Fermion Many-Body Systems III

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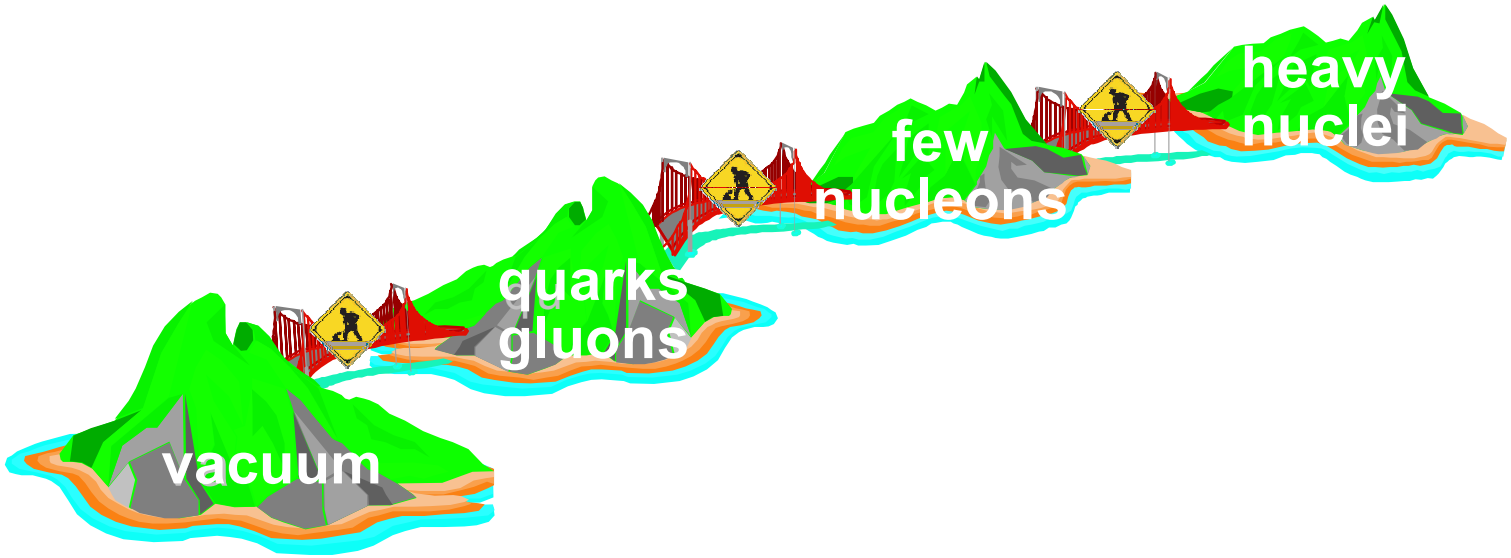
Outline

Introduction: Finite Nuclei

Density Functional Theory (DFT)

Future: Many-Body Challenges

The Islands of Hadronic and Nuclear Physics



quark-gluon plasma QCD	nucleon QCD	few-body systems free NN force	many-body systems effective NN force

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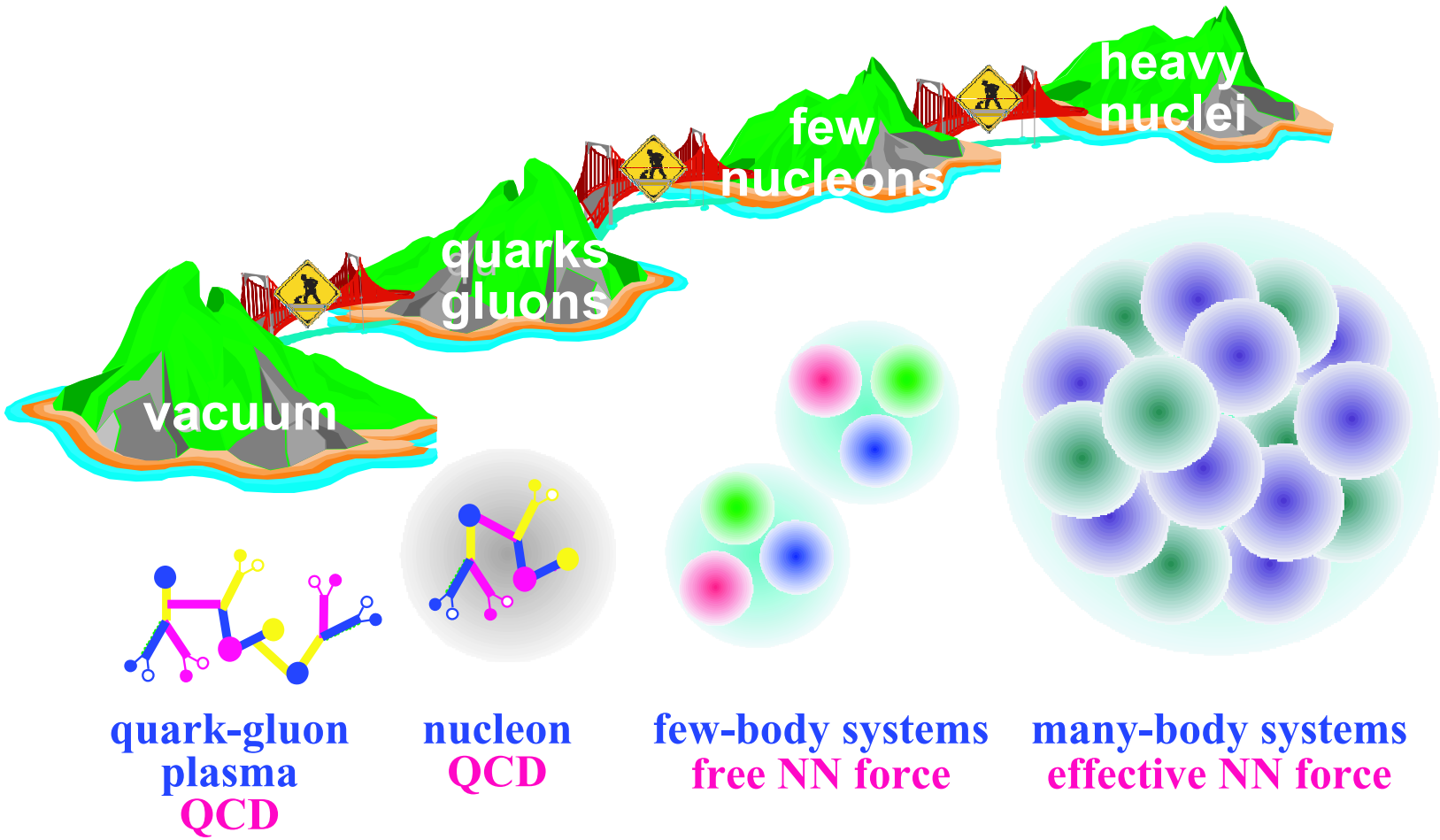

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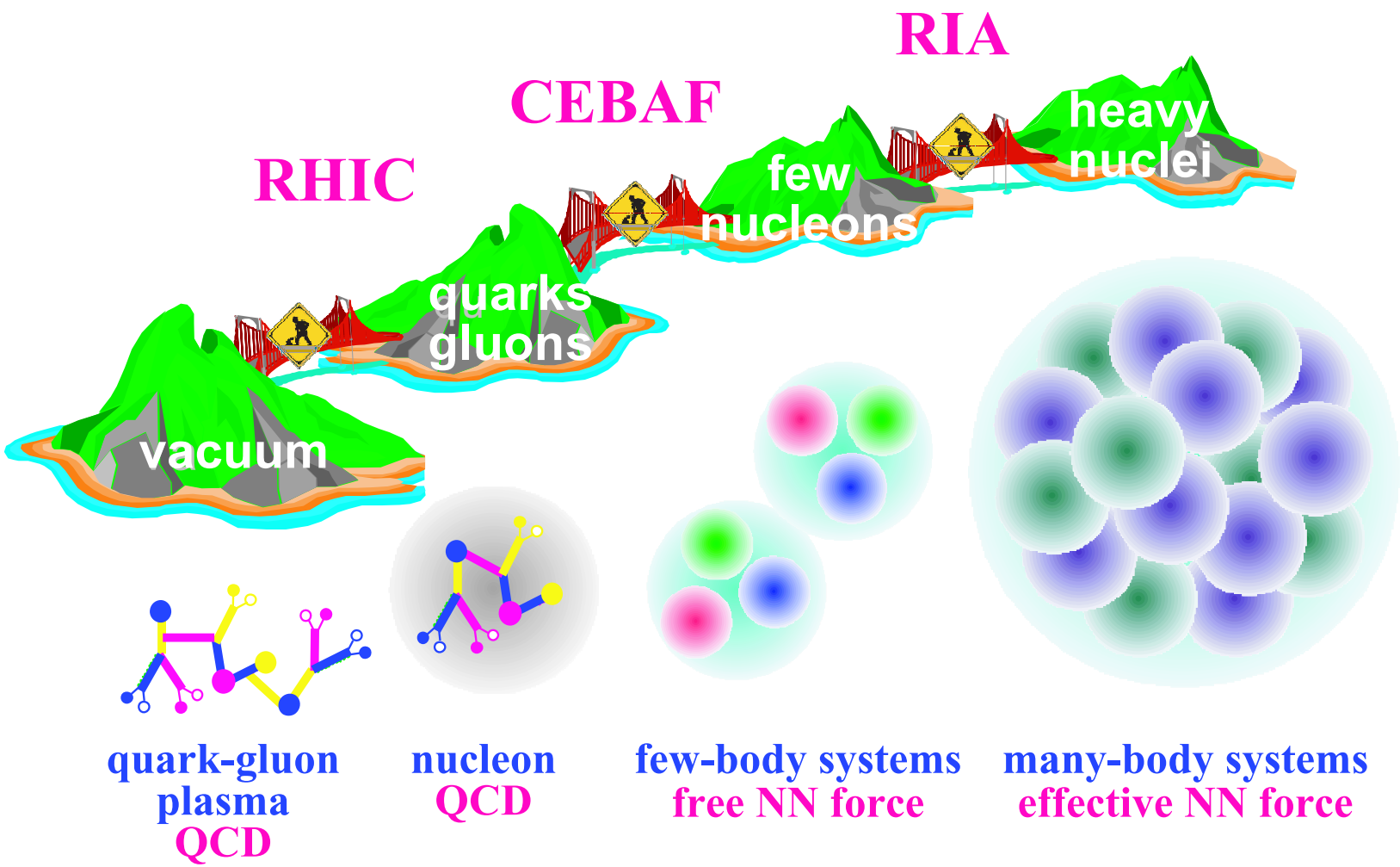

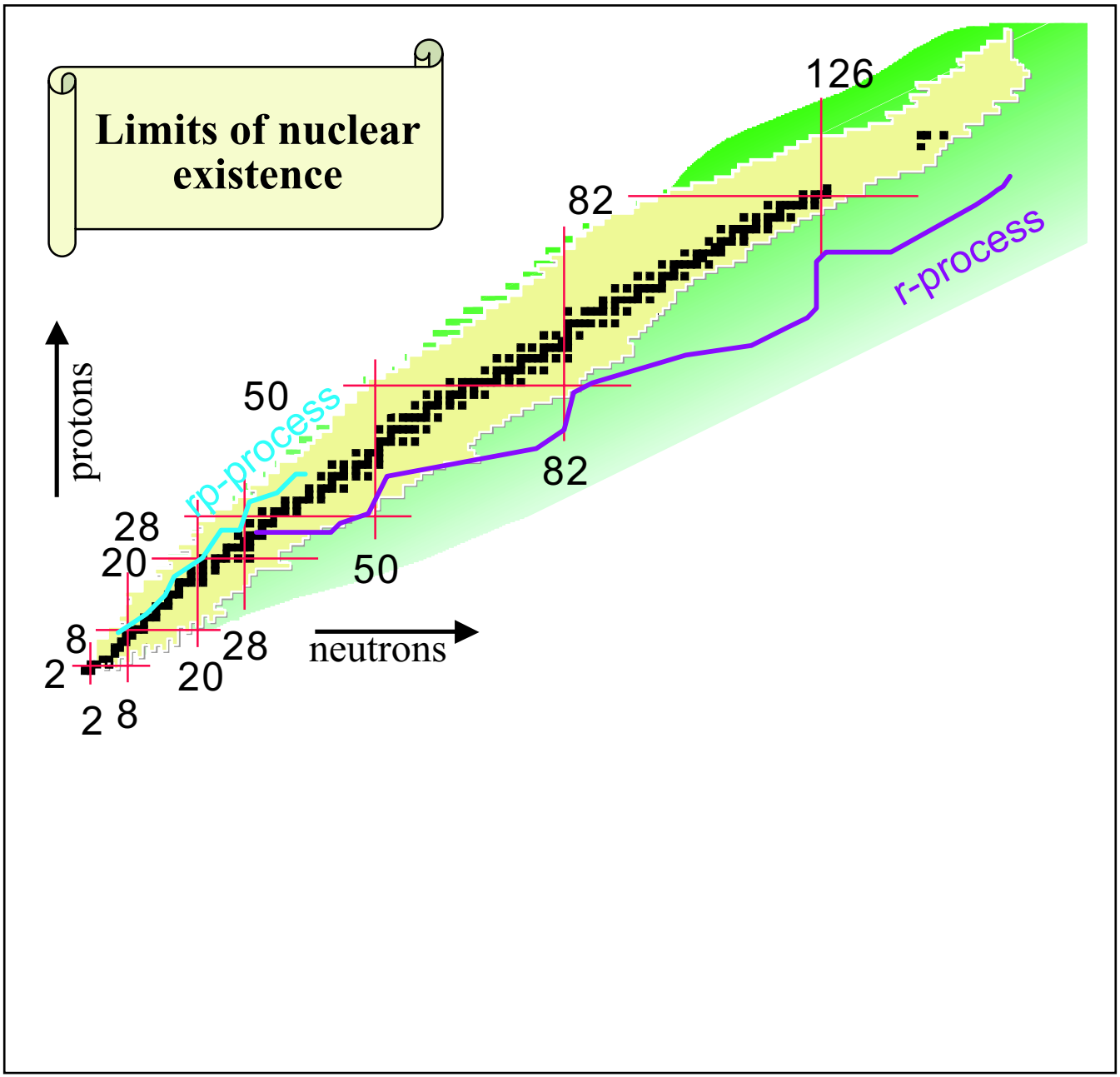
Limits of nuclear existence
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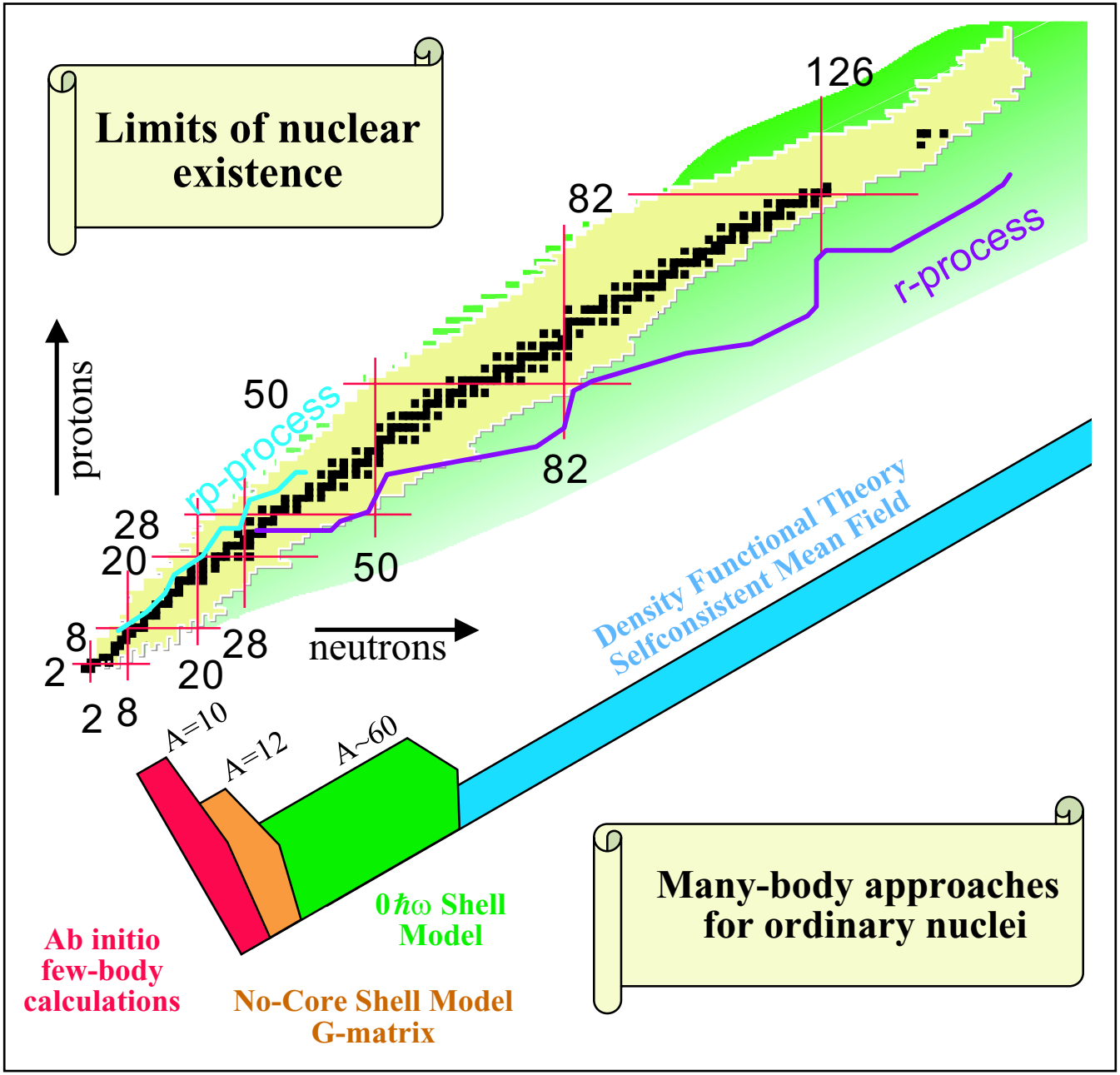
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Selfconsistent Mean Field
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Ab initio few-body calculations
No-Core Shell Model G-matrix
Many-body approaches for ordinary nuclei

Monte Carlo Calculations of Many-Body Systems

- For smaller systems (finite or in a box with pbc's)
  $\Longrightarrow$ approximate energy and full many-body wave function
  - Variational, diffusion, path integral, Green's function MC
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  - Variational, diffusion, path integral, Green's function MC
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- Variational Monte Carlo (VMC): Estimate $\langle E \rangle = \int d\mathbf{R}\, \rho(\mathbf{R})\, E_L(\mathbf{R})$
  - local energy $E_L(\mathbf{R}) = \frac{H\psi_T(\mathbf{R})}{\psi_T(\mathbf{R})}$ with trial wave function $\psi_T(\mathbf{R})$
  - probability distribution $\rho(\mathbf{R}) = \frac{\psi_T^2(\mathbf{R})}{\int d\mathbf{R}\, \psi_T^2(\mathbf{R})}$
  - accept step to $\mathbf{R}'$ if $p = \psi_T^2(\mathbf{R}')/\psi_T^2(\mathbf{R}) \geq 1$,
    else if $p < 1$ accept with probability p
  - minimize $\langle E \rangle$ or variance of $E_L(\mathbf{R})$ with respect to variational parameters in $\psi_T(\mathbf{R})$
  - gives upper bound to ground state E
- Requires very good trial wave function for reliable results

- DMC and GFMC exploit S–equation in imaginary time
  $\Longrightarrow$ diffusion!

$$-\hbar\frac{\partial}{\partial\tau}\Psi(\mathbf{R},\tau) = -\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}}\Psi(\mathbf{R},\tau) + V(\mathbf{R})\Psi(\mathbf{R},\tau)$$

  - Use Metropolis to propagate to large $\tau \Longrightarrow$ projects ground state

$$\Psi(\mathbf{R},\tau) = \int d\mathbf{R}'\, G(\mathbf{R},\mathbf{R}',\tau)\,\Psi(\mathbf{R}',\tau)$$

  - Take many steps with small τ approximation to G
  - Generates "walker representation" of wave function (a set of $\mathbf{R}_i$'s)
    $\Longrightarrow$ can only represent a positive density

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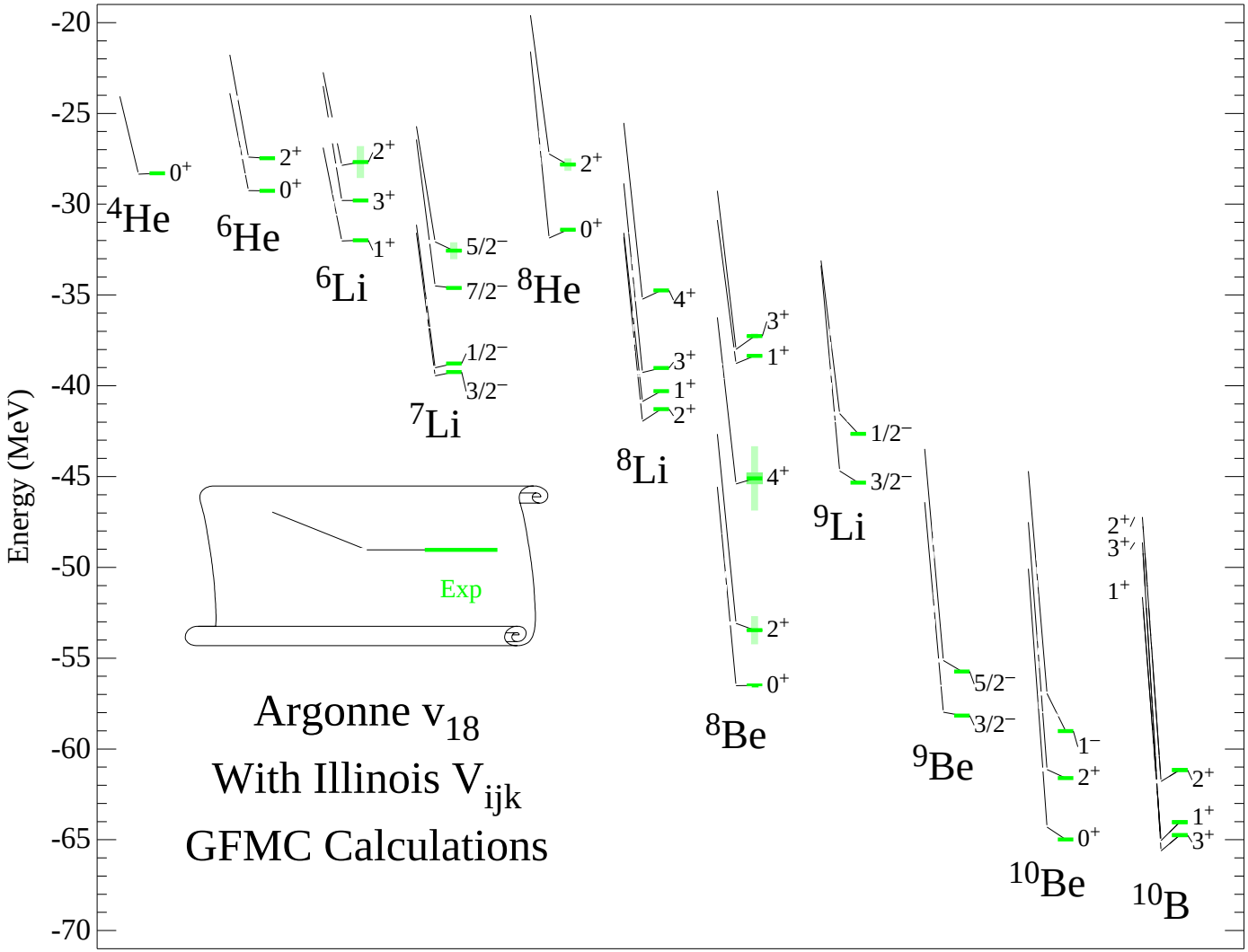
- Fermion sign problem for diffusion, path integral, GFMC
  - for fermions, even ground-state wavefunction changes sign (anti-symmetric)
  - if trial function provides good representation of nodes, solve in regions with nodal boundary conditions ("fixed node")

Monte Carlo (GFMC) Calculations of Light Nuclei

Carlson, Pandharipande, Pieper, Wiringa



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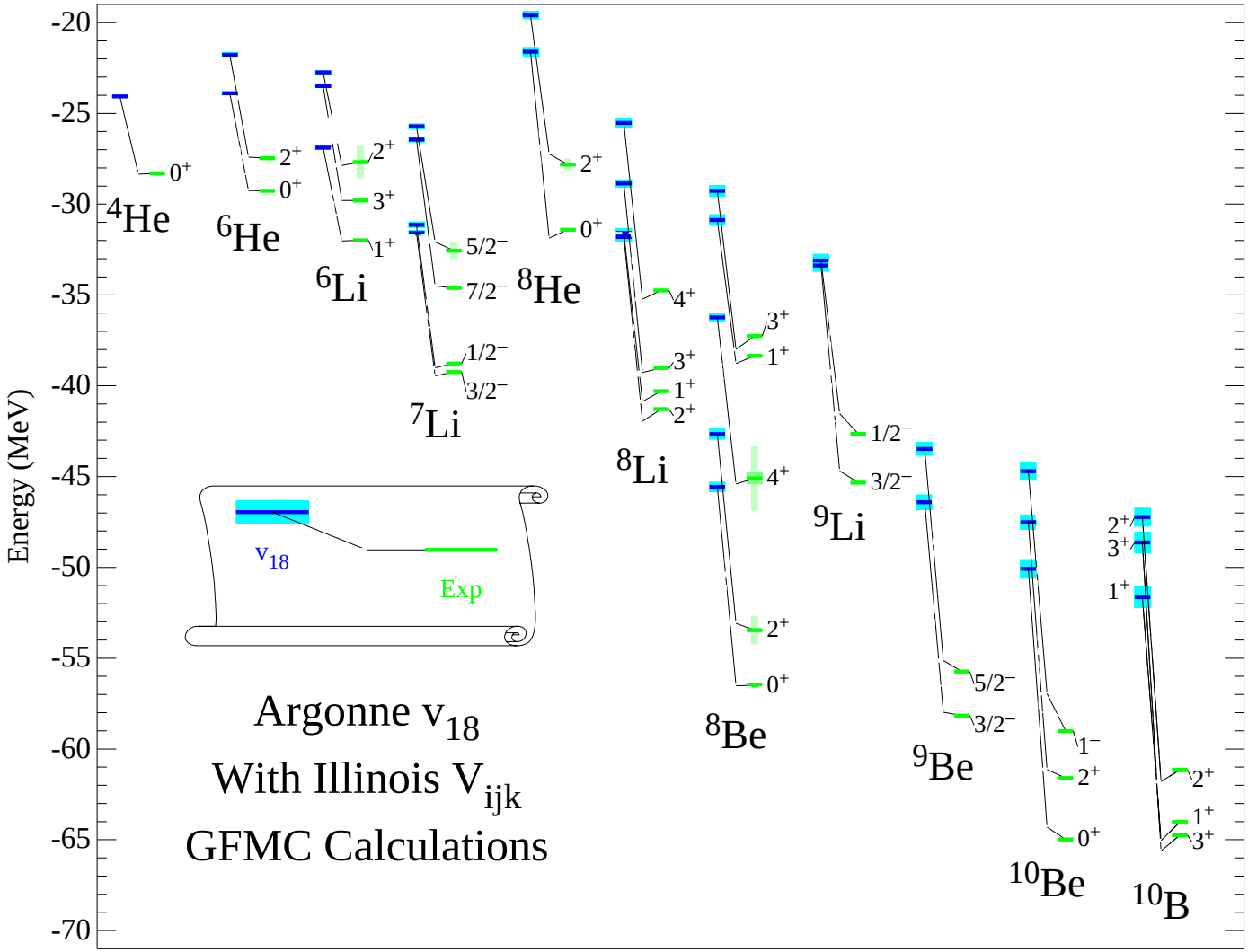

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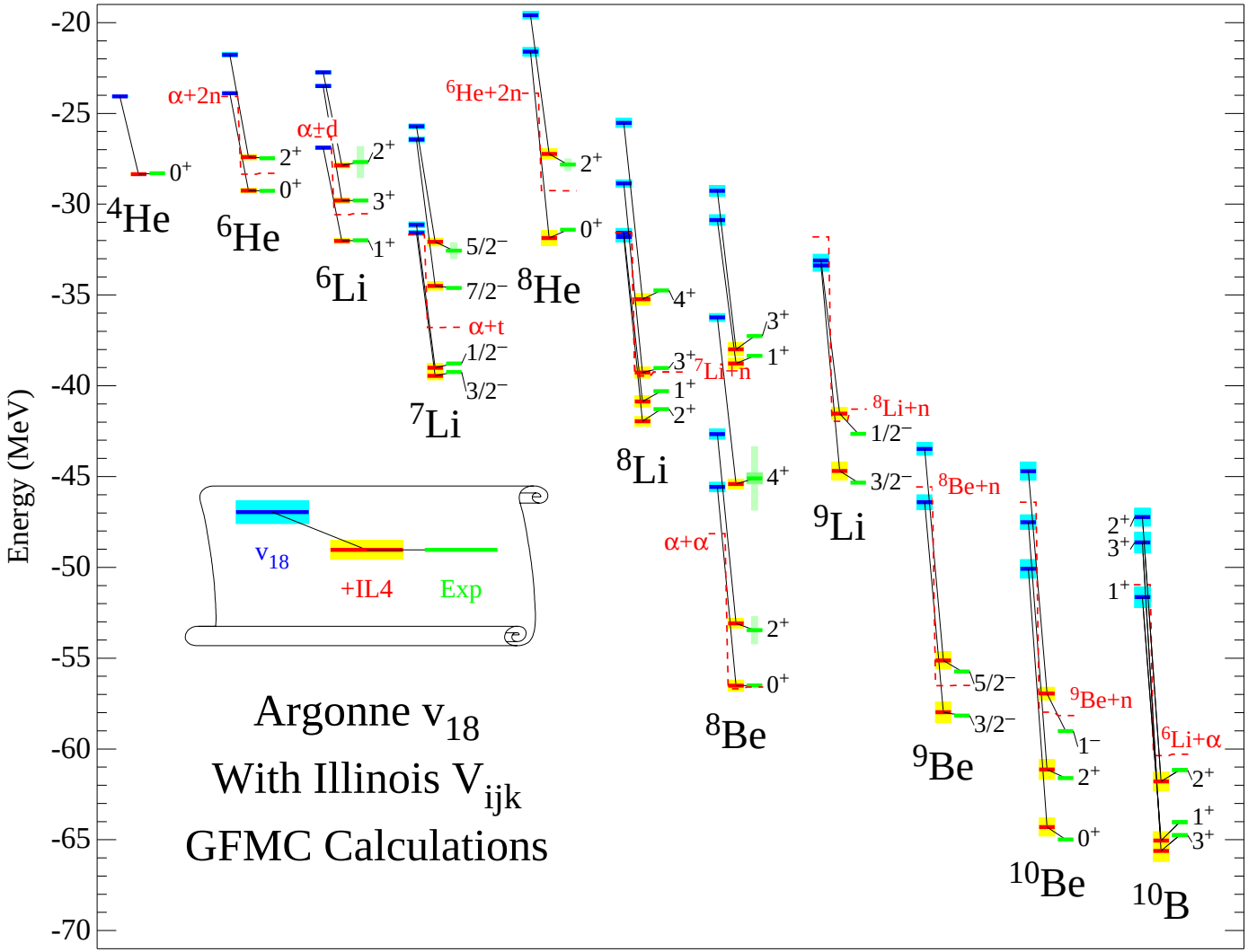
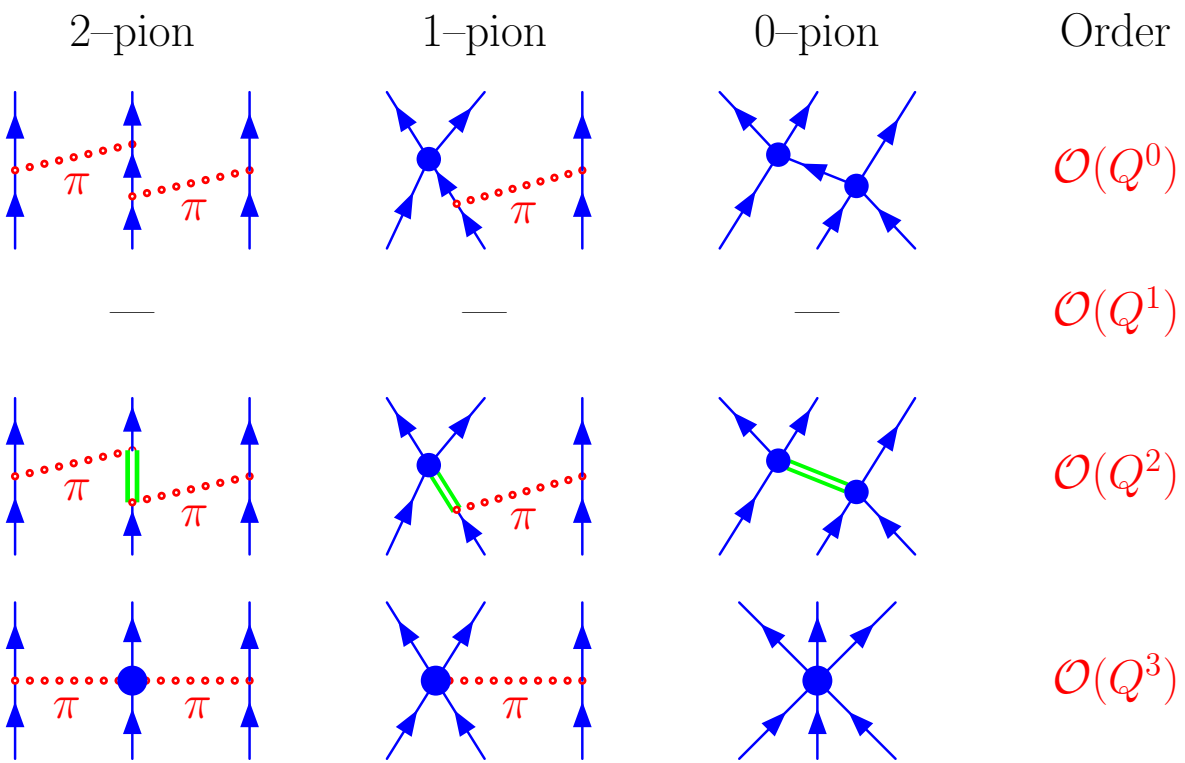


Chiral EFT: Systematic Many-Body Forces

- Contribution of $(n+1)$–body potential relative to n–body:

$$\frac{\langle V_{(n+1)N} \rangle}{\langle V_{nN} \rangle} \sim \mathcal{O}\left(\frac{Q}{\Lambda_\chi}\right)^2$$

- Hierarchy of three-body forces:



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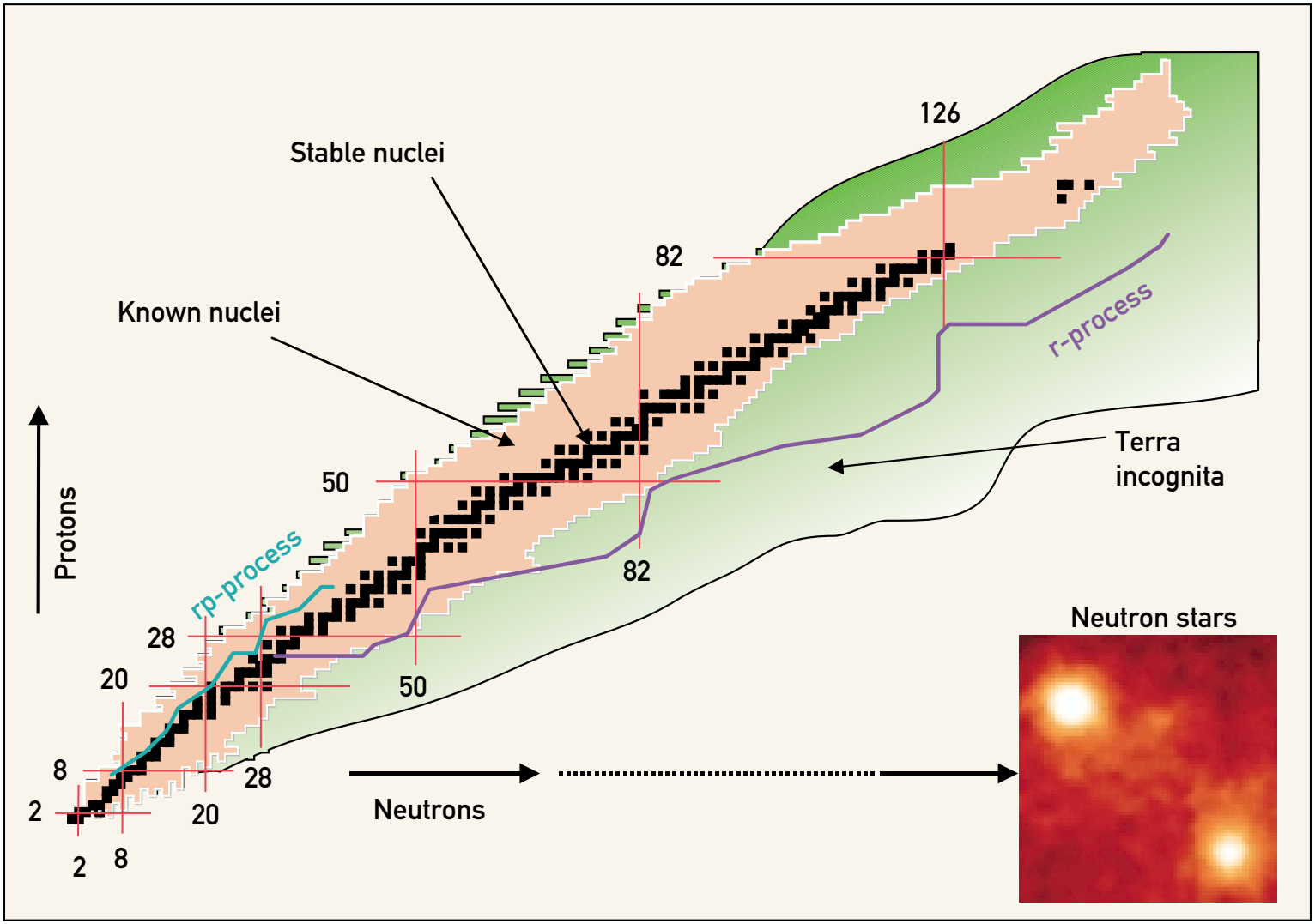

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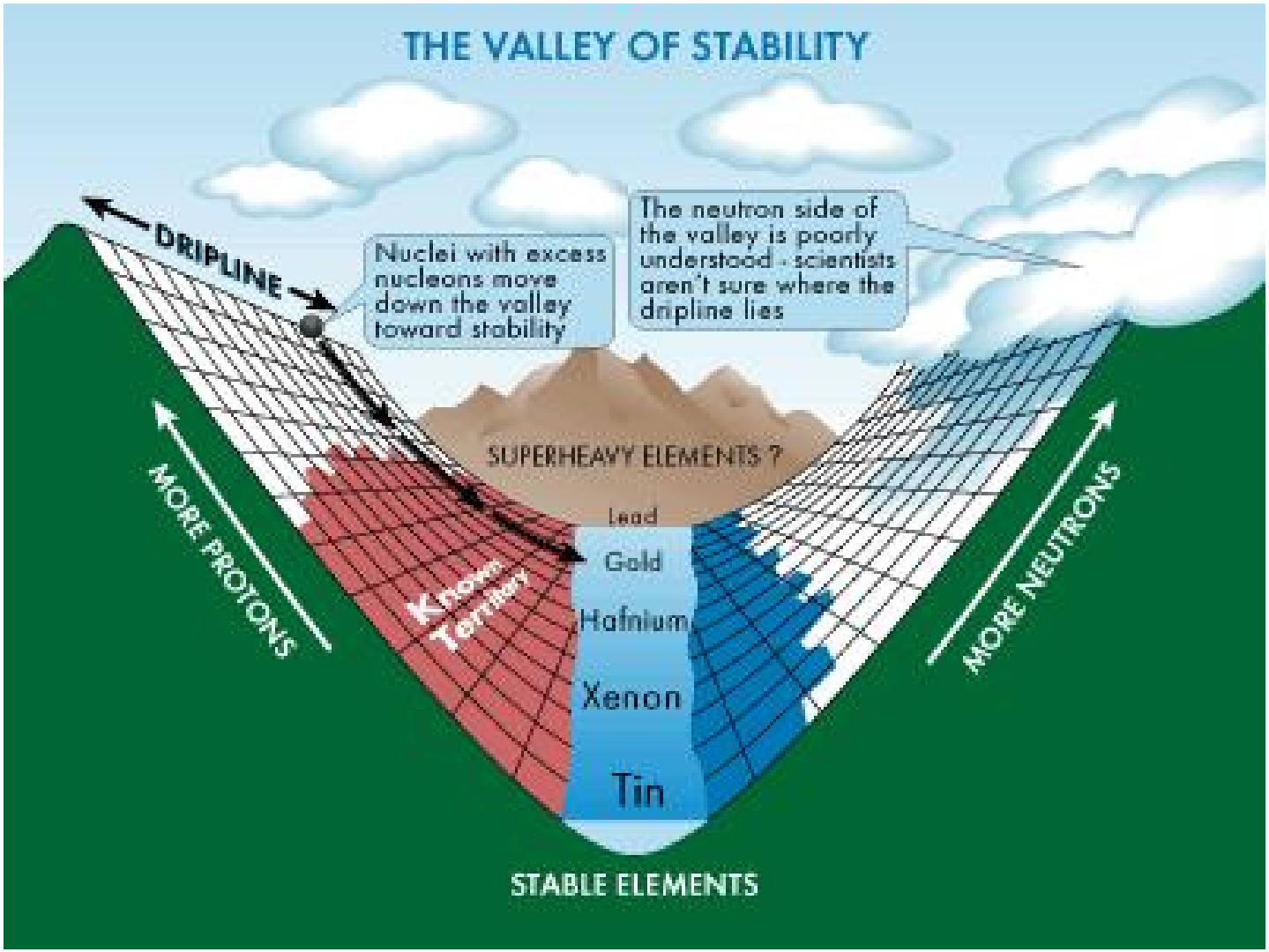

Skyrme Hartree-Fock Energy Functionals

- Skyrme energy density functional (for $N = Z$):

$$\begin{aligned}\mathcal{E}[\rho,\tau,\mathbf{J}] &= \frac{1}{2M}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1+5t_2)\rho\tau \\ &\quad + \frac{1}{64}(9t_1-5t_2)(\nabla\rho)^2 - \frac{3}{4}W_0\rho\nabla\cdot\mathbf{J} + \frac{1}{32}(t_1-t_2)\mathbf{J}^2\end{aligned}$$

  - where $\rho(x) = \sum_\alpha |\phi_i(x)|^2$ and $\tau(x) = \sum_\alpha |\nabla\phi_i(x)|^2$ (and $\mathbf{J}$)

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- Minimize $E = \int d\mathbf{x}\,\mathcal{E}[\rho,\tau,\mathbf{J}]$ by varying the (normalized) ϕ_i's

$$\left(-\nabla\frac{1}{2M^*(\mathbf{x})}\nabla + U(\mathbf{x}) + \frac{3}{4}W_0\nabla\rho\cdot\frac{1}{i}\nabla\times\sigma\right)\phi_\alpha(\mathbf{x}) = \epsilon_\alpha\,\phi_\alpha(\mathbf{x})$$

where the effective mass $M^*(\mathbf{x})$ is given by

$$\frac{1}{2M^*(\mathbf{x})} = \frac{1}{2M} + \left[\frac{3}{16}\,t_1 + \frac{5}{16}\,t_2\right]\,\rho(\mathbf{x})$$

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- Iterate until ϕ_i's and ϵ_α's are self-consisent

Questions and Criticisms of Skyrme HF

- Typical [e.g., SkIII] model parameters (in units of MeV-fm^n):
  $t_0 = -1129 \quad t_1 = 395 \quad t_2 = -95 \quad t_3 = 14000 \quad W_0 = 120$
  - These seem large; is there an expansion?
  - Where does $\rho^{2+\alpha}$ come from?
  - Parameter Fitting [von Neumann via Fermi via Dyson]:
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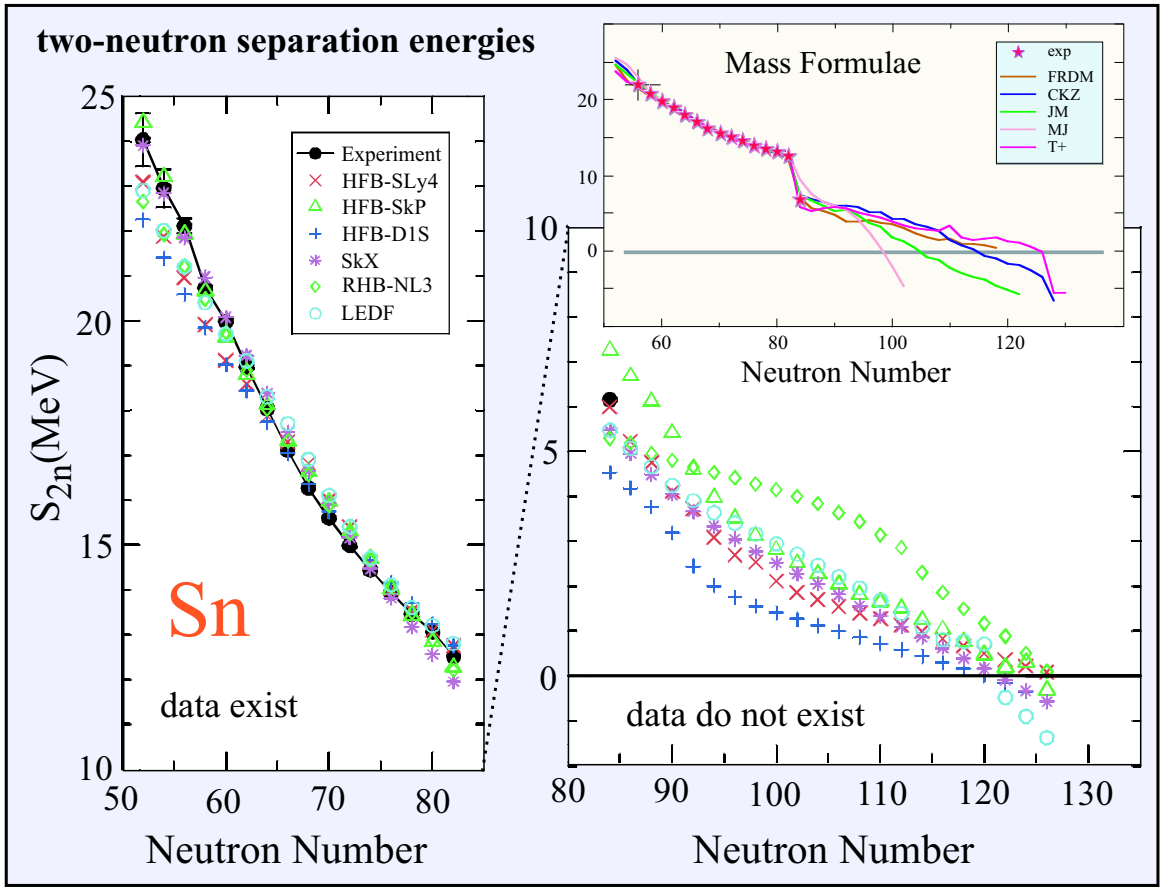
- How does Skyrme HF relate to NN (and NNN) forces?

Problems with Extrapolations

- Mass formulas and energy functionals do well where there is data, but elsewhere . . .



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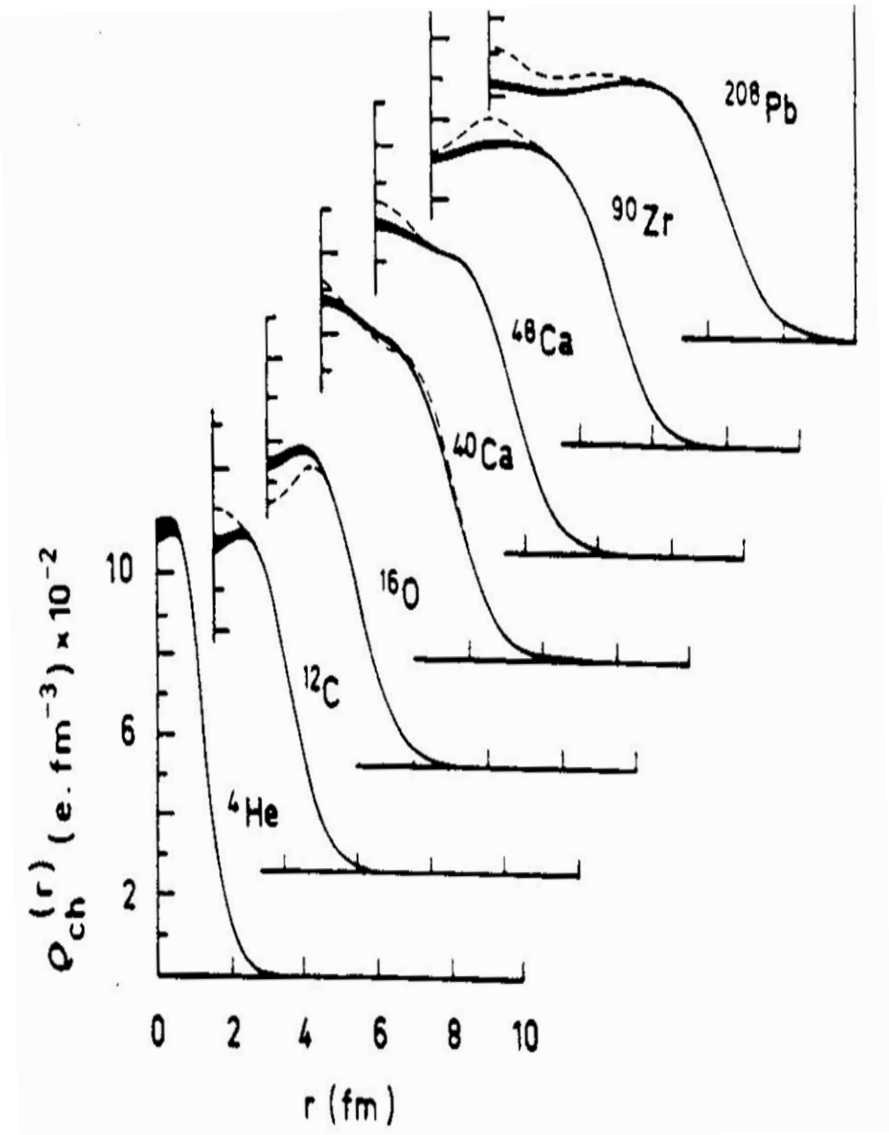
- New insight into analytic structure of functional
  - e.g., logs in low-density expansion in $k_F a_s$ from renormalization group

Density Functional Theory (DFT)

- Hohenberg-Kohn: There exists an energy functional $E_v[n]$ ...

$$E_v[n] = F_{\rm HK}[n] + \int d^3x\, v(\mathbf{x}) n(\mathbf{x})$$

- $F_{\rm HK}$ is *universal* (same for any external v) $\Longrightarrow$ H_2 to DNA!



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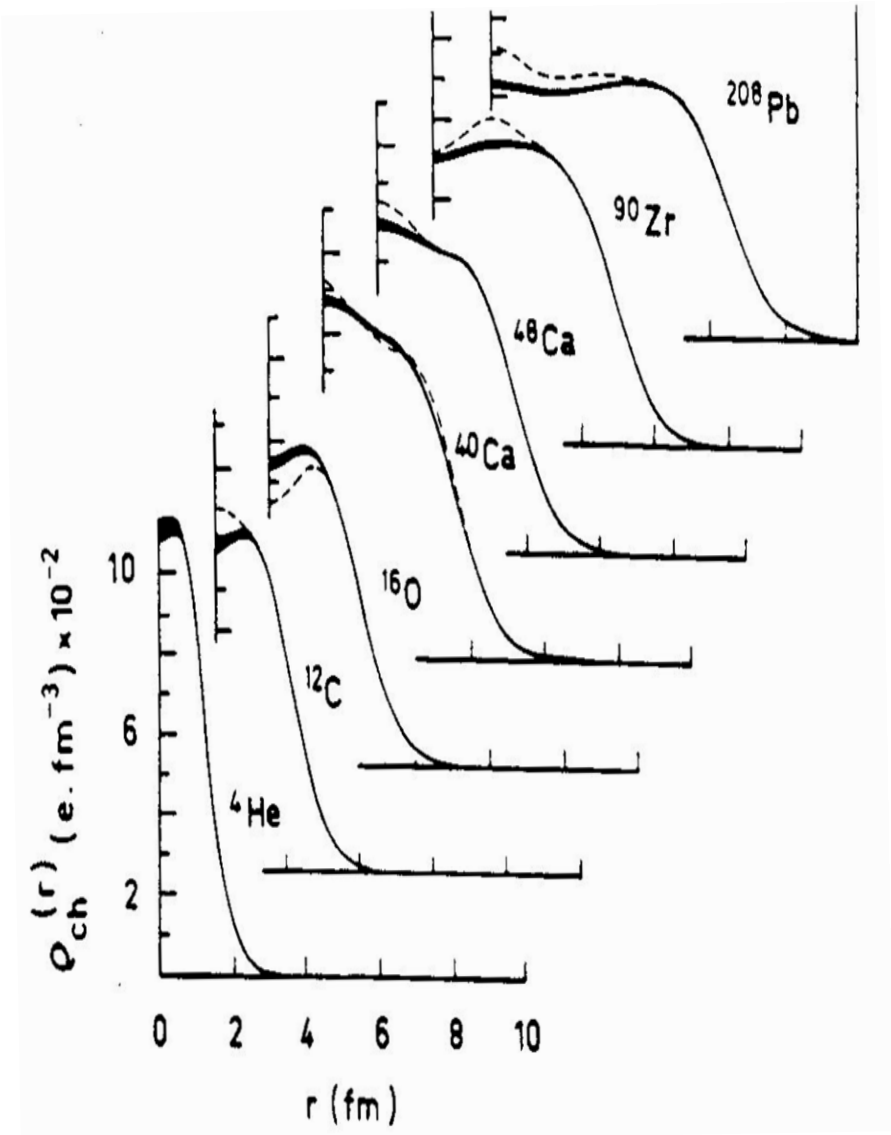

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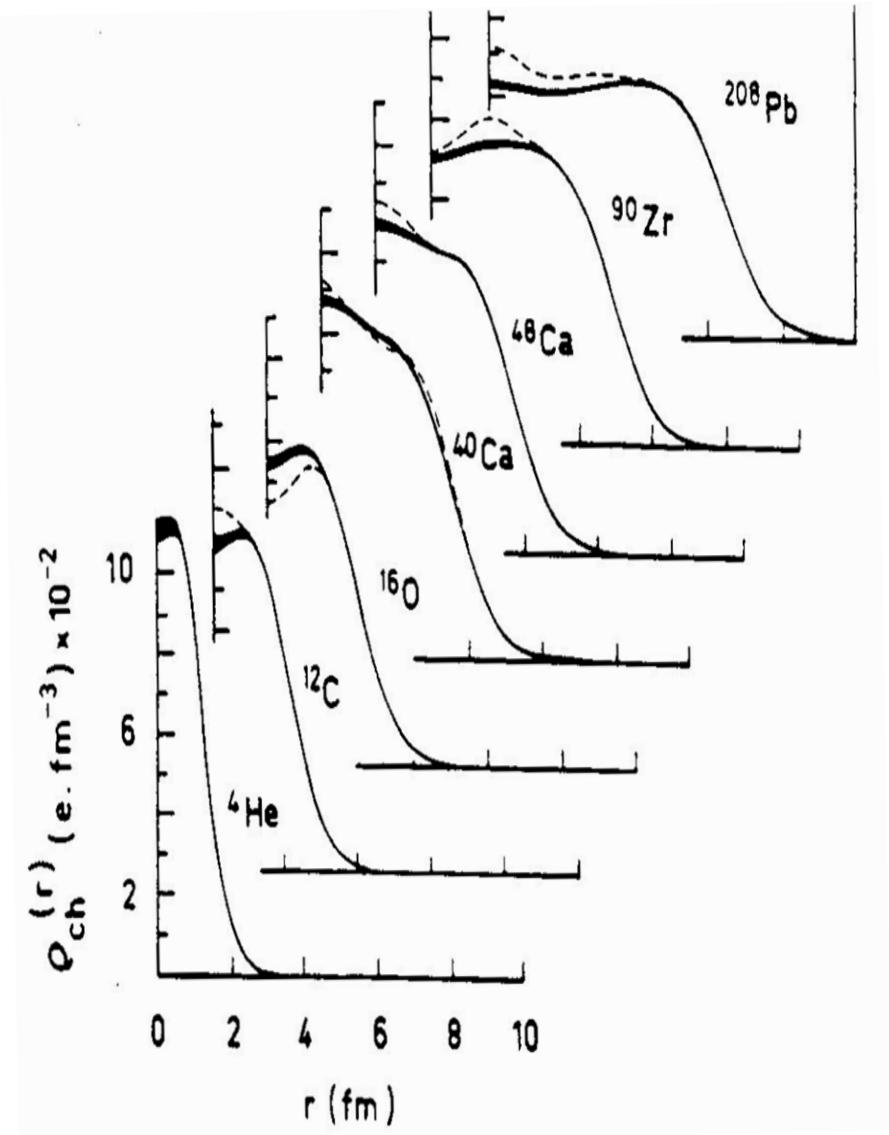
- Kohn-Sham procedure similar to nuclear "mean field" calculations



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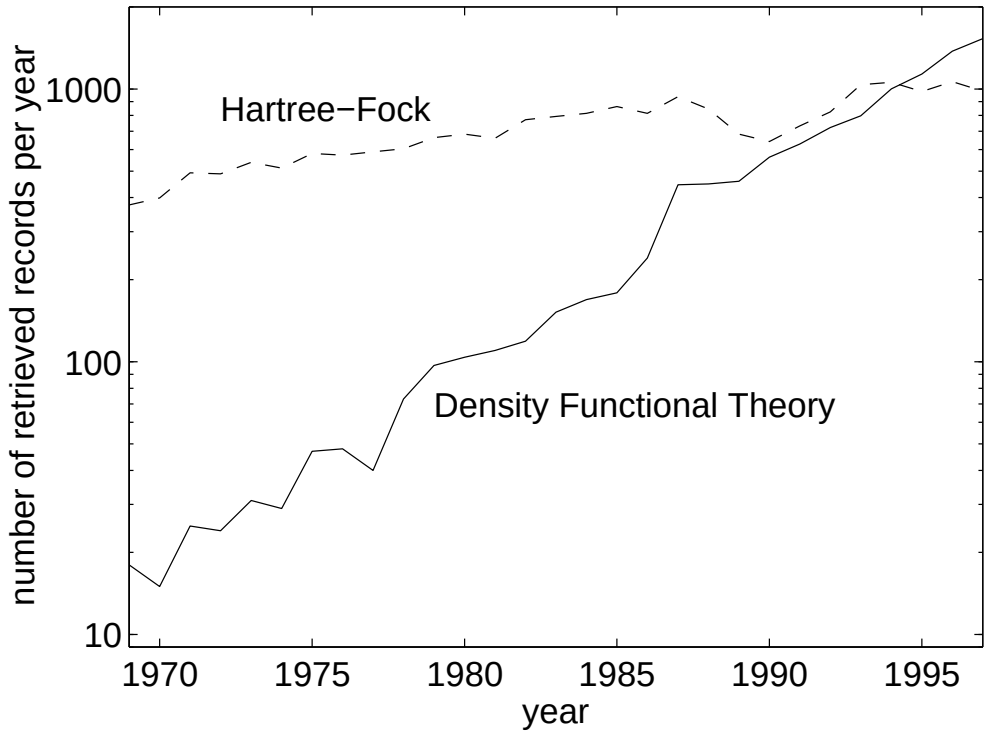
- Dominant application: inhomogeneous electron gas
- Interacting point electrons in static potential of atomic nuclei
- “Ab initio” calculations of atoms, molecules, crystals, surfaces



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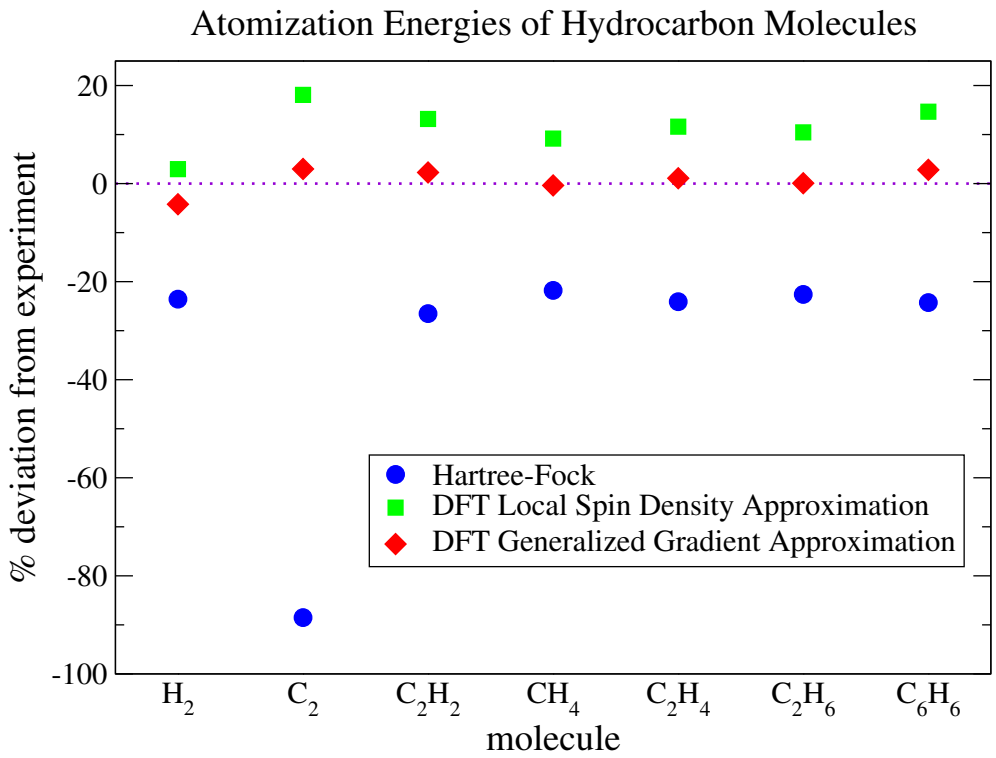

Quotes From the DFT Literature

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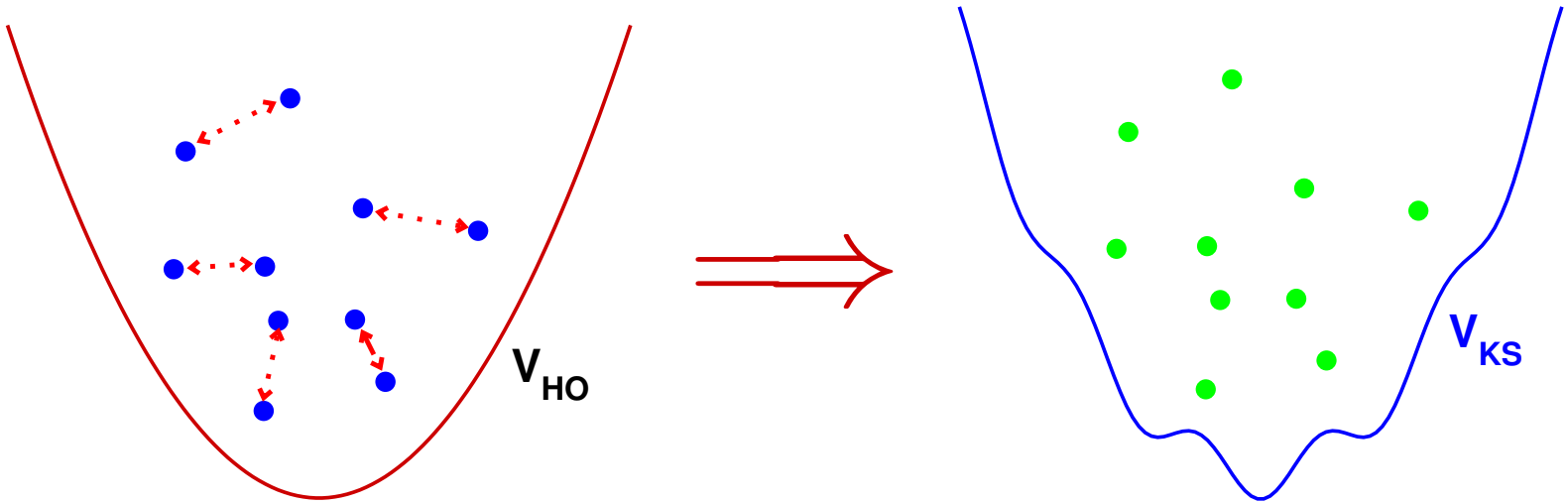
Meta-Generalized Gradient Approximation (Perdew et al., 1999)

"Some say that 'there is no systematic way to construct density functional approximations.' But there are more or less systematic ways, and the approach taken . . . here is one of the former."

Kohn-Sham DFT



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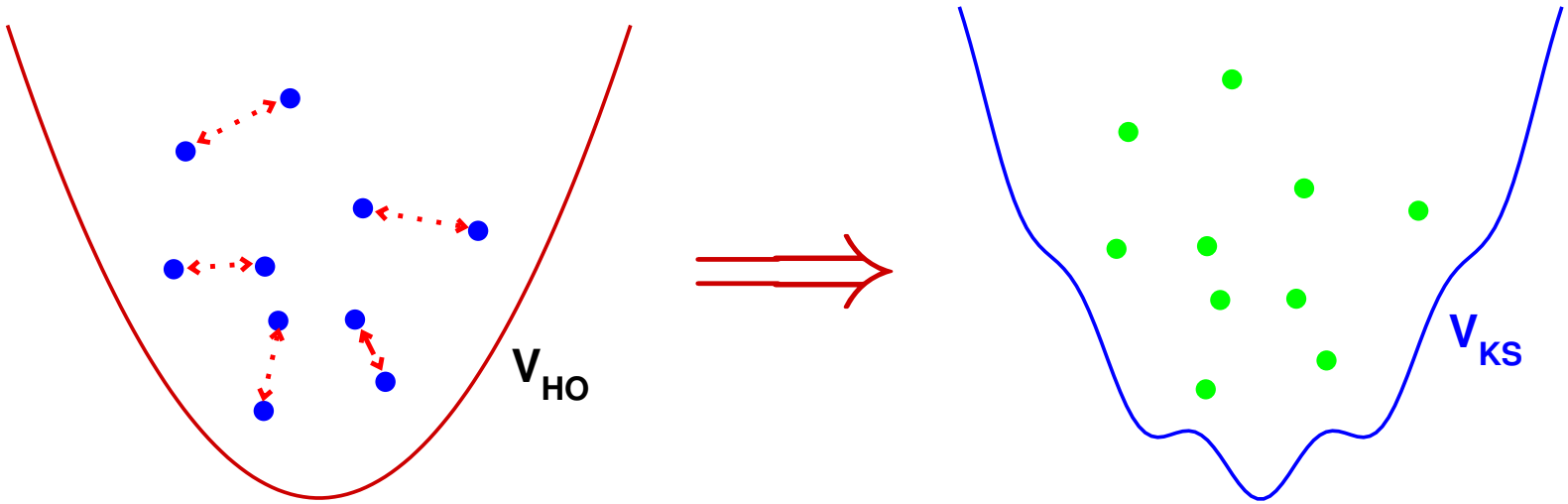


- Interacting density with $v_{\rm HO}$ $\equiv$ Non-interacting density with $v_{\rm KS}$
- Orbitals $\{\phi_i(\mathbf{x})\}$ in local potential $v_{\rm KS}([n],\mathbf{x})$ [but no $M^*(\mathbf{x})$]

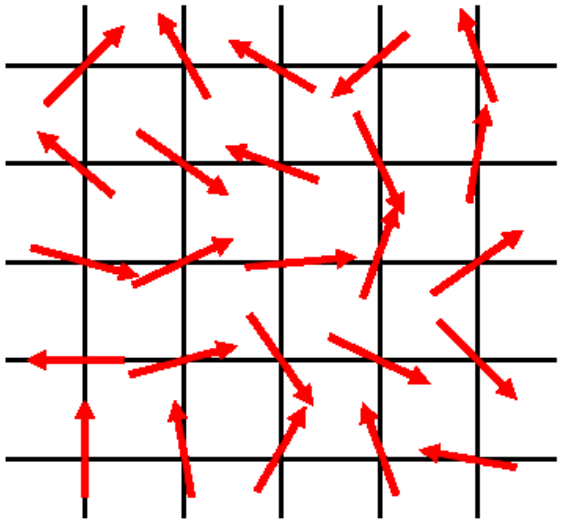
$$[-\nabla^2/2m + v_{\rm KS}(\mathbf{x})]\phi_i = \epsilon_i\phi_i \implies n(\mathbf{x}) = \sum_{i=1}^{N} |\phi_i(\mathbf{x})|^2$$

  - find Kohn-Sham potential $v_{\rm KS}(\mathbf{x})$ from $\delta E_v[n]/\delta n(\mathbf{x})$
  - Solve self-consistently

Thermodynamic Interpretation of DFT

- Consider a system of spins S_i on a lattice with interaction g
- The partition function has the information about the energy, magnetization of the system:

$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta g \sum_{\{i,j\}} S_i S_j}$$



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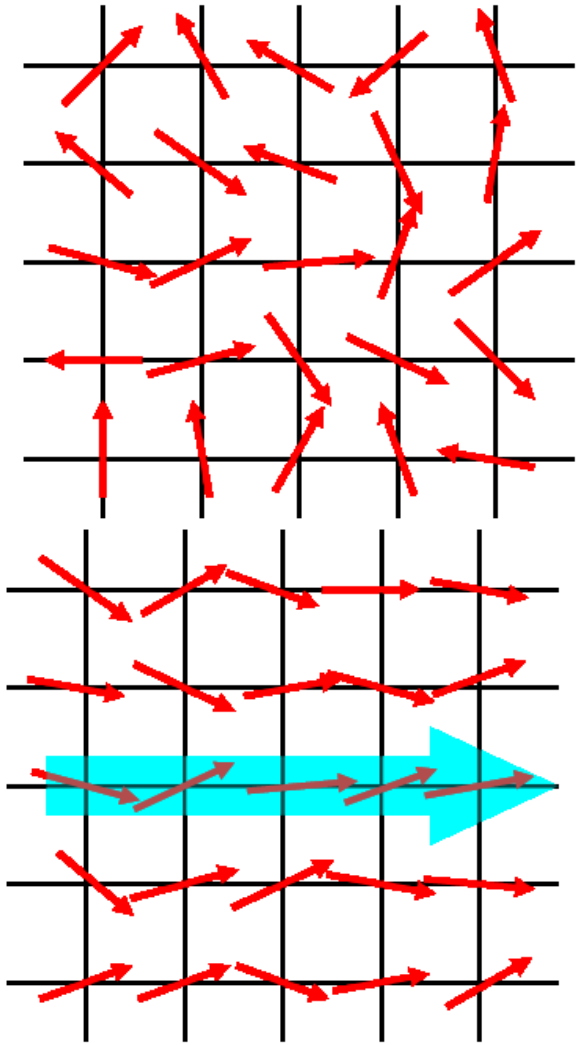
- The magnetization M is

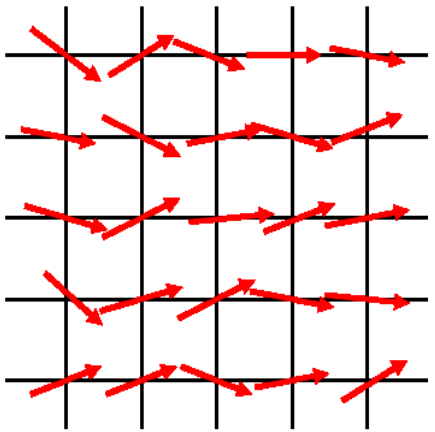
$$\begin{aligned} M &= \left\langle \sum_i S_i \right\rangle \\ &= \frac{1}{\mathcal{Z}} \mathrm{Tr} \left[\left(\sum_i S_i \right) e^{-\beta g \sum_{\{i,j\}} S_i S_j} \right] \end{aligned}$$



Add A Magnetic Probe Source H

- The source probes configurations near the ground state

$$\mathcal{Z}[H] = e^{-\beta F[H]} = \mathrm{Tr}\, e^{-\beta(g\sum_{\{i,j\}} S_i S_j - H\sum_i S_i)}$$



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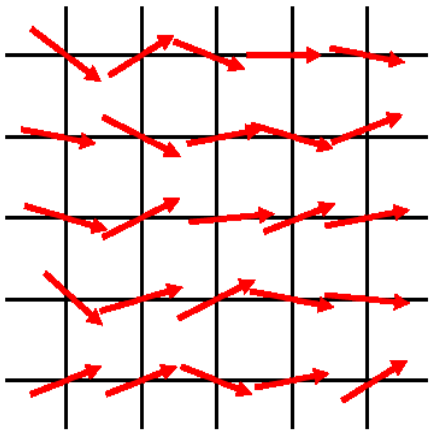
- Variations of the source yield the magnetization

$$M = \left\langle \sum_i S_i \right\rangle_H = -\frac{\partial F[H]}{\partial H}$$



Add A Magnetic Probe Source H

- The source probes configurations near the ground state

$$\mathcal{Z}[H] = e^{-\beta F[H]} = \mathrm{Tr}\, e^{-\beta(g\sum_{\{i,j\}} S_i S_j - H\sum_i S_i)}$$

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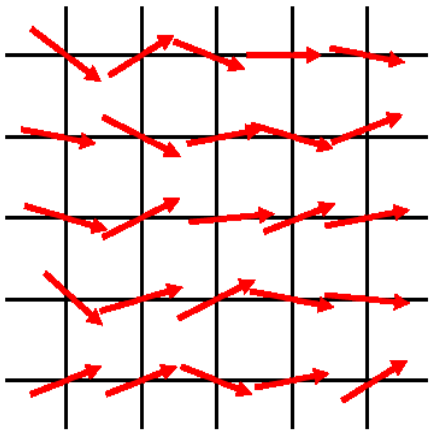

- $F[H]$ is the Helmholtz free energy. Set $H = 0$ (or equal to a real external source) at the end

Legendre Transformation to Effective Action

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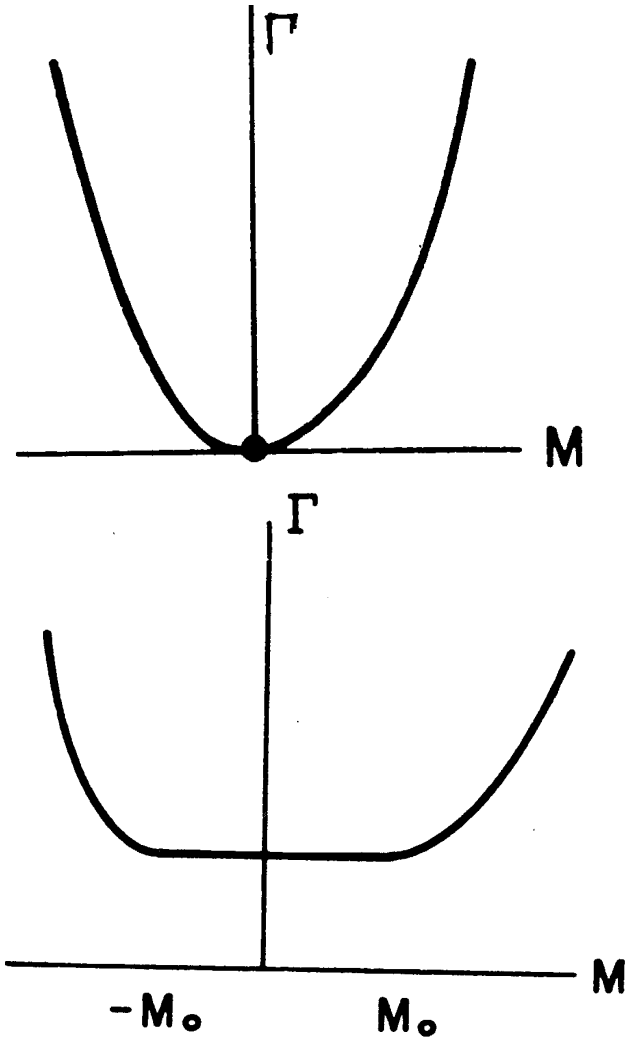

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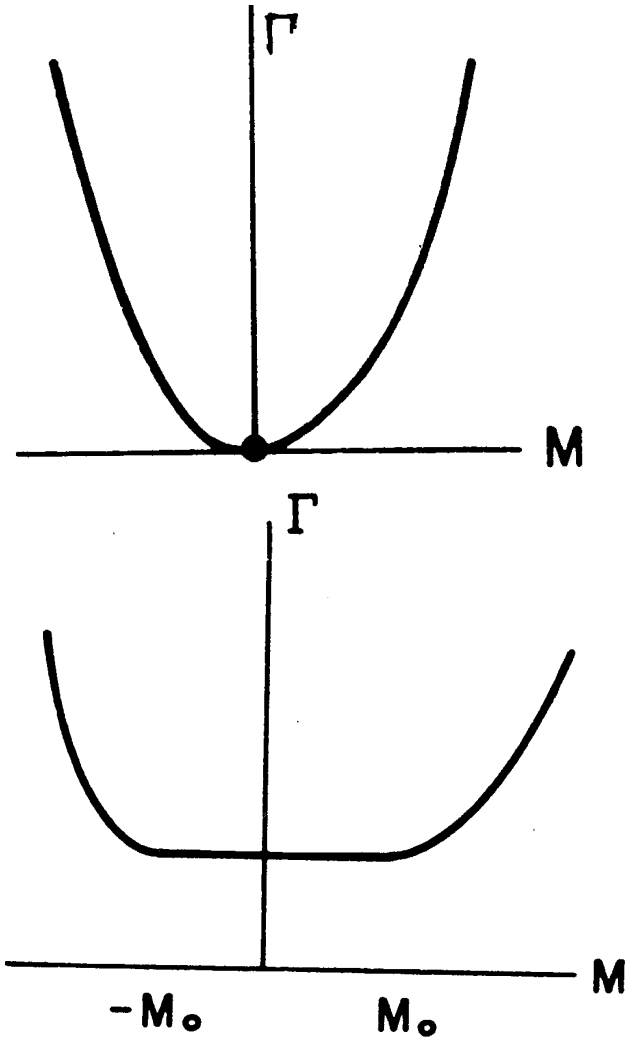
- The ground-state magnetization $M_{\rm gs}$ follows by minimizing $\Gamma[M]$:

$$H = \frac{\partial \Gamma[M]}{\partial M} \longrightarrow \left.\frac{\partial \Gamma[M]}{\partial M}\right|_{M_{\rm gs}} = 0$$



DFT as Analogous Legendre Transformation

- In analogy to the spin system, add source $J(x)$ coupled to density operator $\widehat{n}(x) \equiv \psi^\dagger(x)\psi(x)$ to the partition function:

$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H}+J\,\widehat{n})} \longrightarrow \int \mathcal{D}[\psi^\dagger]\mathcal{D}[\psi]\, e^{-\int [\mathcal{L}+J\,\psi^\dagger\psi]}$$

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- Invert to find $J[n]$ and Legendre transform from J to n:

$$\Gamma[n] = -W[J] + \int J\, n \quad \text{with} \quad J(x) = \frac{\delta \Gamma[n]}{\delta n(x)} \longrightarrow \left.\frac{\delta \Gamma[n]}{\delta n(x)}\right|_{n_{\mathrm{gs}}(\mathbf{x})} = 0$$

$\Longrightarrow$ For static $n(\mathbf{x})$, $\Gamma[n] \propto$ the DFT energy functional F_{HK}!

What can EFT do for DFT?

- Effective action as a path integral $\Longrightarrow$ construct $W[J]$, order-by-order in EFT expansion
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$$n(x) = \frac{\delta W_0[J_0]}{\delta J_0(x)} \quad \text{and} \quad J_0(x)|_{n=n_{\rm gs}} = \left.\frac{\delta \Gamma_{\rm interacting}[n]}{\delta n(x)}\right|_{n=n_{\rm gs}}$$

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- Interpretation: J_0 is the external potential that yields for a noninteracting system the exact density
  - This is the Kohn-Sham potential!
  - Two conditions on $J_0 \Longrightarrow$ Self-consistency

Kohn-Sham J_0 According to the EFT Expansion

- Simplifying with the local density approximation (LDA)

$$J_0(\mathbf{x}) = \left[$$

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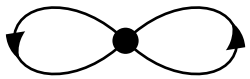
LO : 

$$J_0(\mathbf{x}) = \left[-\frac{(\nu-1)}{\nu}\frac{4\pi a_0}{M}\rho(\mathbf{x}) \right.$$

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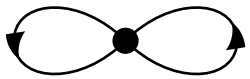

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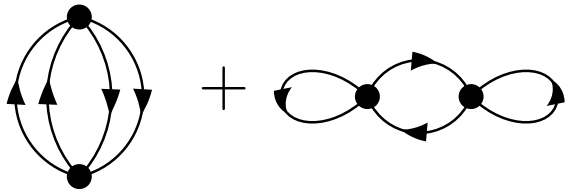

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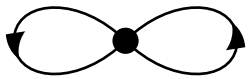

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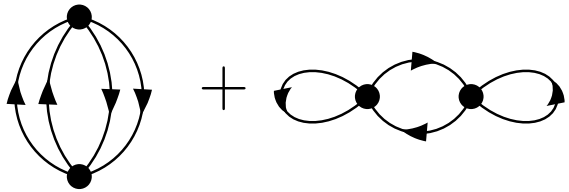

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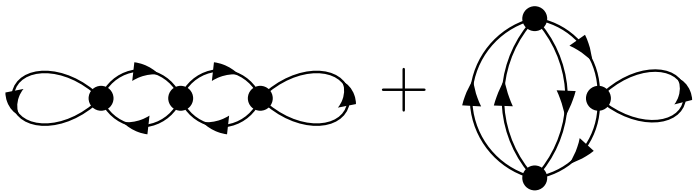

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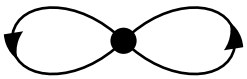

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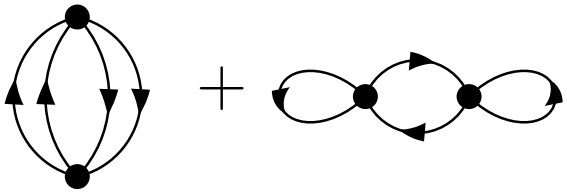

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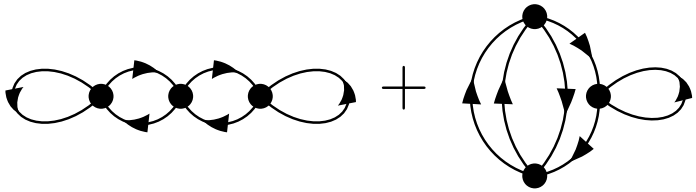

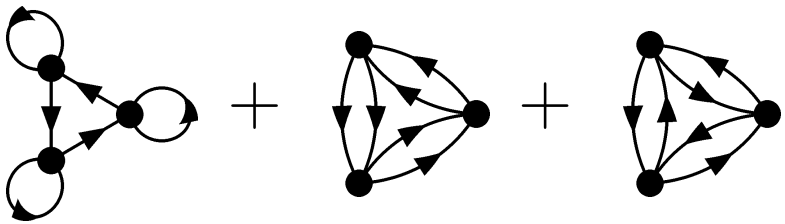

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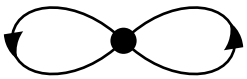

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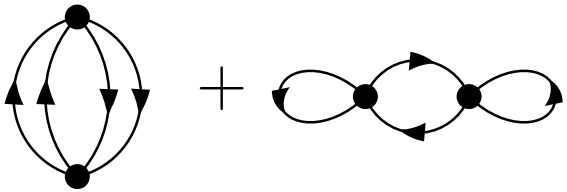

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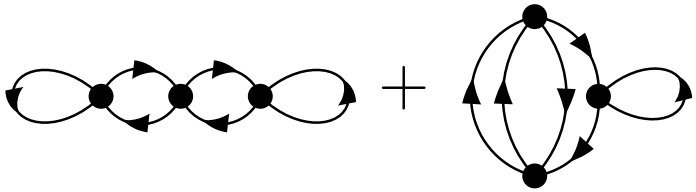

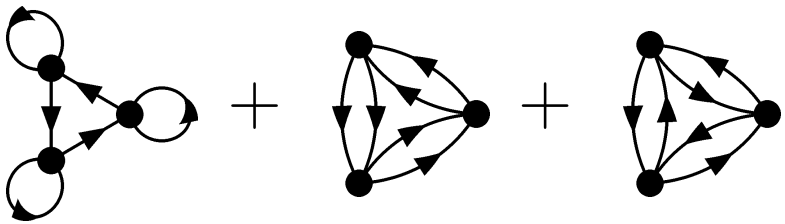

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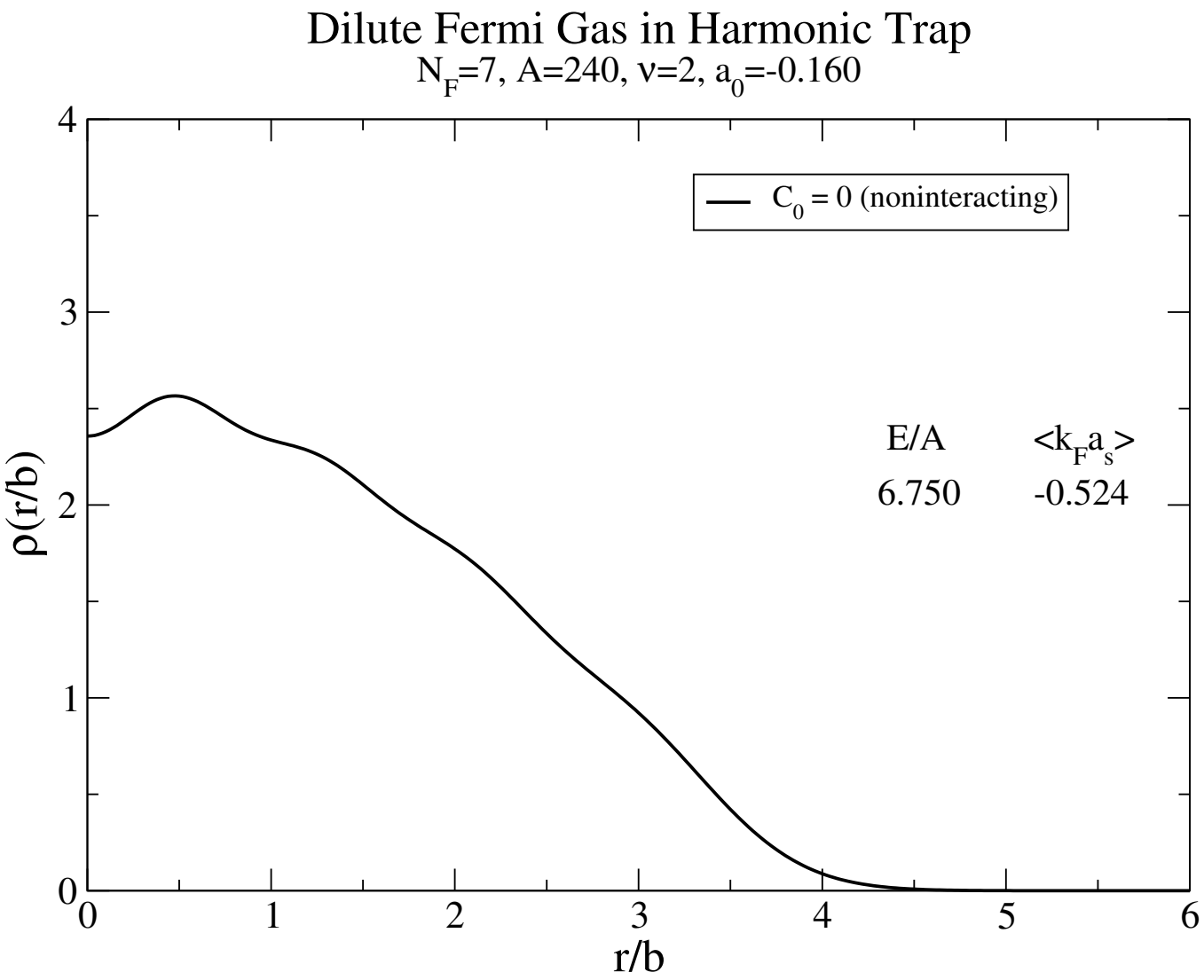
Looks like a Skyrme Hartree-Fock calculation!

Check Out An Example



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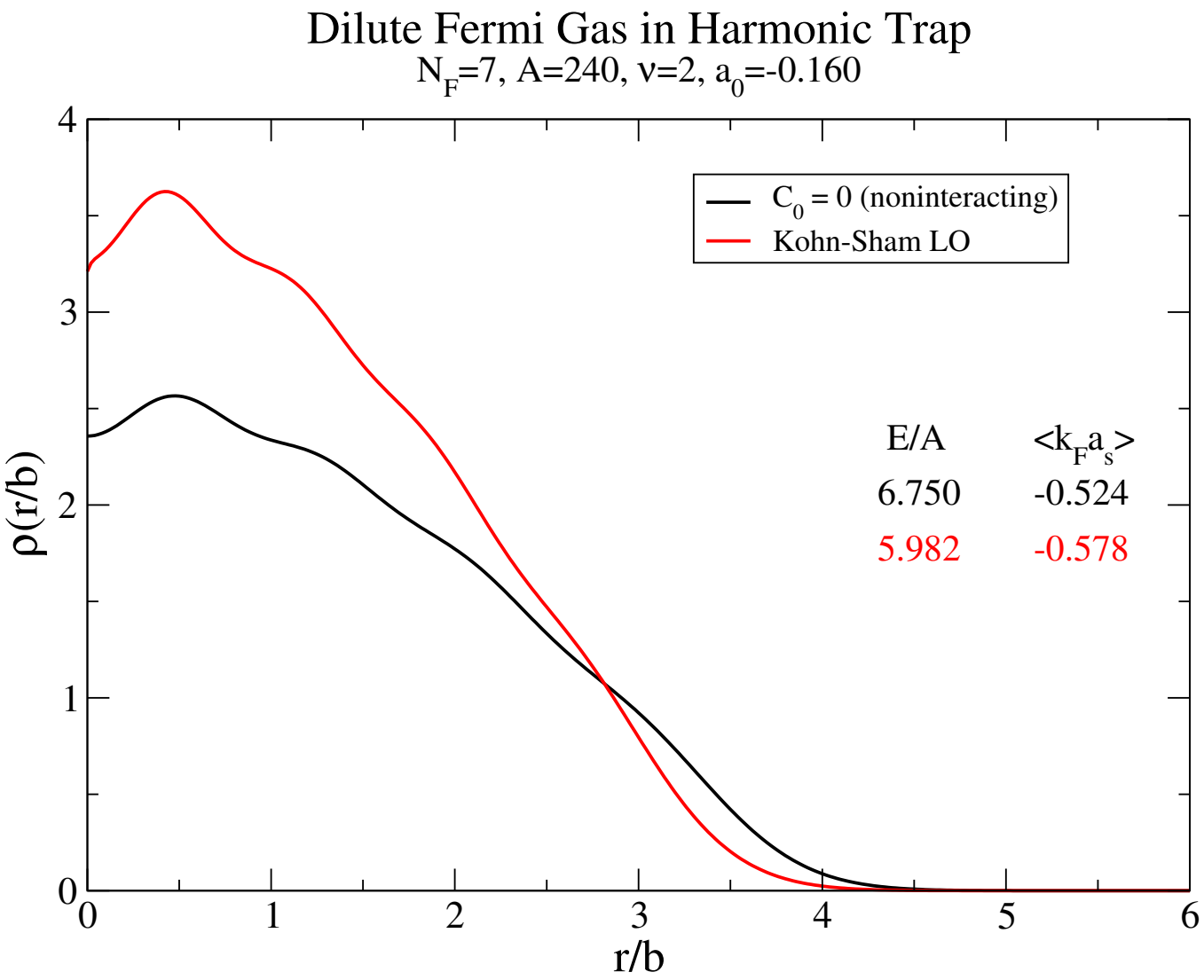

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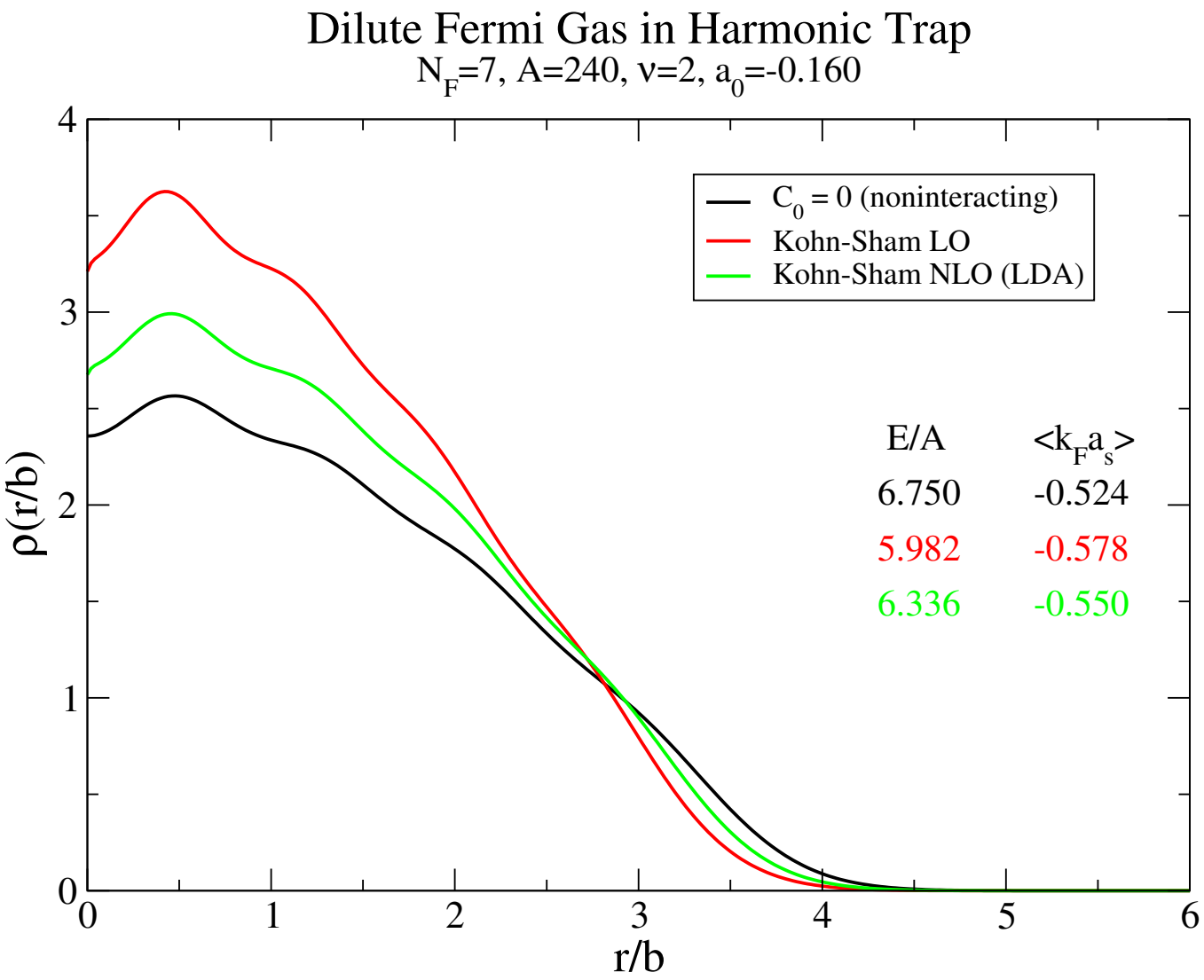

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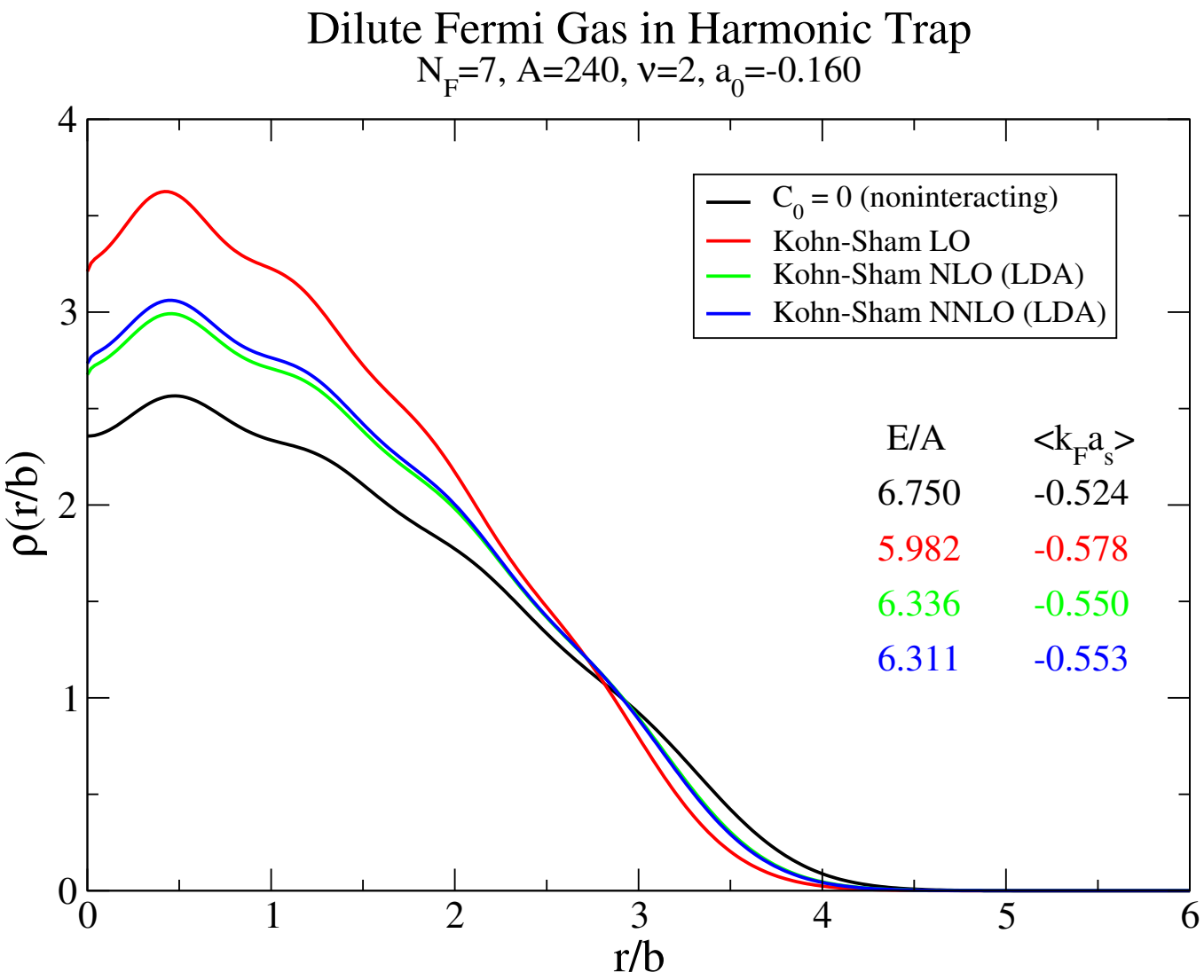
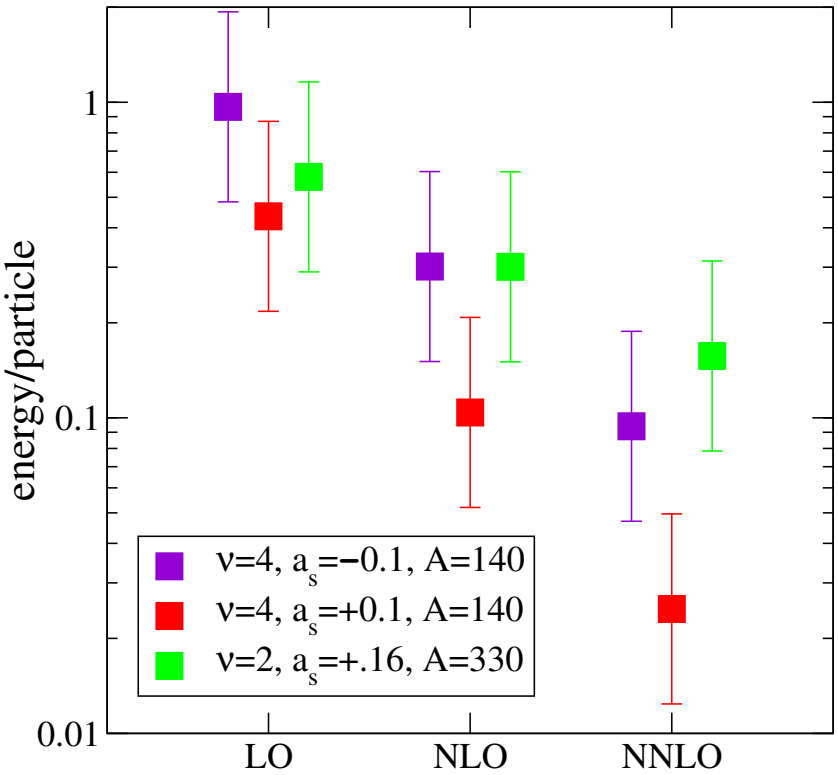


Power Counting Terms in Energy Functionals

- Scale contributions according to average density or $\langle k_F \rangle$



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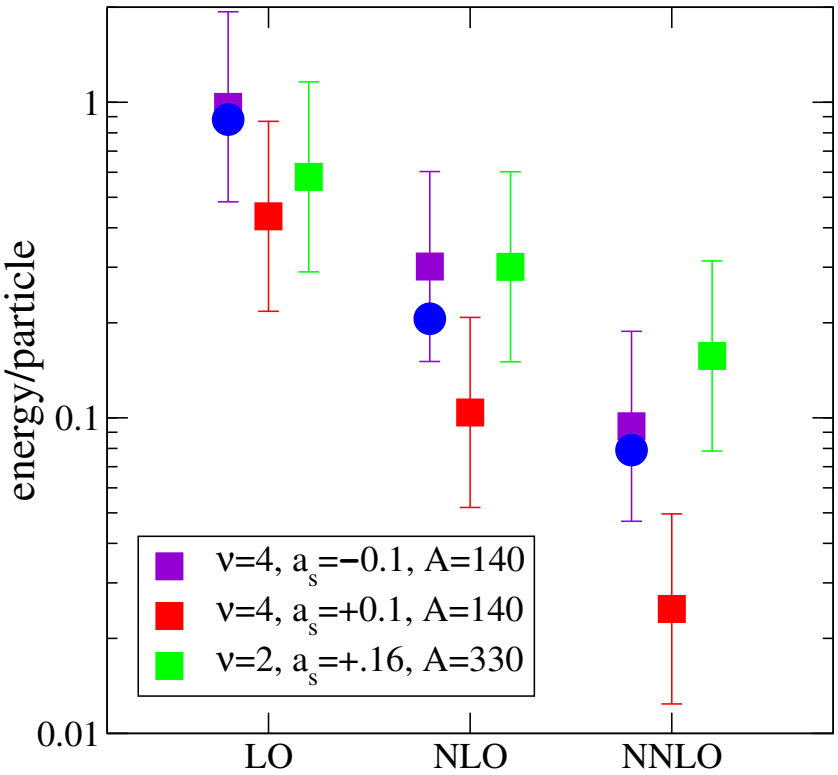

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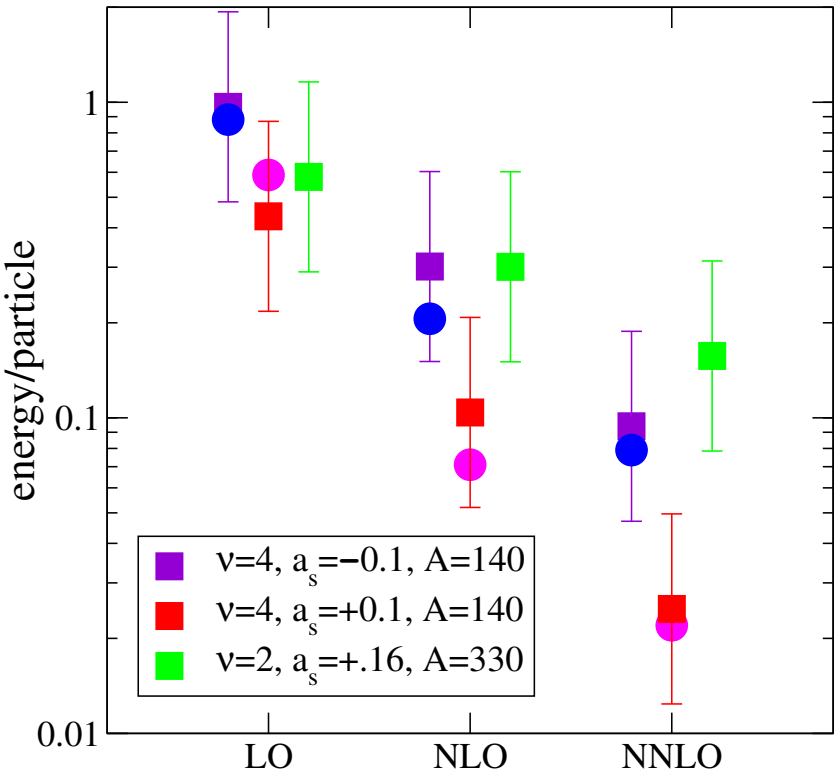

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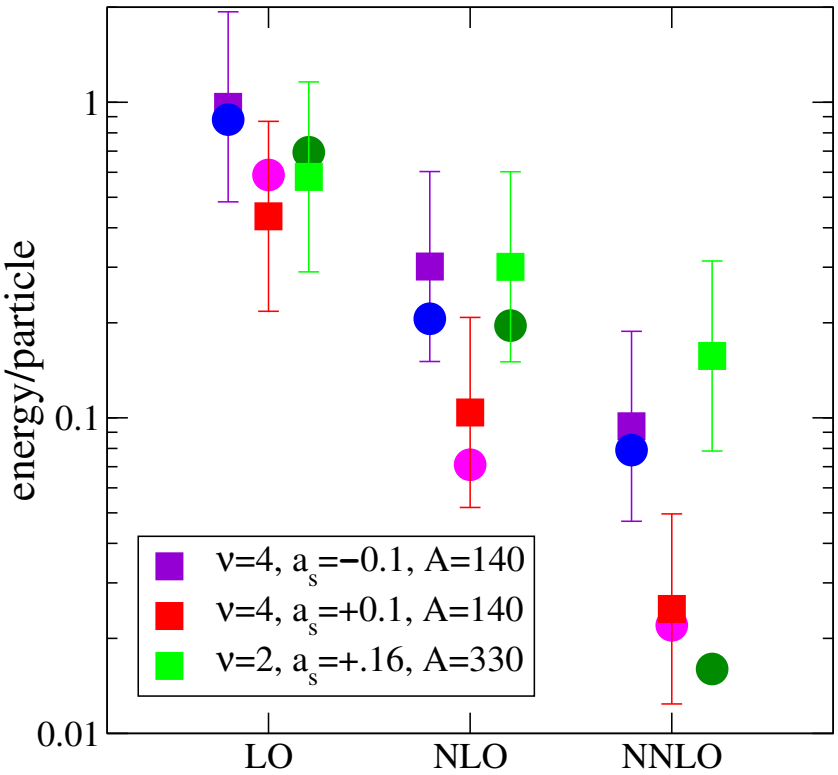

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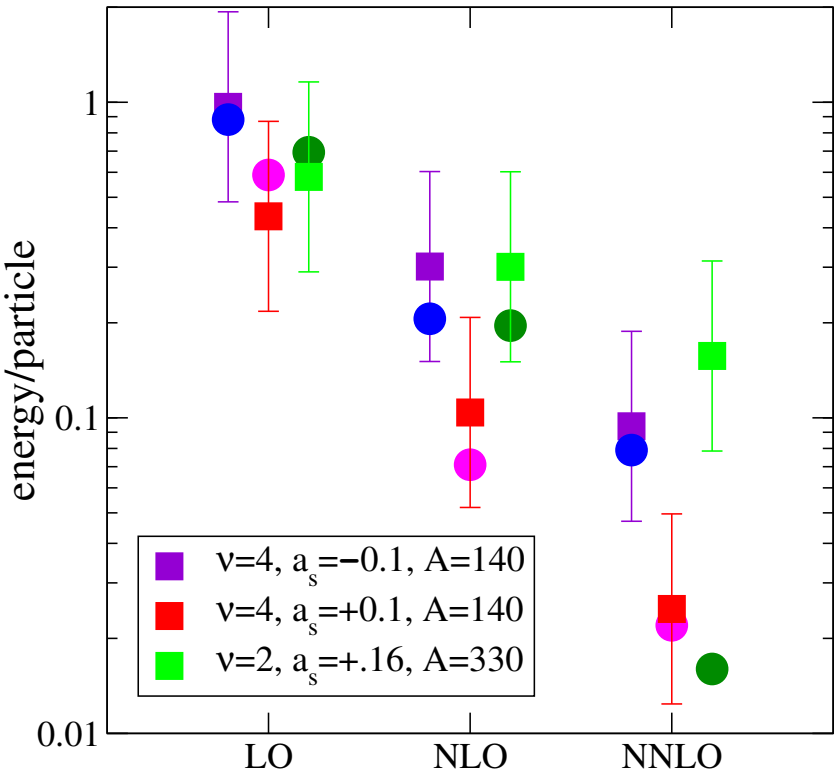
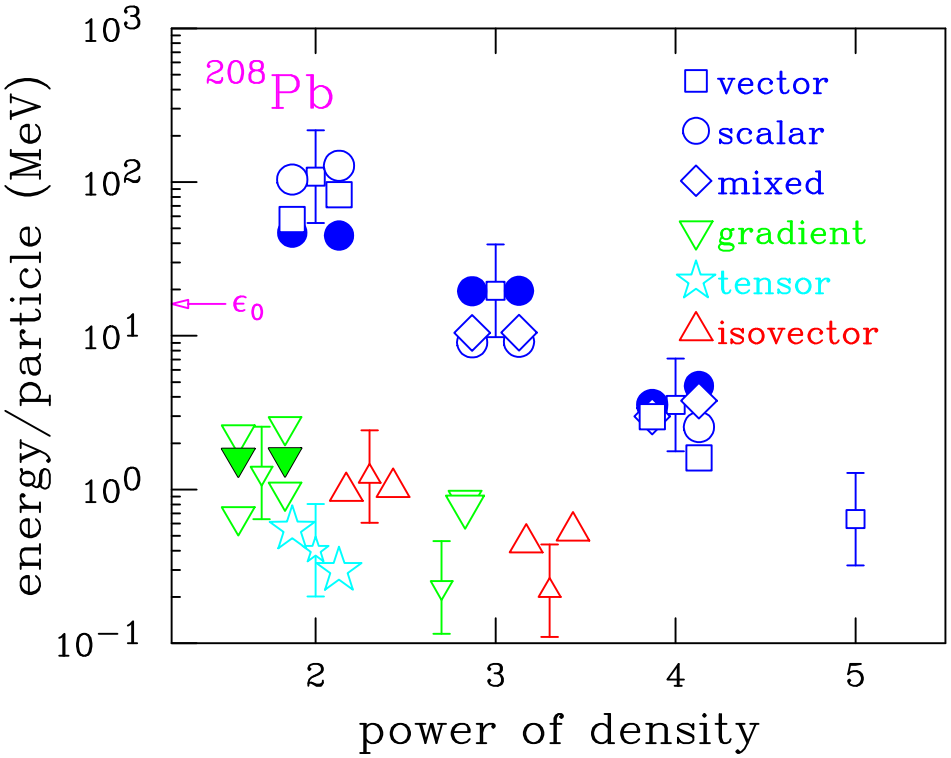


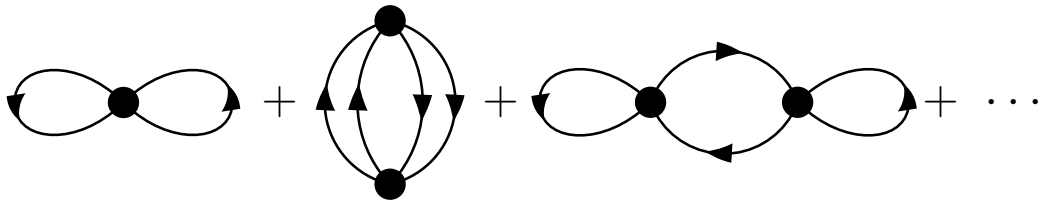


- Accurate estimates $\Longrightarrow$ truncation errors understood

Kohn-Luttinger-Ward Theorem (1960)

- $T \to 0$ diagrammatic expansion of $\Omega(\mu, V, T)$ in external $v(\mathbf{x})$
  $\Longrightarrow$ same as $F(N, V, T \equiv 0)$ with μ_0 and no anomalous diagrams

$$\Omega(\mu, V, T) = \Omega_0(\mu) \; +$$



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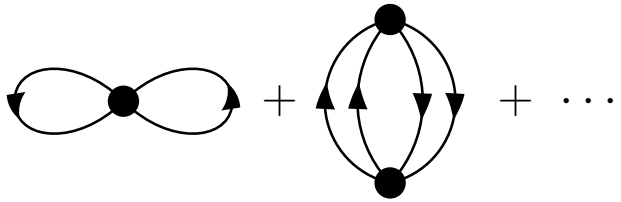
$$\xrightarrow{T \to 0} \quad F(N, V, T = 0) = E_0(N) \; +$$



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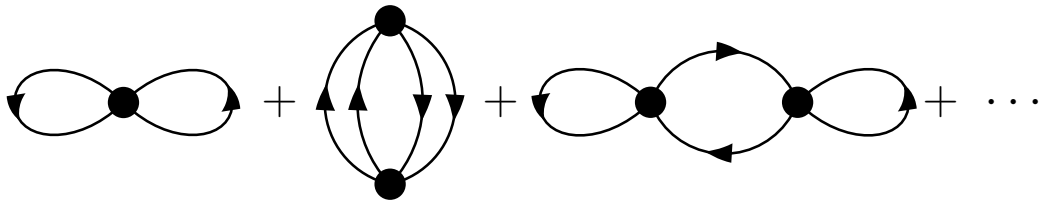

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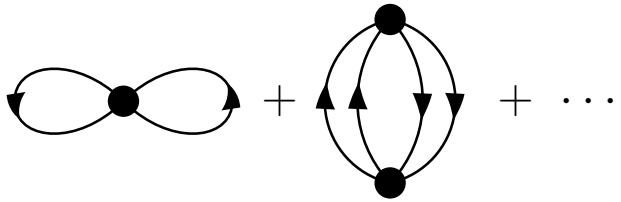

with $G_0(\mu_0)$

- Uniform Fermi system with no external potential (degeneracy ν):

$$\mu_0(N) = (6\pi^2 N/\nu V)^{2/3} \equiv k_{\rm F}^2/2M \equiv \epsilon_F^0$$

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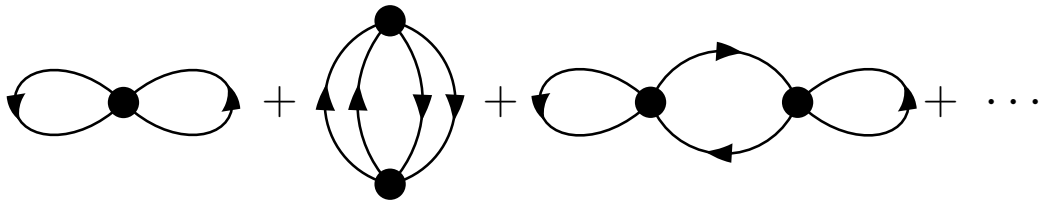
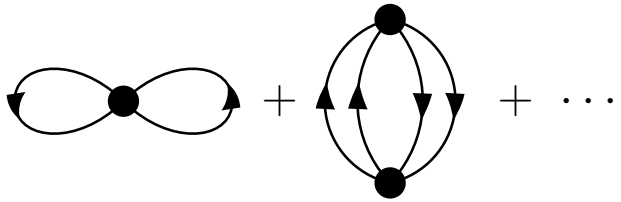
- $T \to 0$ diagrammatic expansion of $\Omega(\mu, V, T)$ in external $v(\mathbf{x})$
  $\Longrightarrow$ same as $F(N, V, T \equiv 0)$ with μ_0 and no anomalous diagrams

$$\Omega(\mu, V, T) = \Omega_0(\mu) \; +$$



with $\mathcal{G}_0(\mu, T)$

$$\xrightarrow{T\to 0} \quad F(N, V, T = 0) = E_0(N) \; +$$



with $G_0(\mu_0)$

- Uniform Fermi system with no external potential (degeneracy ν):

$$\mu_0(N) = (6\pi^2 N/\nu V)^{2/3} \equiv k_{\rm F}^2/2M \equiv \epsilon_F^0$$

- *If* symmetry of non-interacting and interacting systems agree

Kohn-Luttinger Inversion Method [F & W, sec. 30]

- Find $F(N) = \Omega(\mu) + \mu N$ with $\mu(N)$ from $N(\mu) = -(\partial\Omega/\partial\mu)_{TV}$

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$$\begin{aligned} \Omega(\mu) &= \Omega_0(\mu) + \Omega_1(\mu) + \Omega_2(\mu) + \cdots \\ \mu &= \mu_0 + \mu_1 + \mu_2 + \cdots \\ F(N) &= F_0(N) + F_1(N) + F_2(N) + \cdots \end{aligned}$$

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$$0 = [\partial\Omega_1/\partial\mu]_{\mu=\mu_0} + \mu_1[\partial^2\Omega_0/\partial\mu^2]_{\mu=\mu_0} \Longrightarrow \mu_1 = -\frac{[\partial\Omega_1/\partial\mu]_{\mu=\mu_0}}{[\partial^2\Omega_0/\partial\mu^2]_{\mu=\mu_0}}$$

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- Same pattern to all orders: μ_i is determined by functions of μ_0

- Apply this inversion to $F = \Omega + \mu N$:

$$F(N) = \underbrace{\Omega_0(\mu_0) + \mu_0 N}_{F_0} + \underbrace{\Omega_1(\mu_0) + \mu_1 N + \mu_1 \left[\frac{\partial \Omega_0}{\partial \mu}\right]_{\mu=\mu_0}}_{F_1}$$

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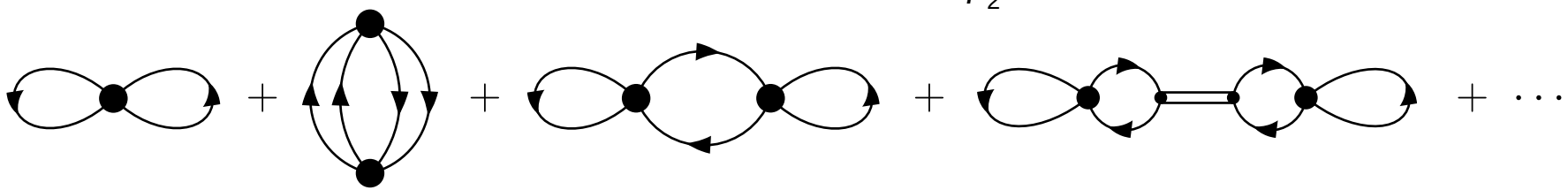
- μ_i always cancels from F_i for $i \geq 1$:

$$F(N) = F_0(N) + \underbrace{\Omega_1(\mu_0)}_{F_1} + \underbrace{\Omega_2(\mu_0) - \frac{1}{2}\frac{[\partial \Omega_1/\partial \mu]^2_{\mu=\mu_0}}{[\partial^2 \Omega_0/\partial \mu^2]_{\mu=\mu_0}} + \cdots}_{F_2}$$



F_1 F_2

Generalizing the KLW Inversion Approach

- Three generalizations $\Longrightarrow$ Kohn-Sham DFT, other sources, and pairing
  1. $\mu N + J(\mathbf{x})\rho(\mathbf{x})$ with $J(\mathbf{x}) = \delta F[\rho]/\delta\rho(\mathbf{x}) \rightarrow 0$ in ground state

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$$+ J_\tau(\mathbf{x})\tau(\mathbf{x}) \quad \text{where} \quad \tau(x) \equiv \langle \nabla\psi^\dagger \cdot \nabla\psi \rangle$$

$$\Longrightarrow M^*(\mathbf{x}) \text{ in the Kohn-Sham equation (cf. Skyrme)}$$

$$\left[-\frac{\nabla^2}{2M} + v_{\rm KS}(\mathbf{x})\right]\psi_\alpha = \epsilon_\alpha\psi_\alpha \implies \left[-\nabla\frac{1}{M^*(\mathbf{x})}\nabla + v_{\rm KS}(\mathbf{x})\right]\psi_\alpha = \epsilon_\alpha\psi_\alpha$$

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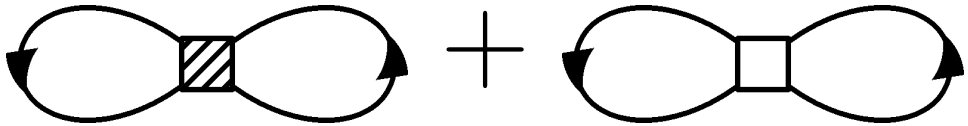
- Same inversion method, but use $[j]_{\rm gs} = j_0 + j_1 + j_2 + \cdots = 0$
  $\Longrightarrow$ solve for j_0 iteratively: from $[j_0]_{\rm old}$ find $[j_0]_{\rm new} = -j_1 - j_2 + \cdots$

Warm-Up Problem: Hartree-Fock Diagrams Only

- Consider bowtie diagram from vertices with derivatives:

$$\mathcal{L}_{\rm eft} = \ldots + \frac{C_2}{16}\left[(\psi\psi)^\dagger(\psi \overleftrightarrow{\nabla}^2 \psi) + \text{ h.c.}\right] + \frac{C_2'}{8}(\psi \overleftrightarrow{\nabla} \psi)^\dagger \cdot (\psi \overleftrightarrow{\nabla} \psi) + \ldots$$



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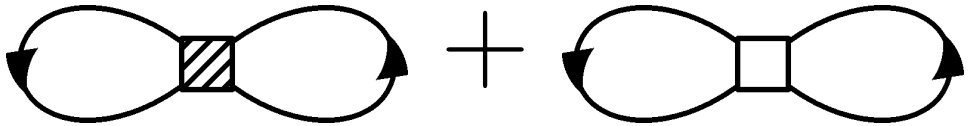

- Energy density in Kohn-Sham LDA ($\nu = 2$):

$$\mathcal{E}_{\rm int} = \ldots + \frac{C_2}{8}\left[\frac{3}{5}\left(\frac{6\pi^2}{\nu}\right)^{2/3}\rho^{8/3}\right] + \frac{3C_2'}{8}\left[\frac{3}{5}\left(\frac{6\pi^2}{\nu}\right)^{2/3}\rho^{8/3}\right] + \ldots$$

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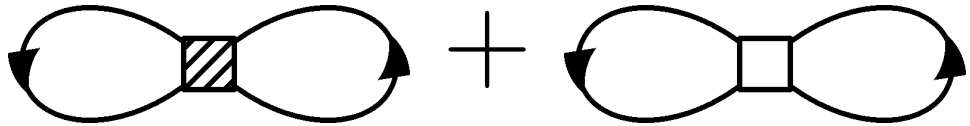

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- Energy density in Kohn-Sham with τ ($\nu = 2$):

$$\mathcal{E}_{\rm int} = \ldots + \frac{C_2}{8}\left[\rho\tau + \frac{3}{4}(\nabla\rho)^2\right] + \frac{3C_2'}{8}\left[\rho\tau - \frac{1}{4}(\nabla\rho)^2\right] + \ldots$$

Pairing in DFT/EFT from Effective Action

- Natural framework for spontaneous symmetry breaking
  - e.g., test for zero-field magnetization M in a spin system
  - introduce an external field H to break rotational symmetry
  - Legendre transform Helmholtz free energy $F(H)$:

$$\text{invert } M = -\partial F(H)/\partial H \quad \Longrightarrow \quad G[M] = F[H(M)] + MH(M)$$

  - since $H = \partial G/\partial M$, minimize G to find ground state

Pairing in DFT/EFT from Effective Action

- With pairing, the broken symmetry is a $U(1)$ [phase] symmetry
  - standard treatment in condensed matter uses auxiliary pairing field $\Delta(x)$
  - to leading order in the loop expansion (mean field) $\Longrightarrow$ BCS approximation
- Here: Combine the EFT expansion and the inversion method
  - external current j coupled to pair density breaks symmetry
  - natural generalization of Kohn-Sham DFT

Generalizing Effective Action to Include Pairing

- Generating functional with sources J, j coupled to densities:

$$Z[J,j] = e^{-W[J,j]} = \int D(\psi^\dagger \psi)\, e^{-\int d^4x\, [\mathcal{L} + J(x)\psi^\dagger_\alpha \psi_\alpha + j(x)(\psi^\dagger_\uparrow \psi^\dagger_\downarrow + \psi_\downarrow \psi_\uparrow)]}$$

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$$\rho(x) \equiv \langle \psi^\dagger(x)\psi(x)\rangle_{J,j} = \left.\frac{\delta W[J,j]}{\delta J(x)}\right|_j$$

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- Effective action $\Gamma[\rho,\phi]$ by functional Legendre transformation:

$$\Gamma[\rho,\phi] = W[J,j] - \int d^4x\, J(x)\rho(x) - \int d^4x\, j(x)\phi(x)$$

- $\Gamma[\rho, \phi] \propto$ ground-state energy functional $E[\rho, \phi]$
  - at finite temperature, the proportionality constant is β

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$$\frac{\delta E[\rho,\phi]}{\delta\rho(\mathbf{x})} = J(\mathbf{x}) \qquad \text{and} \qquad \frac{\delta E[\rho,\phi]}{\delta\phi(\mathbf{x})} = j(\mathbf{x})$$

  - but the sources are zero in the ground state
  - $\Longrightarrow$ determine ground-state $\rho(\mathbf{x})$ and $\phi(\mathbf{x})$ by stationarity:

$$\left.\frac{\delta E[\rho,\phi]}{\delta\rho(\mathbf{x})}\right|_{\rho=\rho_{\rm gs},\phi=\phi_{\rm gs}} = \left.\frac{\delta E[\rho,\phi]}{\delta\phi(\mathbf{x})}\right|_{\rho=\rho_{\rm gs},\phi=\phi_{\rm gs}} = 0$$

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- This is Hohenberg-Kohn DFT extended to pairing!
- So far this is purely formal
  - we need a method to carry out the inversion
  - we will need to renormalize

Kohn-Sham Inversion Method Revisited

- Order-by-order matching in EFT expansion parameter λ

$$\begin{aligned} J[\rho,\phi,\lambda] &= J_0[\rho,\phi] + J_1[\rho,\phi] + J_2[\rho,\phi] + \cdots \\ j[\rho,\phi,\lambda] &= j_0[\rho,\phi] + j_1[\rho,\phi] + j_2[\rho,\phi] + \cdots \\ \widetilde{W}[J,j,\lambda] &= \widetilde{W}_0[J,j] + \widetilde{W}_1[J,j] + \widetilde{W}_2[J,j] + \cdots \\ \widetilde{\Gamma}[\rho,\phi,\lambda] &= \widetilde{\Gamma}_0[\rho,\phi] + \widetilde{\Gamma}_1[\rho,\phi] + \widetilde{\Gamma}_2[\rho,\phi] + \cdots \end{aligned}$$

- 0^{th} order is Kohn-Sham system with potentials $J_0(\mathbf{x})$ and $j_0(\mathbf{x})$
  $\Longrightarrow$ yields the exact densities $\rho(\mathbf{x})$ and $\phi(\mathbf{x})$
  - introduce single-particle orbitals and solve

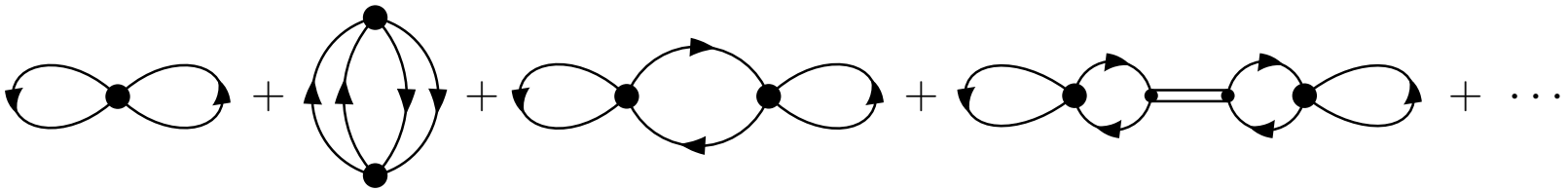
$$\begin{pmatrix} h_0(\mathbf{x}) - \mu_0 & j_0(\mathbf{x}) \\ j_0(\mathbf{x}) & -h_0(\mathbf{x}) + \mu_0 \end{pmatrix} \begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix} = E_i \begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix}$$

$$\text{where} \qquad h_0(\mathbf{x}) \equiv -\frac{\nabla^2}{2M} + v(\mathbf{x}) - J_0(\mathbf{x})$$

with conventional orthonormality relations for u_i, v_i

Diagrammatic Expansion of W_i

- Same diagrams, but with Nambu-Gor'kov Green's functions

$\Gamma_{\text{int}} =$  $+ \cdots$

$$i\mathbf{G} = \begin{pmatrix} \langle T\psi_\uparrow(x)\psi_\uparrow^\dagger(x')\rangle_0 & \langle T\psi_\uparrow(x)\psi_\downarrow(x')\rangle_0 \\ \langle T\psi_\downarrow^\dagger(x)\psi_\uparrow^\dagger(x')\rangle_0 & \langle T\psi_\downarrow^\dagger(x)\psi_\downarrow(x')\rangle_0 \end{pmatrix} \equiv \begin{pmatrix} iG^0_{\text{ks}} & iF^0_{\text{ks}} \\ iF^{0\,\dagger}_{\text{ks}} & -iG^0_{\text{ks}} \end{pmatrix}$$

- In frequency space, the Green's functions are

$$iG^0_{\text{ks}}(\mathbf{x},\mathbf{x}';\omega) = \sum_i \left[\frac{u_i(\mathbf{x})\,u_i^*(\mathbf{x}')}{\omega - E_i + i\eta} + \frac{v_i(\mathbf{x}')\,v_i^*(\mathbf{x})}{\omega + E_i - i\eta}\right]$$

$$iF^0_{\text{ks}}(\mathbf{x},\mathbf{x}';\omega) = -\sum_i \left[\frac{u_i(\mathbf{x})\,v_i^*(\mathbf{x}')}{\omega - E_i + i\eta} - \frac{u_i(\mathbf{x}')\,v_i^*(\mathbf{x})}{\omega + E_i - i\eta}\right]$$

Kohn-Sham Self-Consistency Procedure

- Same iteration procedure as in Skyrme or RMF with pairing
- In terms of the orbitals, the fermion density is

$$\rho(\mathbf{x}) = 2\sum_i |v_i(\mathbf{x})|^2$$

and the pair density is

$$\phi(\mathbf{x}) = \sum_i [u_i^*(\mathbf{x})v_i(\mathbf{x}) + u_i(\mathbf{x})v_i^*(\mathbf{x})]$$

- The chemical potential μ_0 is fixed by $\int \rho(\mathbf{x}) = A$
- Diagrams for $\widetilde{\Gamma}[\rho,\phi] = -E[\rho,\phi]$ (with LDA+) yields KS potentials

$$J_0(\mathbf{x})\Big|_{\rho=\rho_{\rm gs}} = \left.\frac{\delta\widetilde{\Gamma}_{\rm int}[\rho,\phi]}{\delta\rho(\mathbf{x})}\right|_{\rho=\rho_{\rm gs}} \quad \text{and} \quad j_0(\mathbf{x})\Big|_{\phi=\phi_{\rm gs}} = \left.\frac{\delta\widetilde{\Gamma}_{\rm int}[\rho,\phi]}{\delta\phi(\mathbf{x})}\right|_{\phi=\phi_{\rm gs}}$$

Renormalization

- Even at leading order, divergences from $\langle \psi_\uparrow^\dagger \psi_\downarrow^\dagger + \psi_\downarrow \psi_\uparrow \rangle$
  - cf. renormalization of relativistic scalar density $\rho_s = \langle \overline{\psi} \psi \rangle$
- Gap equation from self-consistency of j_0 has linear divergence

$$j_0 = -j_1 = -\frac{1}{2} C_0 \phi \overset{\text{uniform}}{=} -\frac{1}{2} C_0 \int \frac{d^3k}{(2\pi)^3} \frac{j_0}{\sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}}$$

  - Standard plan: renormalize as with scattering amplitude
  - Papenbrock & Bertsch $\Longrightarrow$ dim. reg. with minimal subtraction
  - In fact, much trickier . . . stay tuned!
- In finite system, use derivative expansion technology
  - developed for one-loop relativistic vacuum calculations
  - cf. Bulgac et al., cutoff regularization and renormalization

Summary: Many-Body Effective Field Theory

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- Some of the challenges . . .
  - Connect to chiral EFT (see N. Kaiser and W. Weise)
  - Consistent treatment of pairing in higher orders (renormalization)
  - Systematic gradient expansions for DFT
  - Additional expansions for large scattering lengths
  - Relativistic DFT/EFT (nuclear and atomic)
  - Ab initio QCD calculations of nuclei?

Ab Initio QCD Calculations of Nuclei?

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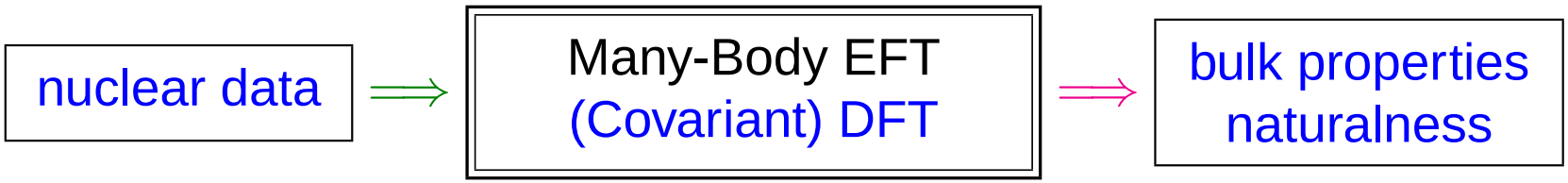

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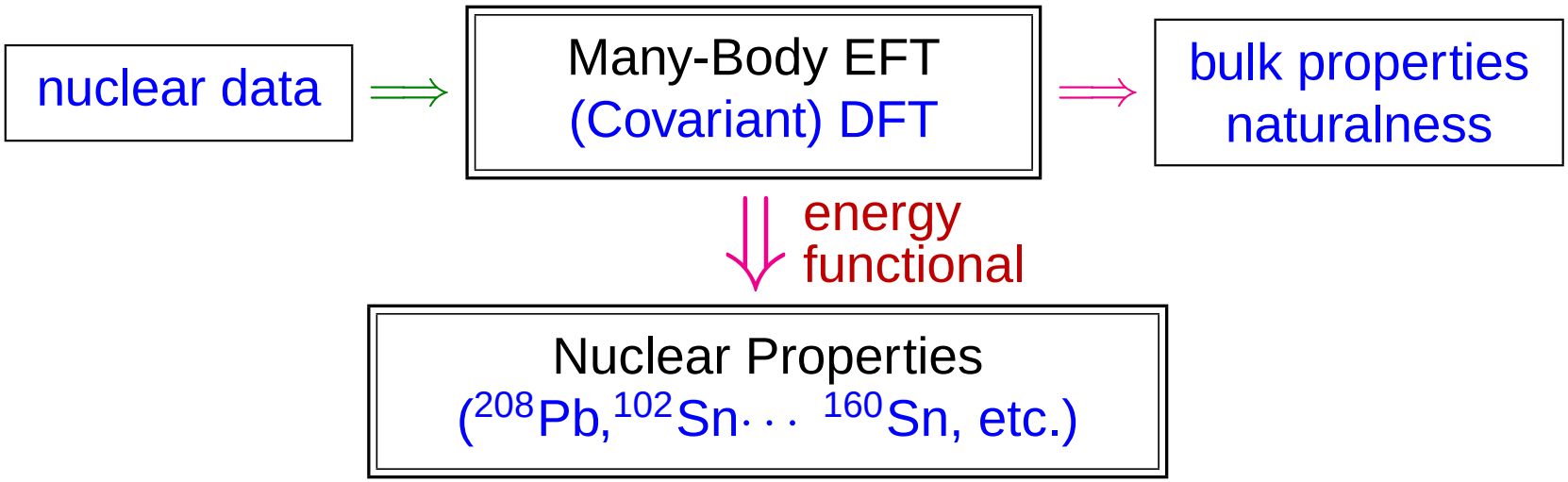

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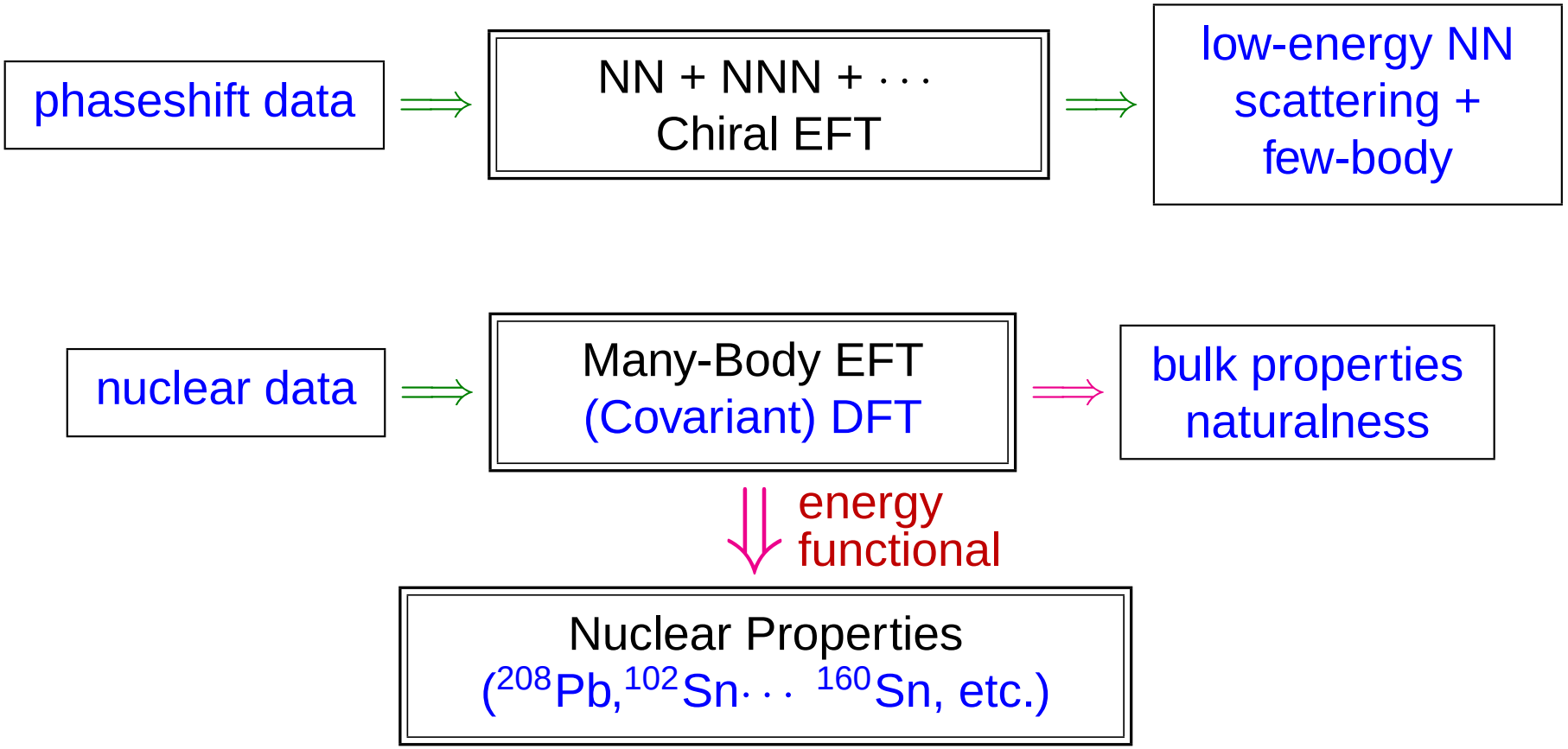

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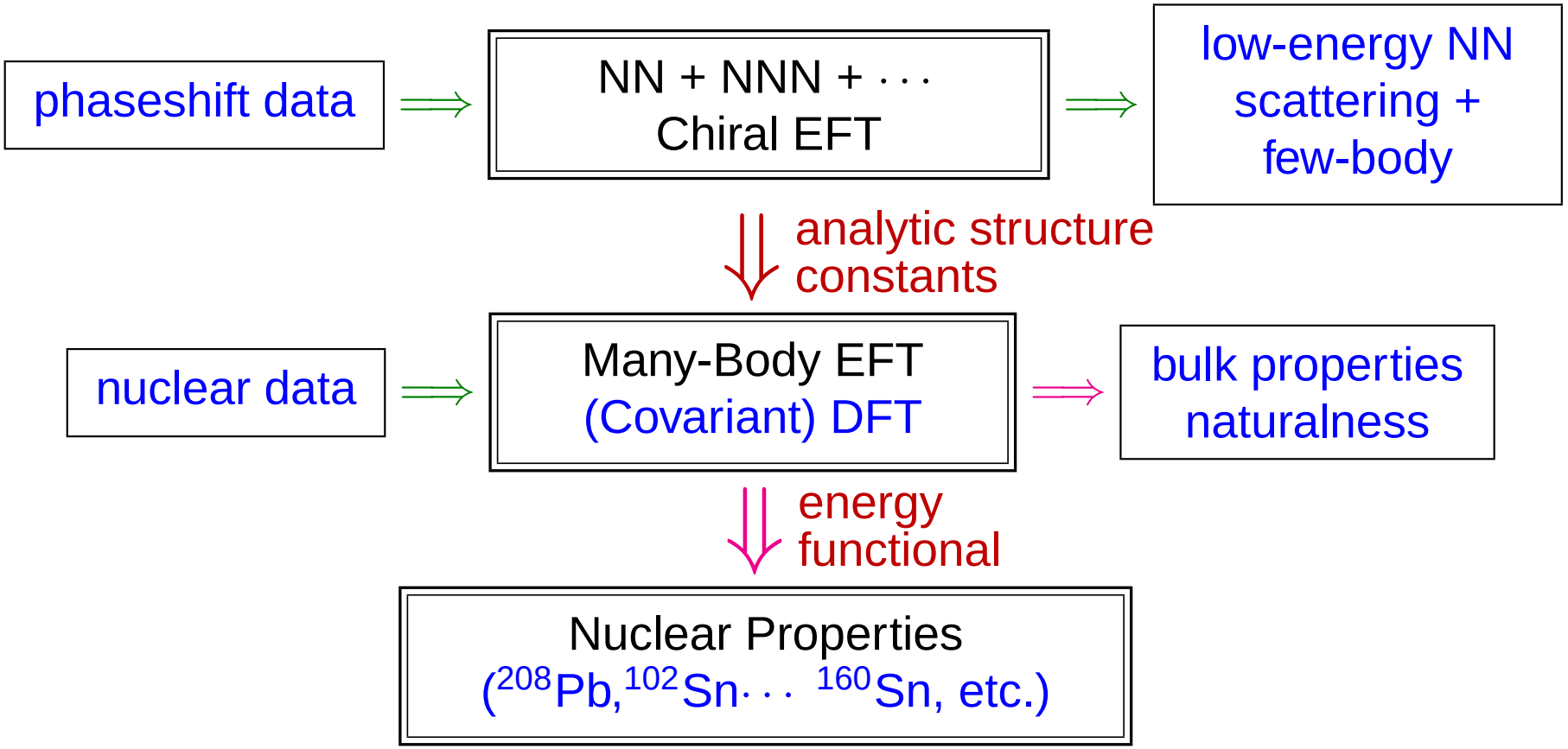

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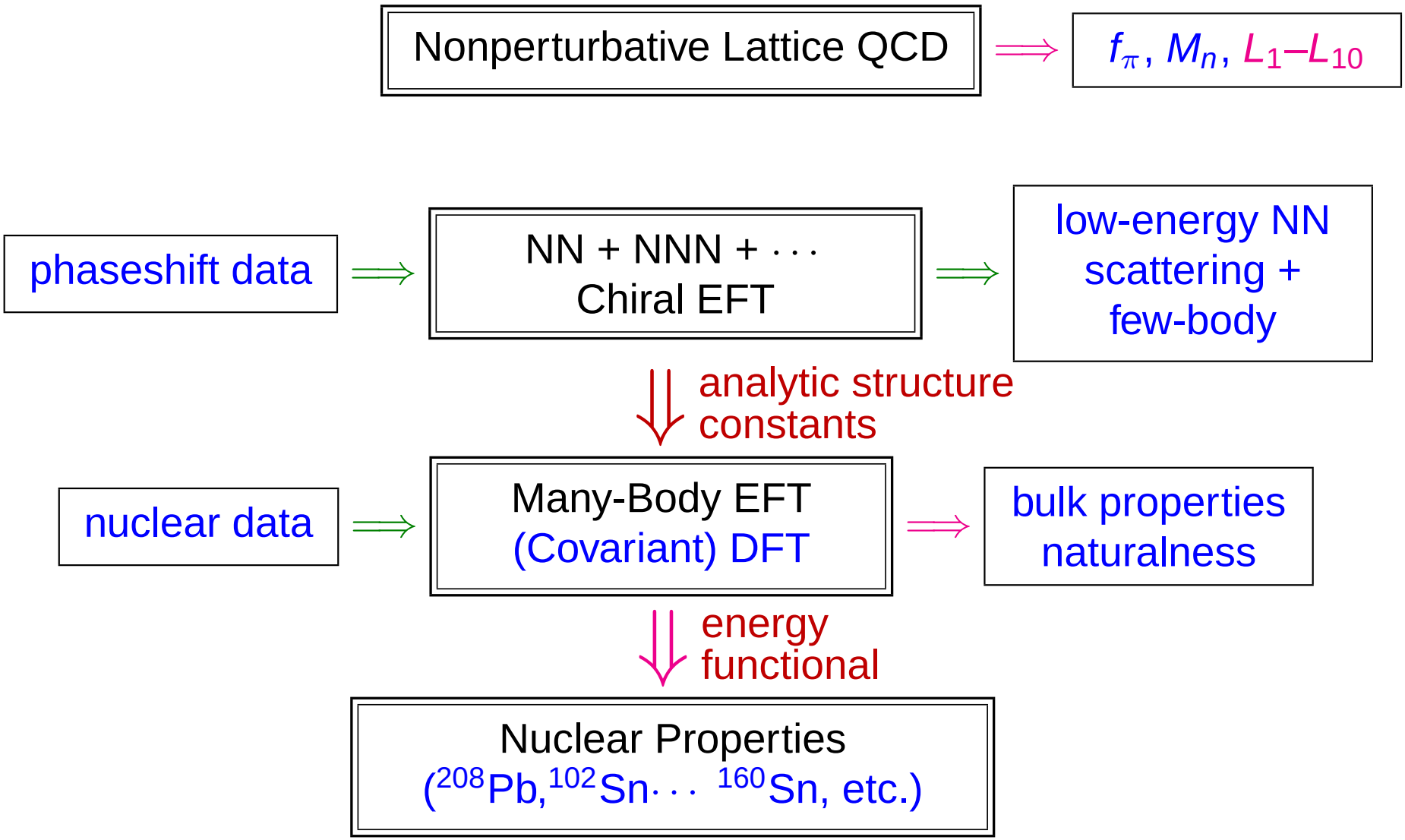

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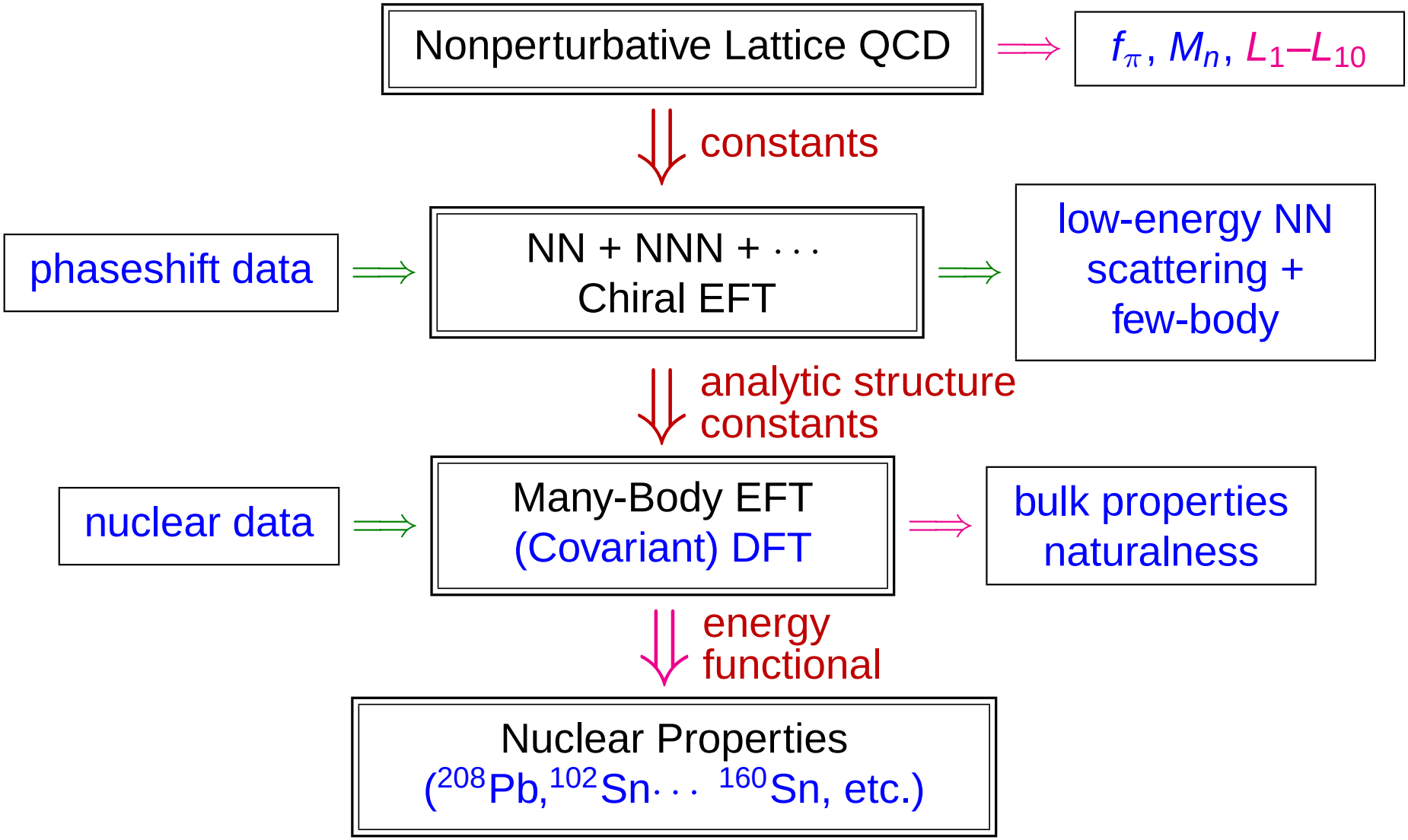

(Nuclear) Many-Body Physics: "Old" vs. "New"

One Hamiltonian for all problems and energy/length scales	Infinite # of low-energy potentials; different resolutions $\Longrightarrow$ different dof's and Hamiltonians
Find the "best" potential	There is no best potential $\Longrightarrow$ use a convenient one!
Two-body data may be sufficient; many-body forces as last resort	Many-body data needed and many-body forces inevitable
Avoid divergences	Exploit divergences
Choose diagrams by "art"	Power counting determines diagrams and truncation error