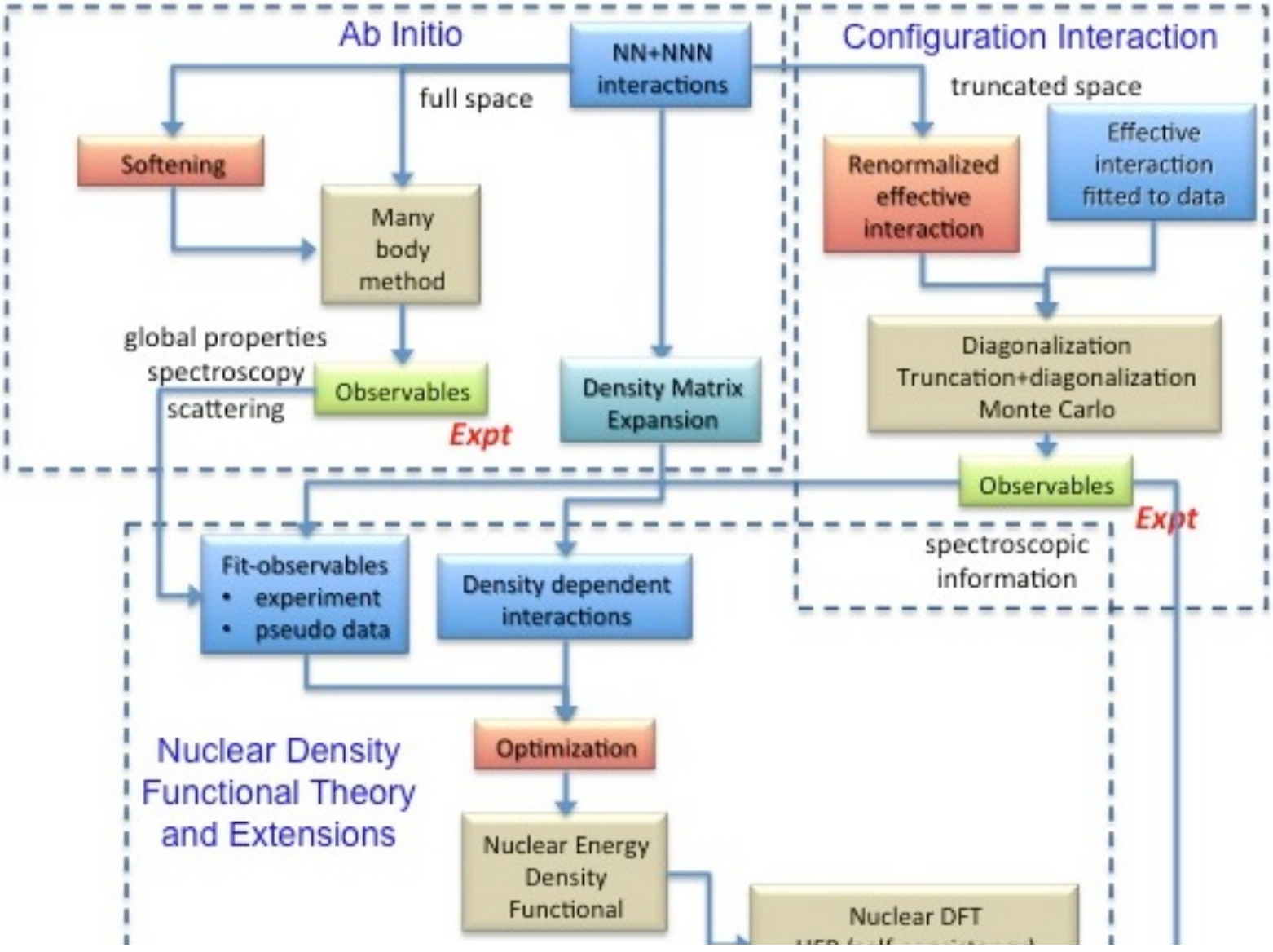
- overview
- status and plans

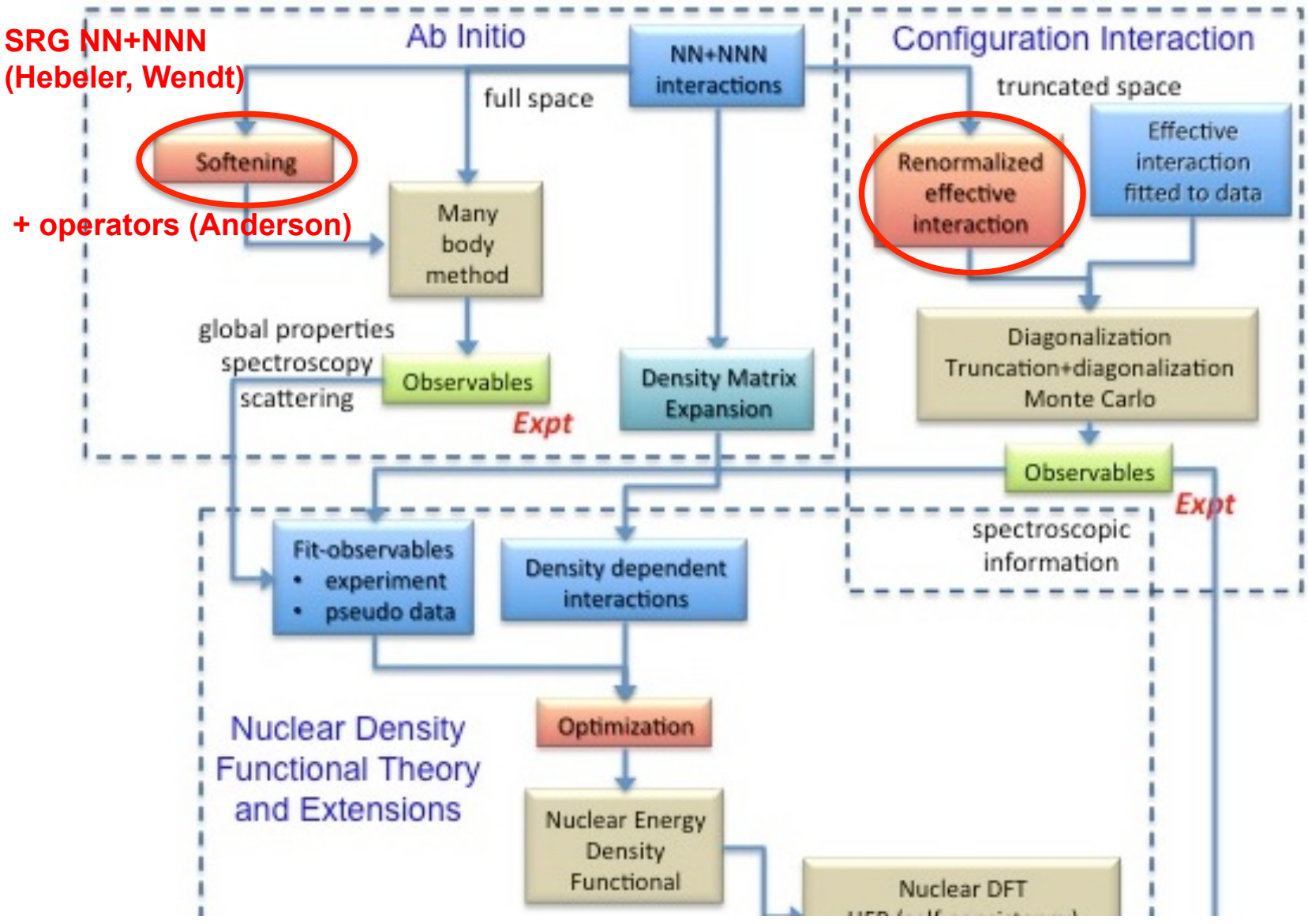


Role and Goals of the Ab Initio Functionals Group

From last year's CPR: (previous talks) (today's talks)

- Develop low-momentum NN and NNN interactions and operators as input to ab initio wave function methods and nuclear matter (Hebeler, Wendt, Anderson)
- Develop nuclear matter calculations with controlled theoretical errors as input to microscopic functionals (Hebeler)
- Construct ab initio functionals in the form of a generalized Skyrme interaction, with theoretical error bars, and understand conceptual issues (Drut, Bogner, Hergert)
- Validate the functionals against ab initio wave function methods (Maris, Kortelainen, Holt)
- Provide guidance to DFT Applications on novel density dependencies for EDF's based on microscopic input (Stoitsov, Hergert, Holt)


Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT


SRG NN+NNN
(Hebeler, Wendt)
+ operators (Anderson)
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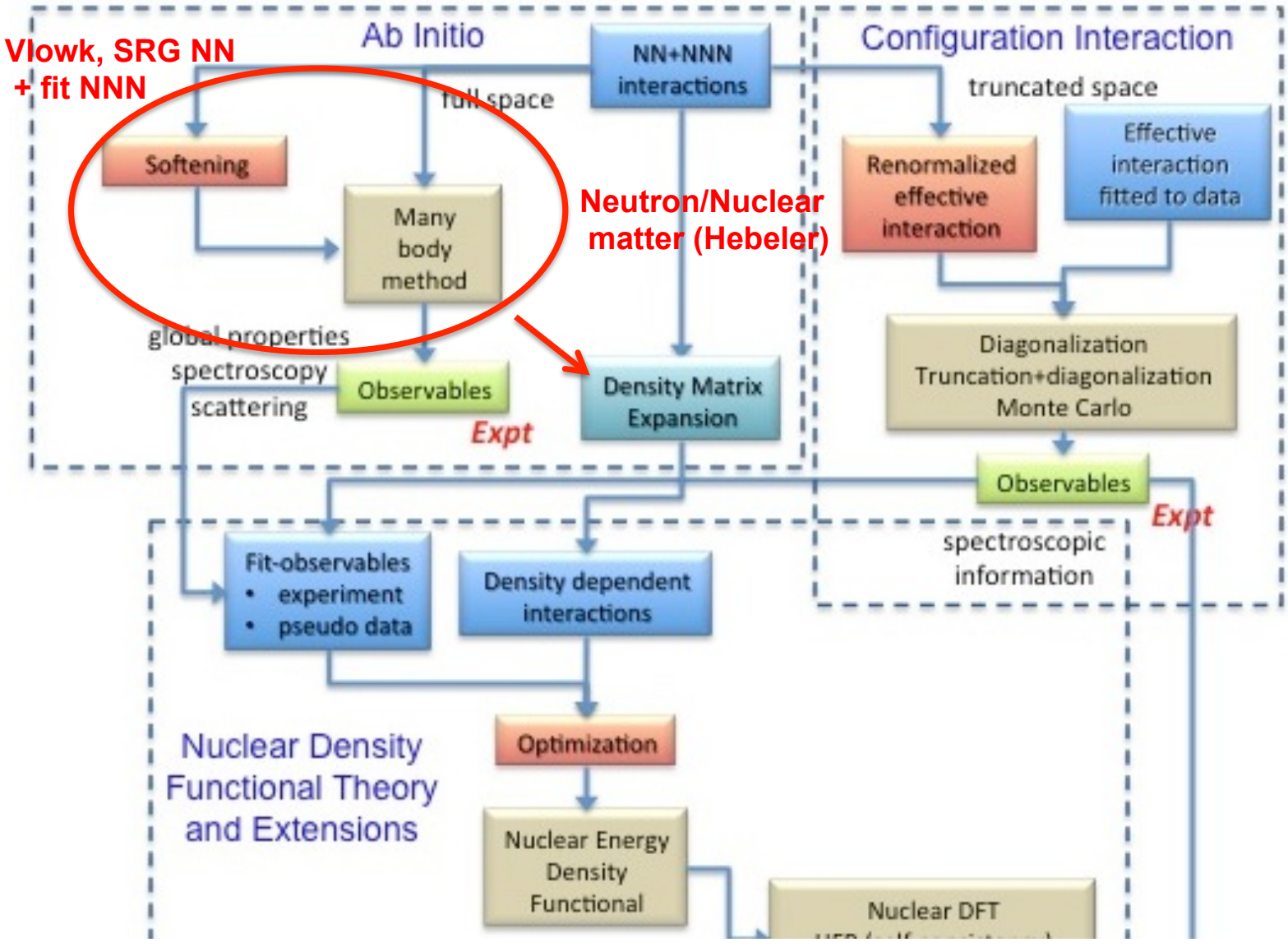
Vlowk, SRG NN
+ fit NNN
Ab Initio
NN+NNN
interactions
full space
Softening
Many
body
method
Neutron/Nuclear
matter (Hebeler)
global properties
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Density Matrix
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and Extensions
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Density
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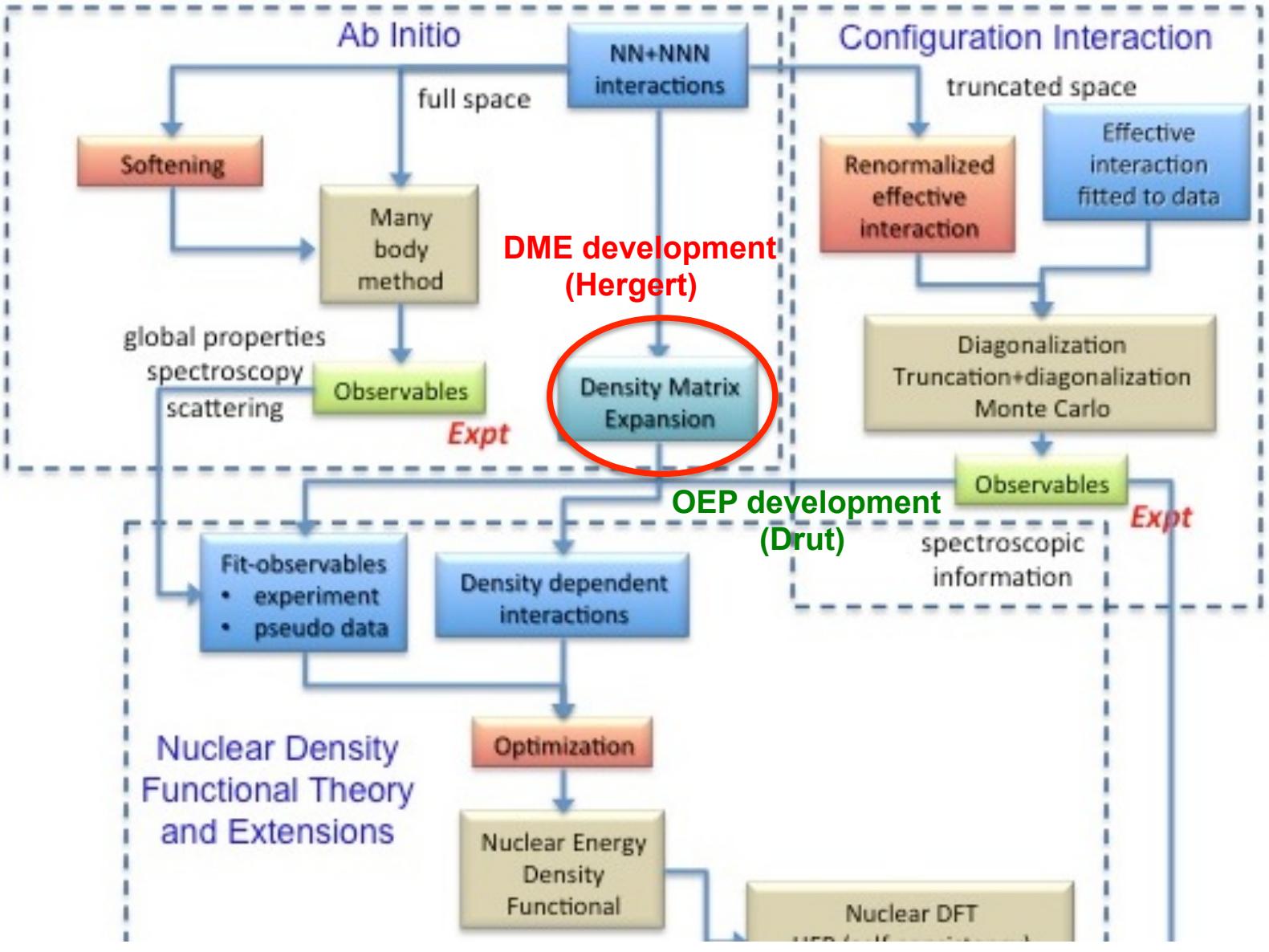
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DME development (Hergert)
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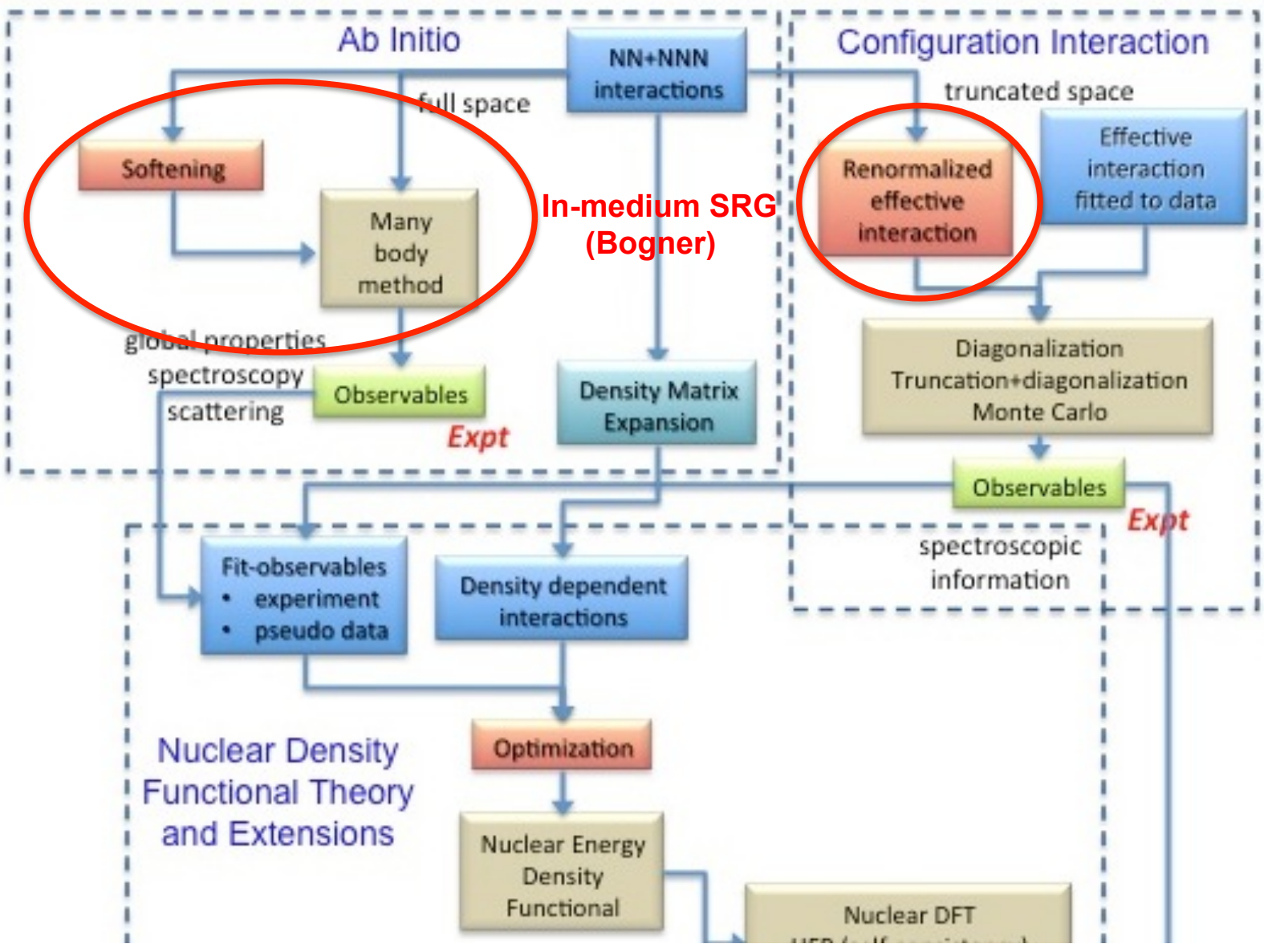
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In-medium SRG (Bogner)
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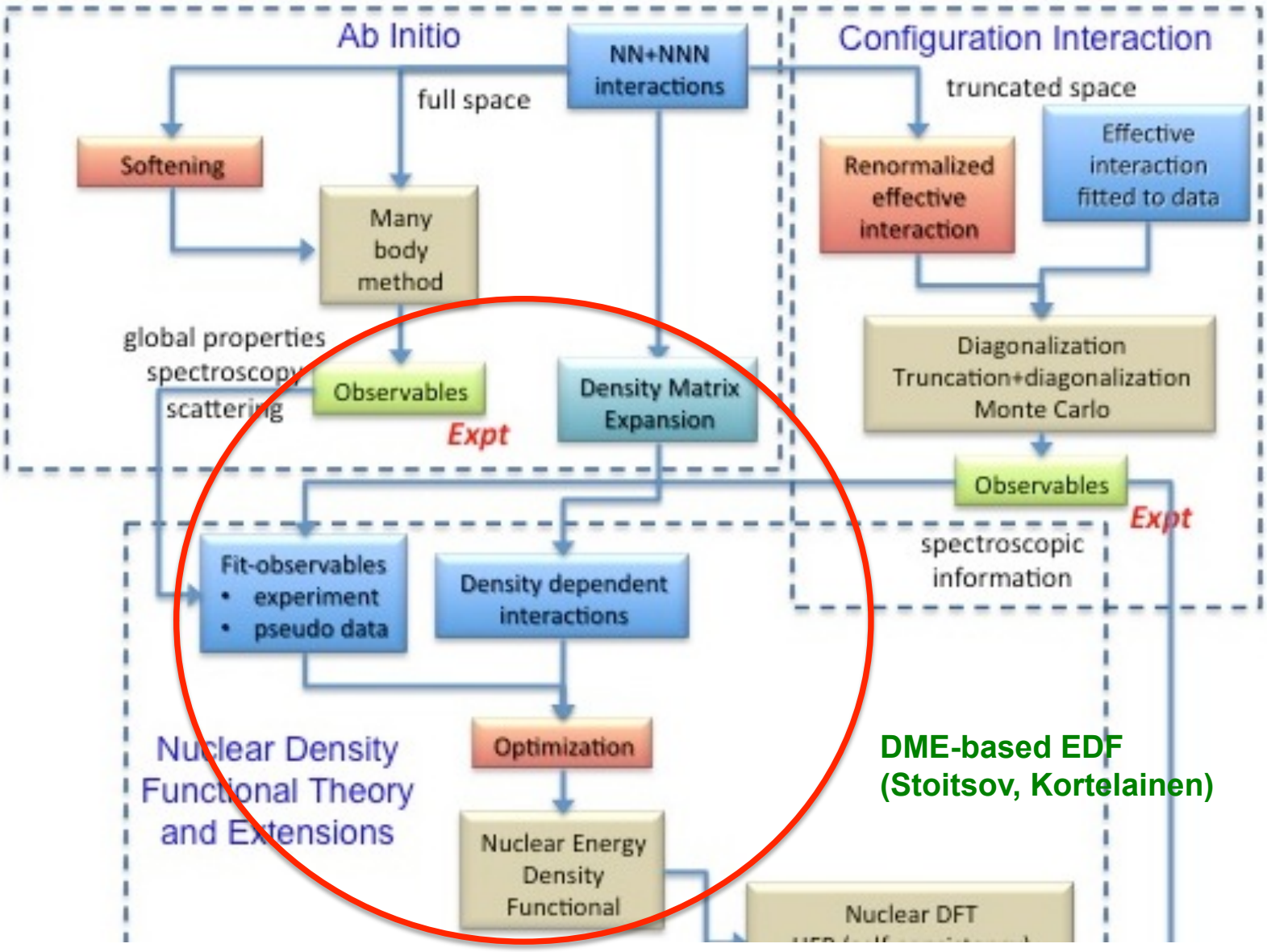
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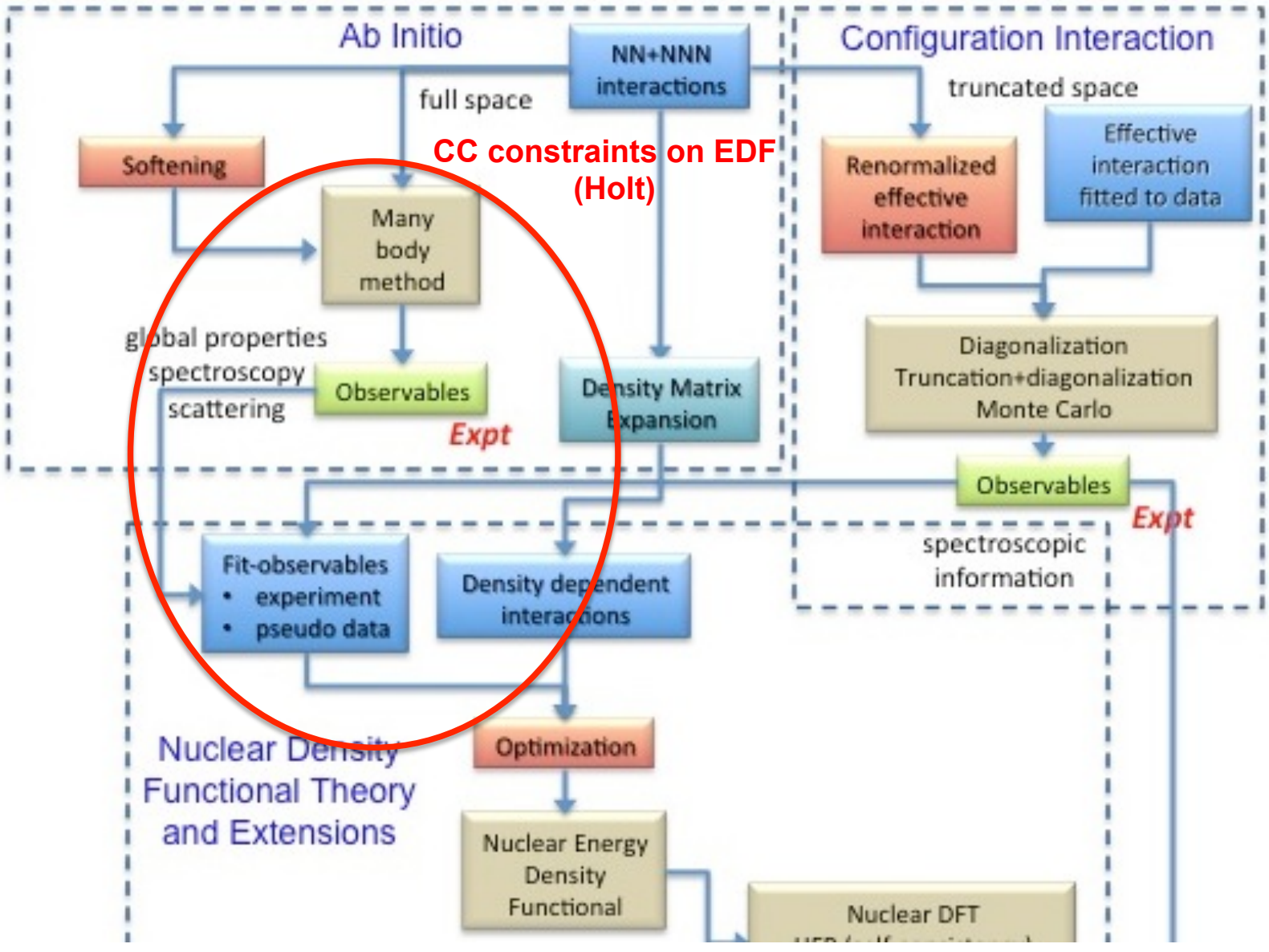
Nuclear DFT
DME-based EDF
(Stoitsov, Kortelainen)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CC constraints on EDF (Holt)
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Progress reports in this session

- Kai Hebeler, Neutron/nuclear matter/pairing with 3NF
  [presented by Furnstahl]
- Kyle Wendt, SRG developments
- Eric Anderson, SRG-evolved operators
- Scott Bogner, In-medium SRG

Coffee break

- Heiko Hergert, HFB/DME and QRPA calculations
- Jason Holt, Constraints on explicit nuclear density functionals from coupled-cluster theory

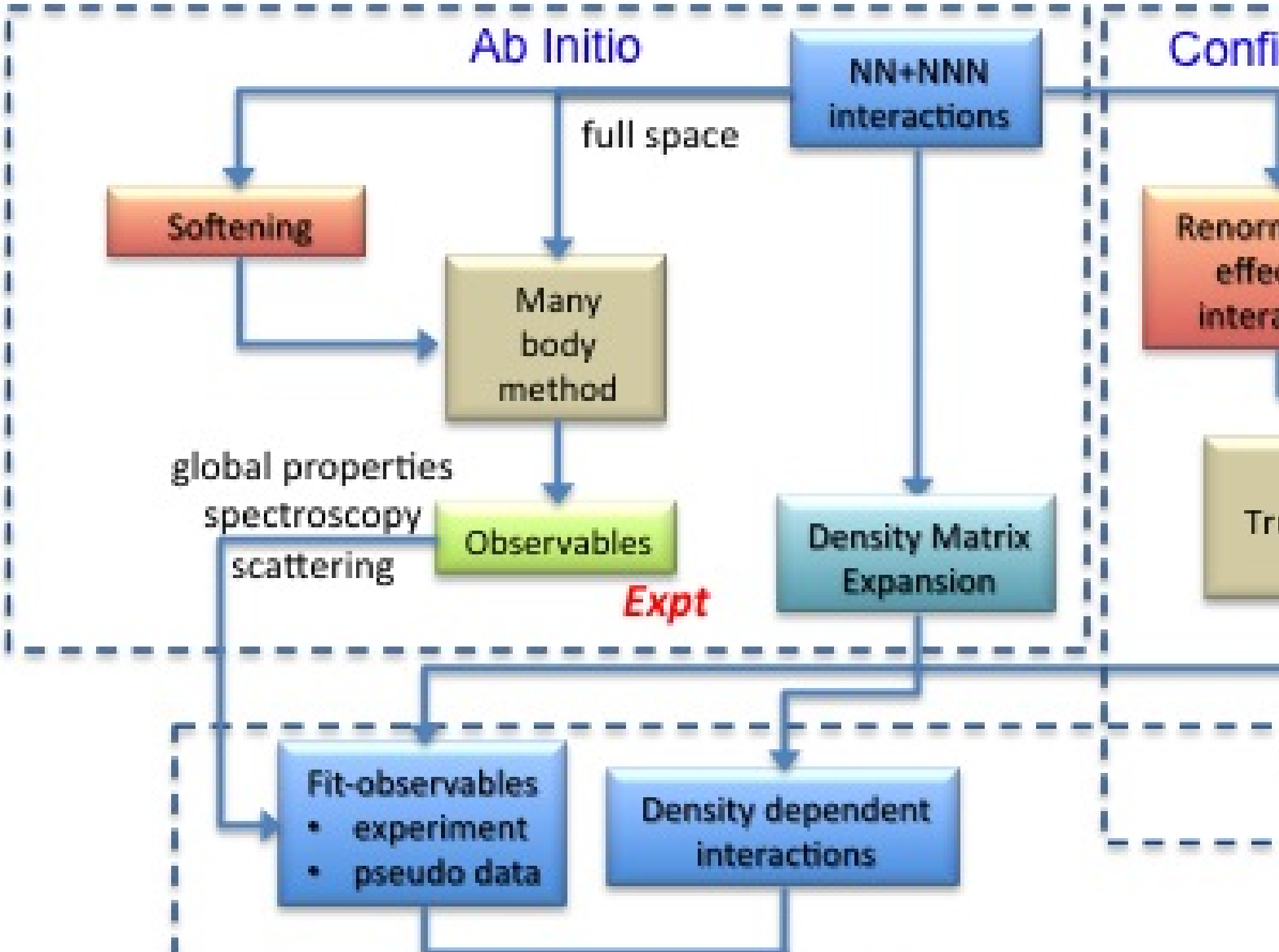
Ab Initio Nuclear DFT Deliverables

Plan for Year-5 from Continuation Progress Report

- Perform neutron drop benchmarks starting from NN and NNN interactions and validate against ab-initio calculations.
- Develop and test improved DME functionals that go beyond HF (microscopic pairing; constrain volume terms from BHF).
- Develop the Optimized Effective Potential (OEP) method for 3D-HFB; compare with HF, HF-DME, and ab initio.
- Use in-medium SRG to develop valence shell model Hamiltonians and effective operators for open-shell nuclei.

Other deliverables from CPR

- Apply *NN* + *NNN* low-*k* SRG interactions in p-shell with NCFC
- SRG: develop few-body operators, test factorization, explore alternative generators to control many-body operators
- Improve and test infinite matter on which DME relies; initial steps toward Monte Carlo and CC calculations
- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.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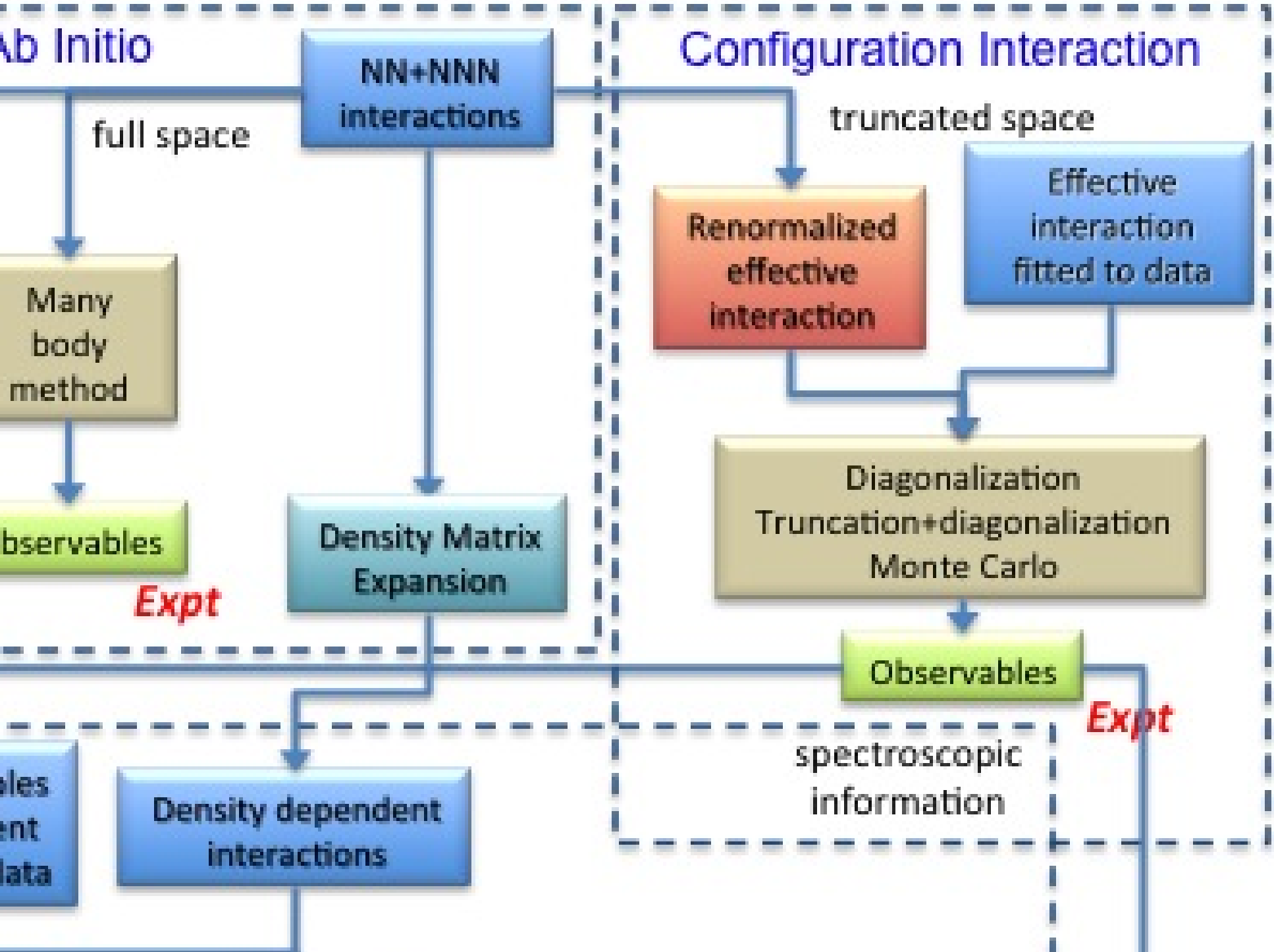
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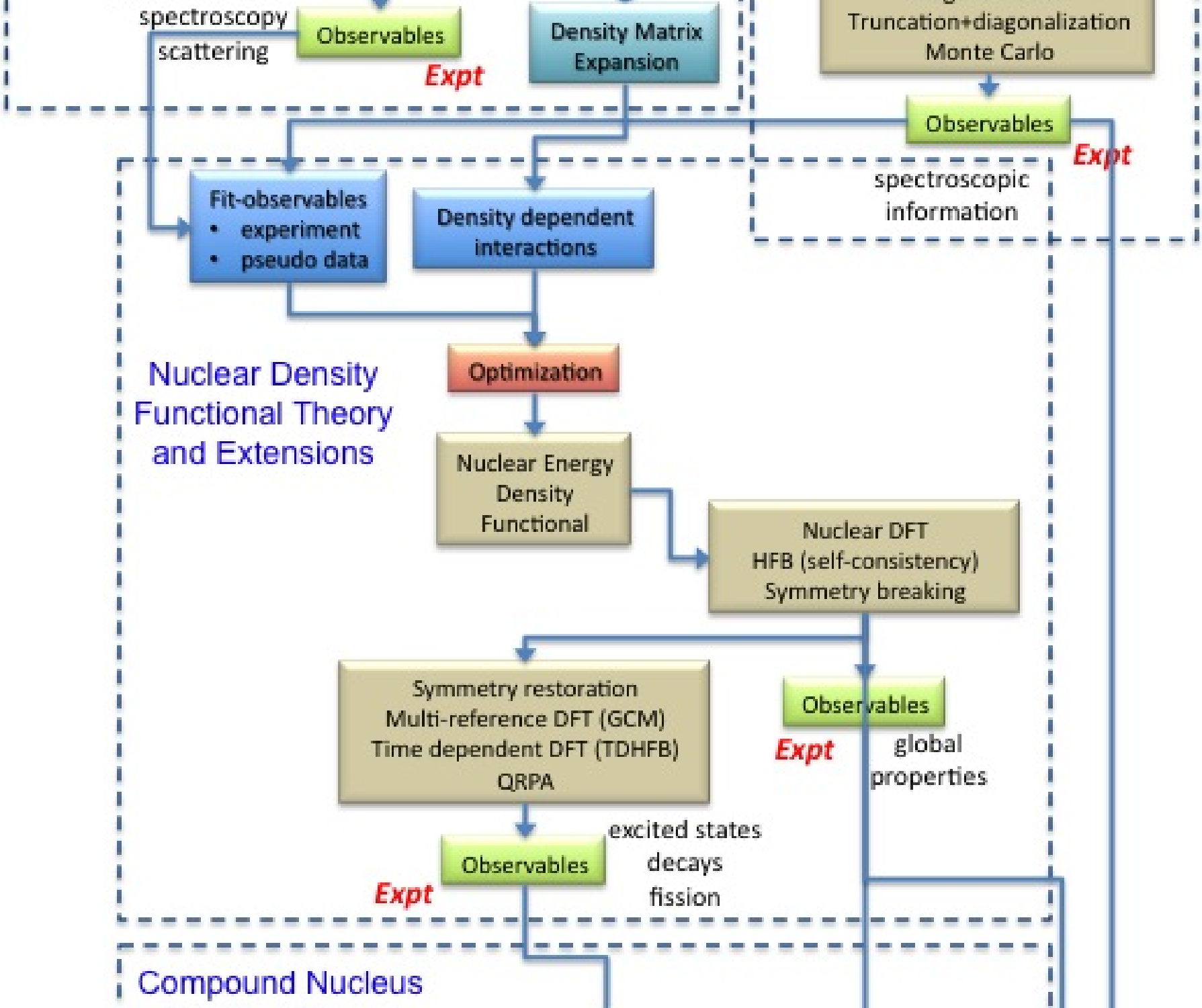
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Optimization
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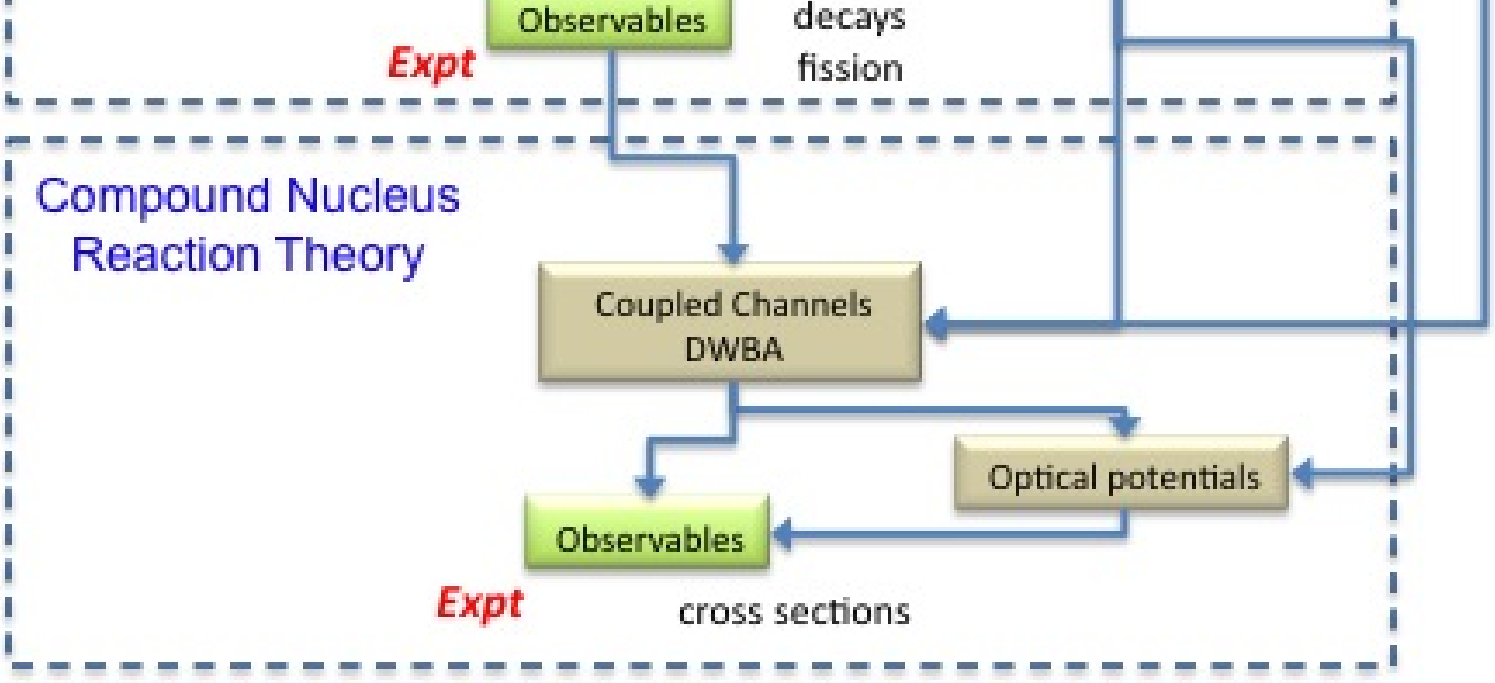
Nuclear DFT
HFB (self-consistency)
Symmetry breaking
Symmetry restoration
Multi-reference DFT (GCM)
Time dependent DFT (TDHFB)
QRPA
Observables
Expt
global properties
excited states
decays
fission
Observables
Expt
Compound Nucleus


Observables
decays
fission
Expt
Compound Nucleus
Reaction Theory
Coupled Channels
DWBA
Optical potentials
Observables
Expt
cross sections