Density Functional Theory (DFT) for Nuclei — What About EFT?

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What is Density Functional Theory (DFT)?

- Hohenberg-Kohn: There exists an energy functional $E_{v_{\text{ext}}}[\rho]$ . . .

$$E_{v_{\text{ext}}}[\rho] = F_{\text{HK}}[\rho] + \int d^3x\, v_{\text{ext}}(\mathbf{x})\rho(\mathbf{x})$$

- F_{HK} is *universal* (same for any external v_{ext}) $\implies H_2$ to DNA!

- Useful if you can approximate the energy functional

- Introduce orbitals and minimize energy functional $\implies E_{gs}, \rho_{gs}$

- Kohn-Sham procedure similar to nuclear "mean field" calculations (e.g., Skyrme HF)
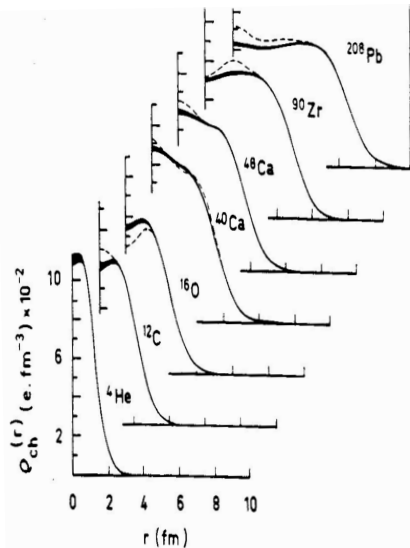
Microscopic Nuclear Structure Methods

- Wave function methods (GFMC/AFMC, NCSM/FCI, CC, . . .)
  - many-body wave functions (in approximate form!)
  - $\Psi(x_1, \cdots, x_A) \implies$ everything (if operators known)
  - limited to $A < 100$? or < 200? or ???

- Green's functions (see W. Dickhoff and D. Van Neck text)
  - response of ground state to removing/adding particles
  - single-particle Green's function $\implies$ expectation value of one-body operators, Hamiltonian
  - energy, densities, single-particle excitations, . . .

- DFT (see C. Fiolhais et al., *A Primer in Density Functional Theory*)
  - LT of response of energy to perturbations of density $J(\mathbf{x})\psi^\dagger \psi$
  - natural framework is effective actions for composite operators $\Gamma[\rho] = \Gamma_0[\rho] + \Gamma_{\text{int}}[\rho]$ (e.g., for EFT/DFT) but also quantum chemistry MBPT+ approach (Bartlett et al.)
  - energy functional $\implies$ plug in candidate density, get out trial energy, minimize (variational?)
 - energy and densities (TDFT $\implies$ excitations)

Paths to a *Nuclear* Energy Functional (EDF)

- Empirical energy functional (Skyrme or RMF)
- Emulate Coulomb DFT: LDA based on precision calculation of uniform system $E[\rho] = \int d\mathbf{r}\, \mathcal{E}(\rho(\mathbf{r}))$ plus constrained gradient corrections ($\nabla \rho$ factors)

- SLDA (Bulgac et al.) for cold atoms
- Fayans and collaborators (e.g., nucl-th/0009034)

$$\mathcal{E}_v = \frac{2}{3}\epsilon_F \rho_0 \left[a_+^v \frac{1 - h_{1+}^v x_+^{1/3}}{1 - h_{2+}^v x_+^{1/3}} x_+^2 \right.$$
$$\left. + a_-^v \frac{1 - h_{1-}^v x_+^{1/3}}{1 - h_{2-}^v x_+^{1/3}} x_-^2 \right]$$

where $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$
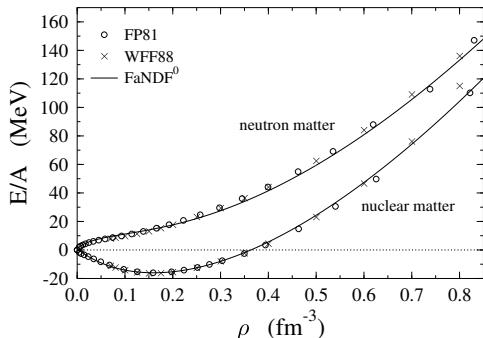
- RG approach (J. Braun, from Polonyi and Schwenk, nucl-th/0403011)
- EDF from perturbative chiral interactions + DME (Kaiser et al.)
- Constructive Kohn-Sham DFT with RG-softened $V_{\chi EFT}$'s

How Can We Use EFT's To Constrain DFT's?

- Constraining the nuclear EOS from fits of energy functionals to nuclei involves uncontrolled extrapolations at present. At low densities, where the pionless EFT is applicable, there are close connections to cold-atom physics. At higher densities inadequately constrained many-body forces are a serious concern. How can EFT help to provide much-needed controlled extrapolations and theoretical error bars?

- Since DFT can be cast in the form of an effective action approach, it is immediately compatible with EFT in principle. How do we implement this in practice? E.g., how to do power counting for the energy functional for a given EFT?

- What are the possible EFT's for nuclear matter? E.g., are nucleon-only degrees of freedom adequate? What is the role of pions and chiral symmetry? Can we write an EFT around the Fermi surface? Does Pauli blocking make the EFT ??(more?) perturbative? Is there a covariant EFT that can explain and improve the successes of "relativistic mean field" phenomenology?

Issues with Empirical EDF's

- Density dependencies might be too simplistic

- Isovector components not well constrained

- No (fully) systematic organization of terms in the EDF

- Difficult to estimate theoretical uncertainties

- What's the connection to many-body forces?

- Pairing part of the EDF not treated on same footing

- and so on . . .

$\Longrightarrow$ How can EFT help?

Comparing LDA Dilute and Skyrme Functionals

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

$$E[\rho, \tau, \mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)(\boldsymbol{\nabla}\rho)^2 \right.$$
$$\left. - \frac{3}{4}W_0\rho\boldsymbol{\nabla}\cdot\mathbf{J} + \frac{1}{16}t_3\rho^{2+\alpha} + \cdots \right\}$$

- Dilute $\rho\tau\mathbf{J}$ energy density functional for $\nu = 4$ ($V_{\text{external}} = 0$)

$$E[\rho, \tau, \mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}C_0\rho^2 + \frac{1}{16}(3C_2 + 5C_2')\rho\tau + \frac{1}{64}(9C_2 - 5C_2')(\boldsymbol{\nabla}\rho)^2 \right.$$
$$\left. - \frac{3}{4}C_2''\rho\boldsymbol{\nabla}\cdot\mathbf{J} + \frac{c_1}{2M}C_0^2\rho^{7/3} + \frac{c_2}{2M}C_0^3\rho^{8/3} + \frac{1}{16}D_0\rho^3 + \cdots \right\}$$

- Same functional as LDA dilute Fermi gas with $t_i \leftrightarrow C_i$
  - Is Skyrme missing non-analytic, NNN, long-range (pion), (and so on) terms? Are proposed extensions enough?
  - Isn't this a short-distance "perturbative" expansion?

Nuclear Energy Density Functional

We consider the EDF in the form,

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

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta\rho_t + \tfrac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^ρ on the isoscalar density ρ_0 as:
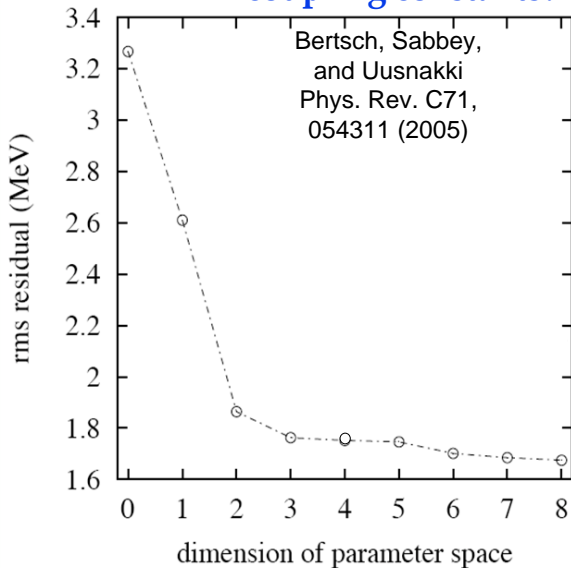
$$C_t^\rho = C_{t0}^\rho + C_{tD}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^\rho, \quad C_{tD}^\rho, \quad C_t^\tau, \quad C_t^{\Delta\rho}, \quad C_t^J, \quad \text{and} \quad C_t^{\nabla J},$$

for $t = 0$ and 1.

How well can we describe masses with 12 coupling constants?

Bertsch, Sabbey,
and Uusnakki
Phys. Rev. C71,
054311 (2005)

Fit to masses

Jacek Dobaczewski

JYVÄSKYLÄN YLIOPISTO

How to extend the nuclear energy density functional beyond the current standard form?

Quest for the spectroscopic-quality functional

⭐ **I.   Density dependence of all the coupling constants**

$$C_t^m(\rho_0, \rho_1) = C_t^m \left[1 + \alpha_t^m \left(1 - \left(\frac{\rho_0}{\rho_{\text{sat}}} \right)^{\gamma_t^m} \right) + \beta_t^m \left(\left(\frac{\rho_1}{\rho_{\text{sat}}} \right)^2 \right)^{\eta_t^m} \right]$$
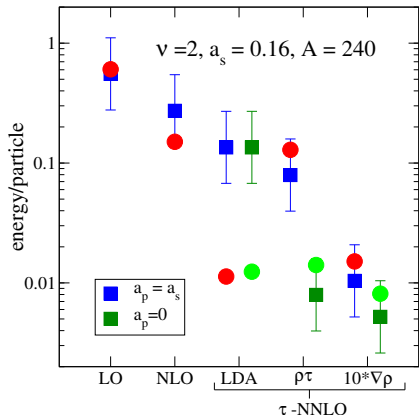
⭐ **II.   Derivatives of higher order up to N³LO:**

$$\rho_{ILkJ'J}^{mn} = \left((\vec{\nabla}^m)_I \left((\vec{k}^n)_L \rho_k \right)_{J'} \right)_J \quad \text{for} \quad k = 0, 1 \quad \text{and} \quad m+n \leq 6$$

⭐ **III. Products of more than two densities, for example:**

$$\rho^2 \tau^2, \quad \rho \tau \Delta \rho, \dots$$

Power Counting Estimates Work for Dilute DFT

- Scale contributions according to average density or $\langle k_F \rangle$
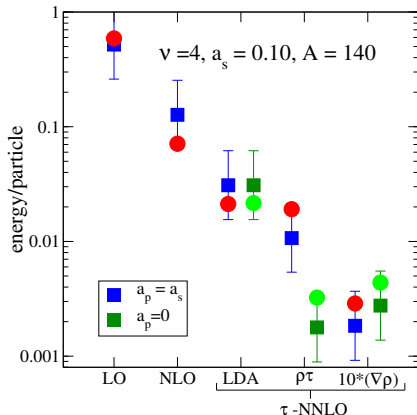
- Reasonable estimates $\implies$ truncation errors understood

Power Counting in Skyrme and RMF Functionals?
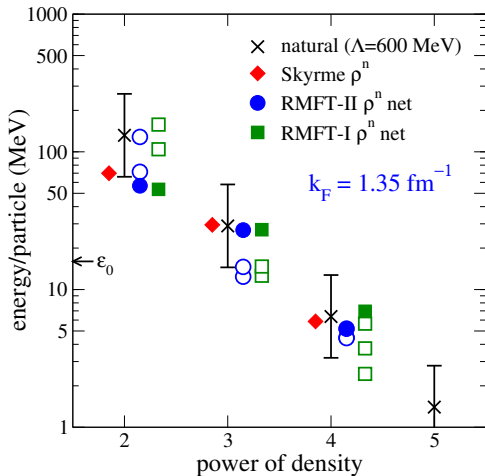
- Old NDA analysis:
  [Friar et al., rjf et al.]

$$c \left[\frac{\psi^\dagger \psi}{f_\pi^2 \Lambda} \right]^l \left[\frac{\nabla}{\Lambda} \right]^n f_\pi^2 \Lambda^2$$

$$\implies \begin{array}{c} \rho \longleftrightarrow \psi^\dagger \psi \\ \tau \longleftrightarrow \nabla \psi^\dagger \cdot \nabla \psi \\ \mathbf{J} \longleftrightarrow \psi^\dagger \nabla \psi \end{array}$$

- Density expansion?

$$\frac{1}{7} \leq \frac{\rho_0}{f_\pi^2 \Lambda} \leq \frac{1}{4}$$

for $1000 \geq \Lambda \geq 500$

- × natural (Λ=600 MeV)
- ◆ Skyrme ρ^n
- ● RMFT-II ρ^n net
- ■ RMFT-I ρ^n net

$k_F = 1.35$ fm^{-1}

ϵ_0

energy/particle (MeV)

power of density

Long-Range Chiral EFT
⟹ Enhanced Skyrme

- Add long-range (π-exchange) contributions in the density matrix expansion (DME)
  - NN/NNN through N²LO derived [SKB,BG]
- Refit the Skyrme parameters
- Test for sensitivies and improved observables (isotope chains)
- Spin-orbit couplings from 2π 3NF particularly interesting
- Can we "see" the pion in medium to heavy nuclei?
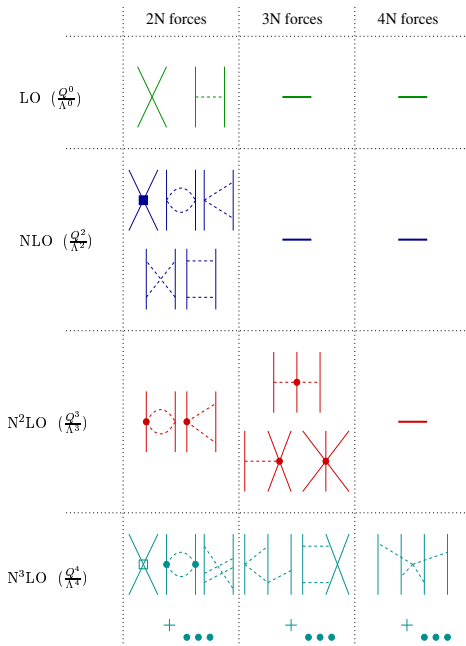
Observables Sensitive to 3N Interactions?

- Study systematics along isotopic chains
- Example: kink in radius shift $\langle r^2 \rangle(A) - \langle r^2 \rangle(208)$
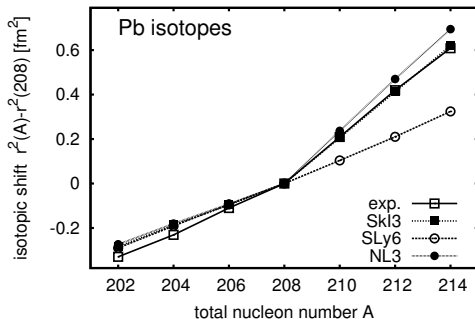

- Associated phenomenologically with behavior of spin-orbit
  - isoscalar to isovector ratio fixed in original Skyrme
- Clues from chiral EFT contributions?
  - Kaiser et al.: ratio of isoscalar to isovector spin-orbit

Scales in Nuclear Matter

- Extrapolation from finite nuclei to $N = Z$ matter:

$$\rho_0 \equiv 2k_F^3/3\pi^2 \approx 0.16\,\text{fm}^{-3} \qquad E_0/A \approx -16\,\text{MeV} \qquad K_0 \approx 200\text{--}300\,\text{MeV}$$

- Fermi momentum $k_F \approx 270\,\text{MeV} \approx 1.35\,\text{fm}^{-1} \approx 2m_\pi$
- Average relative momentum in Fermi sea $\approx 200\,\text{MeV}$
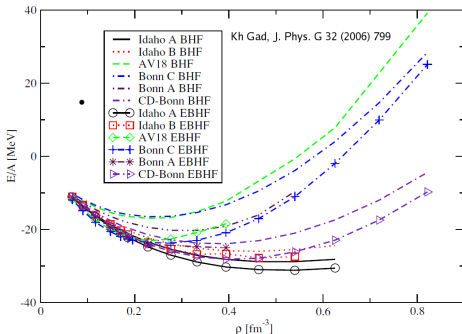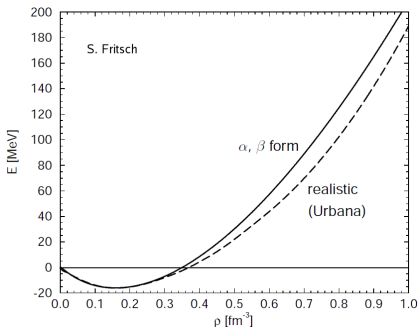
- Can *fit* $\dfrac{E}{A} = \dfrac{3k_F^2}{10M_N} - \dfrac{\alpha k_F^3}{M_N^2} + \dfrac{\beta k_F^4}{M_N^3}$ with $\alpha, \beta \sim 5\text{--}10$

Towards the optimal parameters of a given functional

$$\rho_c, \frac{E^{NM}}{A}, K^{NM}, M_s^{*NM}, a_{sym}^{NM}, L^{NM}, M_v^{*NM}, C_t^{\Delta\rho}, C_t^J, C_t^{\nabla J}$$

Correlation Matrix

1	0.0117	0.0168	0.0203	0.0282	0.0164	0.0020
	1	-0.036	-0.035	-0.032	0.026	-0.0004
		1	-0.020	-0.018	0.0168	-0.0009
			1	-0.019	0.0166	-0.0008
				1	0.0125	-0.0012
					1	0.0010
						1

Preliminary estimates

$$\frac{E^{NM}}{A} \approx -16.05 \text{ MeV},$$

$$\rho_c \approx 0.157 \text{ fm}^{-3},$$

$$K^{NM} \approx 218.5 \text{ MeV},$$

$$M_s^{*NM} \approx 0.997,$$

$$a_{sym}^{NM} = 32.36 \text{ MeV},$$

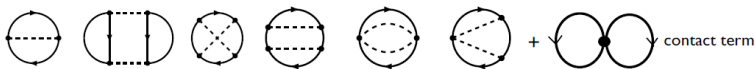$$L^{NM} \approx 46.3 \text{ MeV},$$

$$M_v^{*NM} \approx 1.37,$$

Chiral Dynamics of Nuclear Matter
Munich Group (Kaiser, Fritsch, Weise, . . .)

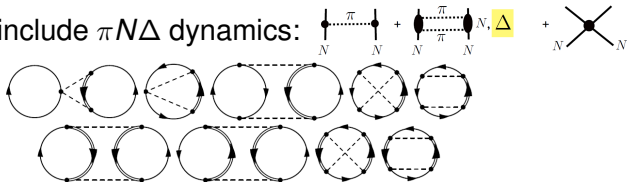- Basic idea: ChPT loop expansion becomes EOS expansion:

$$E(k_{\mathrm{F}}) = \sum_{n=2}^{\infty} k_{\mathrm{F}}^n \, f_n(k_{\mathrm{F}}/m_\pi, \Delta/m_\pi) \qquad [\Delta = M_\Delta - M_N \approx 300\,\mathrm{MeV}]$$

- 1st pass: N's and π's $\Longrightarrow$ count k_{F}'s by medium insertions

  - Saturation from *Pauli-blocking* of iterated 1π-exchange
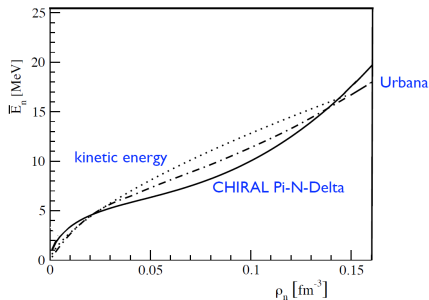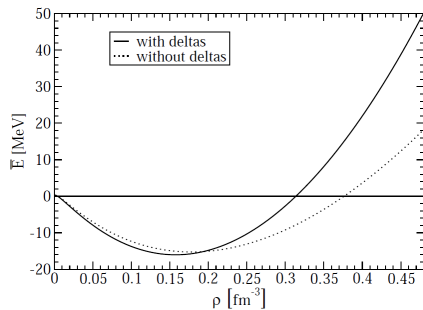 - Problems with single-particle and isospin properties and . . .

- 2nd pass: include $\pi N \Delta$ dynamics:

Chiral Dynamics of Nuclear Matter (cont.)
### Munich Group (Kaiser, Fritsch, Weise, . . .)

- 3-Loop: Fit nuclear matter saturation, predict neutron matter

- Substantial improvement in s.p. properties, spin-stability, . . .
- Issues for perturbative chiral expansion of nuclear matter:
  - higher orders, convergence? power counting?
  - relation of LEC's to free space EFT
- Apply DME to get DFT functional

Near-Term Roadmap for Microscopic Nuclear DFT

- Use a chiral EFT to a given order (e.g., E/M N³LO below)
- Soften with RG (evolve to $\Lambda \approx 2\,\text{fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions (3NF) approximately
- Generate density functional using DME in *k*-space
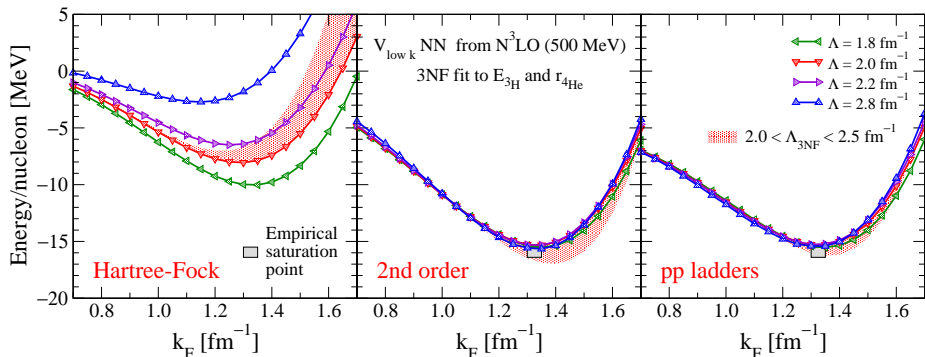
- MBPT organization, not chiral power counting

Orbital Dependent DFT (OEP, OPM, ...) [J. Drut, L. Platter]

- Construct expansion for $\Gamma_{\text{int}}[\rho, \tau, \mathbf{J}, \ldots]$; densities are sums over orbitals solving from Kohn-Sham S-eqn with $J_0(\mathbf{r}), \ldots$
- Self-consistency from $J(\mathbf{r}) = 0 \implies J_0(\mathbf{r}) = \delta\Gamma_{\text{int}}[\rho, \ldots]/\delta\rho(\mathbf{r})$
  - i.e., Kohn-Sham potential is functional derivative of interacting energy functional (or E_{xc}) wrt densities
    - How do we calculate this functional derivative?
- Approximations with explicit $\rho(\mathbf{r})$ dependence: LDA, DME, ...
- Orbital-dependent DFT $\implies$ full derivative via chain rule:

$$J_0(\mathbf{r}) = \frac{\delta\Gamma_{\text{int}}[\phi_\alpha, \varepsilon_\alpha]}{\delta\rho(\mathbf{r})} = \int d\mathbf{r}' \, \frac{\delta J_0(\mathbf{r}')}{\delta\rho(\mathbf{r})} \sum_\alpha \left\{ \int d\mathbf{r}'' \left[\frac{\delta\phi_\alpha^\dagger(\mathbf{r}'')}{\delta J_0(\mathbf{r}')} \frac{\delta\Gamma_{\text{int}}}{\delta\phi_\alpha^\dagger(\mathbf{r}'')} + c.c. \right] \right.$$
$$\left. + \frac{\delta\varepsilon_\alpha}{\delta J_0(\mathbf{r}')} \frac{\partial\Gamma_{\text{int}}}{\partial\varepsilon_\alpha} \right\}$$

- Solve the OPM equation for J_0 using $\chi_s(\mathbf{r}, \mathbf{r}') = \delta\rho(\mathbf{r})/\delta J_0(\mathbf{r}')$

$$\int d^3r' \, \chi_s(\mathbf{r}, \mathbf{r}') \, J_0(\mathbf{r}') = \Lambda_{\text{xc}}(\mathbf{r})$$

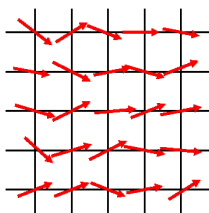- $\Lambda_{\text{xc}}(\mathbf{r})$ is functional of the orbitals ϕ_α, eigenvalues ε_α, and G_{KS}^0

DFT and Effective Actions (Fukuda et al., Polonyi, ...)

- External field $\Longleftrightarrow$ Magnetization
- Helmholtz free energy $F[H]$
  $\Longleftrightarrow$ Gibbs free energy $\Gamma[M]$

$\begin{array}{l} \textit{Legendre} \\ \textit{transform} \end{array} \Longrightarrow \Gamma[M] = F[H] + H\,M$

$H = \dfrac{\partial \Gamma[M]}{\partial M} \xrightarrow[\textit{state}]{\textit{ground}} \left. \dfrac{\partial \Gamma[M]}{\partial M} \right|_{M_{gs}} = 0$
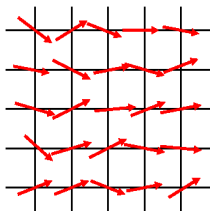

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DFT and Effective Actions (Fukuda et al., Polonyi, ...)

- External field $\Longleftrightarrow$ Magnetization
- Helmholtz free energy $F[H]$
  $\Longleftrightarrow$ Gibbs free energy $\Gamma[M]$

  Legendre transform $\Longrightarrow \Gamma[M] = F[H] + H\,M$

  $H = \dfrac{\partial \Gamma[M]}{\partial M}$ *ground state* $\xrightarrow{}$ $\left.\dfrac{\partial \Gamma[M]}{\partial M}\right|_{M_{\mathrm{gs}}} = 0$

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- Partition function with sources that adjust densities:
  $$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H} + J\,\widehat{\rho})} \quad \Longrightarrow \quad \text{path integral for } W[J]$$

- *Invert* to find $J[\rho]$ and Legendre transform from J to ρ:
  $$\rho(\mathbf{x}) = \frac{\delta W[J]}{\delta J(\mathbf{x})} \quad \Longrightarrow \quad \Gamma[\rho] = W[J] - \int J\,\rho \quad \text{and} \quad J(\mathbf{x}) = -\frac{\delta \Gamma[\rho]}{\delta \rho(\mathbf{x})}$$
  $\Longrightarrow \Gamma[\rho] \propto$ energy functional $E[\rho]$, stationary at $\rho_{\mathrm{gs}}(\mathbf{x})$!

Partition Function in $\beta \to \infty$ Limit [see Zinn-Justin]

- Consider Hamiltonian with time-independent source $J(\mathbf{x})$:

$$\widehat{H}(J) = \widehat{H} + \int J\,\psi^\dagger\psi$$

- *If* ground state is isolated (and bounded from below),

$$e^{-\beta\widehat{H}} = e^{-\beta E_0}\left[|0\rangle\langle 0| + \mathcal{O}\big(e^{-\beta(E_1 - E_0)}\big)\right]$$

- As $\beta \to \infty$, $\mathcal{Z}[J] \Longrightarrow$ ground state of $\widehat{H}(J)$ with energy $E_0(J)$

$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H} + J\widehat{\rho})} \Longrightarrow E_0(J) = \lim_{\beta\to\infty} -\frac{1}{\beta}\log \mathcal{Z}[J] = \frac{1}{\beta}W[J]$$

- Substitute and separate out the pieces:

$$E_0(J) = \langle\widehat{H}(J)\rangle_J = \langle\widehat{H}\rangle_J + \int J\langle\psi^\dagger\psi\rangle_J = \langle\widehat{H}\rangle_J + \int J\,\rho(J)$$

- Expectation value of $\widehat{H}$ in ground state generated by $J[\rho]$

$$\langle\widehat{H}\rangle_J = E_0(J) - \int J\,\rho = \frac{1}{\beta}\Gamma[\rho]$$

Putting it all together . . .

$$\frac{1}{\beta}\Gamma[\rho] = \langle \widehat{H} \rangle_J \xrightarrow{J \to 0} E_0 \quad \text{and} \quad J(x) = -\frac{\delta\Gamma[\rho]}{\delta\rho(x)} \xrightarrow{J \to 0} \left.\frac{\delta\Gamma[\rho]}{\delta\rho(x)}\right|_{\rho_{\text{gs}}(\mathbf{x})} = 0$$

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

- The true ground state (with $J = 0$) is a variational minimum
  - So more sources should be better! (e.g., $\Gamma[\rho, \tau, \mathbf{J}, \cdots]$)
  - [For Minkowski-space version of this, see Weinberg, Vol. II]
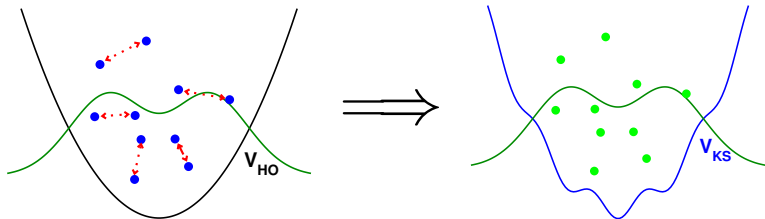- Universal dependence on external potential is trivial:

$$\Gamma_v[\rho] = W_v[J] - \int J\,\rho = W_{v=0}[J+v] - \int [(J+v)-v]\,\rho = \Gamma_{v=0}[\rho] + \int v\,\rho$$

  - But functionals change with resolution or field redefinitions
    $\Longrightarrow$ only stationary points are observables
- If uniform, can find spontaneously broken ground state;
  if finite system, must deal with zero modes

Kohn-Sham DFT for $v_{ext} = V_{HO}$ Harmonic Trap
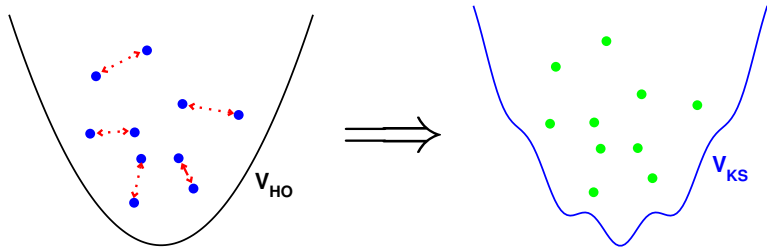
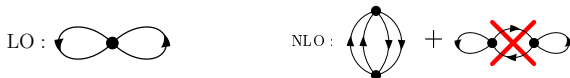# **Kohn-Sham DFT for $v_{\text{ext}} = V_{\text{HO}}$ Harmonic Trap**

- Interacting density in V_{HO} $\equiv$ Non-interacting density in V_{KS}
- Orbitals $\{\psi_i(\mathbf{x})\}$ in local potential $V_{\text{KS}}([\rho], \mathbf{x})$

$$[-\boldsymbol{\nabla}^2/2m + V_{\text{KS}}(\mathbf{x})]\psi_i = \varepsilon_i \psi_i \implies \rho(\mathbf{x}) = \sum_{i=1}^{A} |\psi_i(\mathbf{x})|^2$$
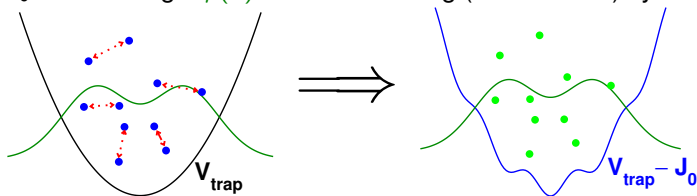
- Find Kohn-Sham potential $V_{\text{KS}}([\rho], \mathbf{x})$ from $\delta E_{v_{\text{ext}}}[\rho]/\delta\rho(\mathbf{x})$
- Solve self-consistently

Construct $W[J]$ and then $\Gamma[\rho]$ order-by-order

- Diagrammatic *expansion* (e.g., use EFT power counting)

- Inversion method $\implies$ Split source $J = J_0 + J_1 + \ldots$
  - J_0 *chosen* to get $\rho(\mathbf{x})$ in noninteracting (Kohn-Sham) system:

  - cf. $H = (H_0 + U) + (V - U)$ with freedom to choose U
  - Orbitals $\{\psi_i(\mathbf{x})\}$ in local potential $V_{\text{KS}}([\rho], \mathbf{x}) \implies$ propagators

$$[-\boldsymbol{\nabla}^2/2m + V_{\text{KS}}(\mathbf{x})]\psi_i = \varepsilon_i\psi_i \implies \rho(\mathbf{x}) = \sum_{i=1}^{A} |\psi_i(\mathbf{x})|^2$$

- Self-consistency from $J(\mathbf{x}) = 0 \implies J_0(\mathbf{x}) = \delta\Gamma_{\text{int}}[\rho]/\delta\rho(\mathbf{x})$