

# Covariant Effective Field Theory for a Dilute Fermi System

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- Effective action approach to EFT-based Kohn-Sham DFT
- Renormalization for short-range interactions
- Density functional theory (DFT) single-particle spectra

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Supported in part by the NSF and the DOE.

# Covariant DFT as Legendre Transformation

- To probe the system, add a source  $V^\mu(\mathbf{x})$  coupled to current operator  $\hat{j}^\mu(\mathbf{x}) \equiv \bar{\psi}(\mathbf{x})\gamma^\mu\psi(\mathbf{x})$  to the partition function:

$$\mathcal{Z}[V] = e^{-W[V]} \sim \text{Tr} e^{-\beta(\hat{H} + V \cdot \hat{j})} \longrightarrow \int \mathcal{D}[\psi^\dagger] \mathcal{D}[\psi] e^{-\int [\mathcal{L} + V_\mu \bar{\psi} \gamma^\mu \psi]}$$

- The (time-dependent) current  $j^\mu(\mathbf{x})$  in the presence of  $V^\mu(\mathbf{x})$  is

$$j^\mu(\mathbf{x}) = (\rho_v(\mathbf{x}), \mathbf{j}_v(\mathbf{x})) \equiv \langle \bar{\psi}(\mathbf{x})\gamma^\mu\psi(\mathbf{x}) \rangle_V = \frac{\delta W[V]}{\delta V_\mu(\mathbf{x})}$$

- Invert to find  $V^\mu[j]$  and Legendre transform from  $V^\mu$  to  $j^\mu$ :

$$\Gamma[j] = -W[V] + \int V \cdot j \quad \text{with} \quad V^\mu(\mathbf{x}) = \frac{\delta \Gamma[j]}{\delta j_\mu(\mathbf{x})} \longrightarrow \left. \frac{\delta \Gamma[j]}{\delta j_\mu(\mathbf{x})} \right|_{j_{\text{gs}}(\mathbf{x})} = 0$$

$\implies$  For static  $j^\mu(\mathbf{x})$ ,  $\Gamma[j] \propto$  the DFT energy functional  $E[\rho_v]$ !

## What About the Scalar Density?

- Can add additional sources and Legendre transformations
- In nonrelativistic DFT, add to Lagrangian  $+ \eta(\mathbf{x}) \nabla\psi^\dagger \nabla\psi$

$$\Gamma[\rho, \tau] = W[\mathbf{J}, \eta] - \int \mathbf{J}(\mathbf{x})\rho(\mathbf{x}) - \int \eta(\mathbf{x})\tau(\mathbf{x})$$

$\implies$  Skyrme HF energy functional  $E[\rho, \tau, \mathbf{J}]$  of density *and* kinetic energy density (see A. Bhattacharyya talk DF06)

- In covariant DFT, add to Lagrangian  $+ \mathbf{S}(\mathbf{x})\bar{\psi}\psi$

$$\Gamma[j^\mu, \rho_s] = W[V^\mu, \mathbf{S}] - \int V(\mathbf{x}) \cdot j(\mathbf{x}) - \int \mathbf{S}(\mathbf{x})\rho_s(\mathbf{x})$$

$\implies$  RMF energy functional  $E[\rho_v, \rho_s]$  [with  $j^\mu = (\rho_v, \mathbf{0})$ ]

# Kohn-Sham DFT Via Inversion [Fukuda et al.]

- Hierarchy (e.g., EFT expansion)  $\implies$  order-by-order matching

$$W[V] = W_0[V] + W_1[V] + W_2[V] + \dots$$

$$V[\rho_V] = V_0[\rho_V] + V_1[\rho_V] + V_2[\rho_V] + \dots$$

$$\Gamma[\rho_V] = \Gamma_0[\rho_V] + \Gamma_1[\rho_V] + \Gamma_2[\rho_V] + \dots$$

- Zeroth order is a **noninteracting** system with potential  $V_0(\mathbf{x})$

$$\Gamma_0[\rho_V] = W_0[V_0] - \int d^4\mathbf{x} V_0(\mathbf{x})\rho_V(\mathbf{x}) \implies \rho_V(\mathbf{x}) = \frac{\delta W_0[V_0]}{\delta V_0(\mathbf{x})}$$

$\implies$  this is the Kohn-Sham system with the **exact** density!

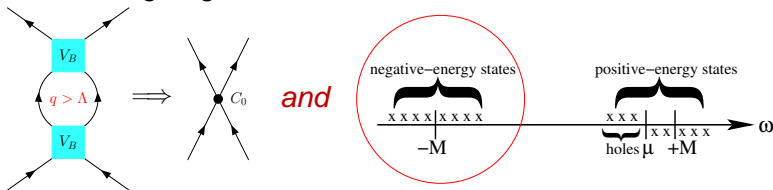
- Diagonalize  $W_0[V_0]$  by introducing KS orbitals  $\implies$  Dirac equation
- Find  $V_0$  for the ground state by completing self-consistency loop:

$$V_0 \rightarrow W_1 \rightarrow \Gamma_1 \rightarrow V_1 \rightarrow W_2 \rightarrow \Gamma_2 \rightarrow \dots \implies V_0(\mathbf{x}) = \frac{\delta \tilde{E}_{\text{int}}[\rho_V]}{\delta \rho_V(\mathbf{x})} \propto \sum_i \frac{\delta \Gamma_i[\rho_V]}{\delta \rho_V(\mathbf{x})}$$

# Power Counting Lost / Power Counting Regained

- Gasser, Sainio, and Svarc  $\implies$  ChPT for  $\pi N$  with relativistic  $N$ 's
  - loop and momentum expansions don't agree  
 $\implies$  systematic power counting lost
  - heavy-baryon EFT restores power counting by  $1/M$  expansion
- Hua-Bin Tang (1996) [and with Paul Ellis]:

*"... EFT's permit useful low-energy expansions only if we absorb **all** of the hard-momentum effects into the parameters of the Lagrangian."*

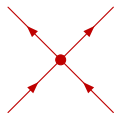


- Becher/Leutwyler IR  $\implies$  Schindler-Gegelia-Scherer version

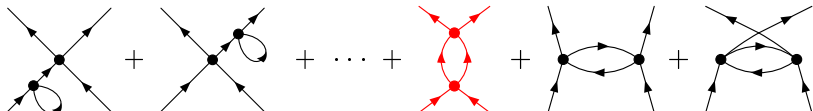
# Consequences for Free-Space Natural Fermions

- Tadpoles,  $N\bar{N}$  loops in free space vanish!
- Leading order (LO) has scalar, vector, etc. vertices

$$\mathcal{L}_{\text{eft}} = \dots - \frac{C_s}{2} (\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{C_v}{2} (\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) + \dots \implies$$



- At NLO, only **particle-particle loop** survives IR



- **Only forward-going nucleons contribute**  
 $\implies$  same scattering amplitude as nonrel. DR/MS for small  $k$

# Laboratory for Covariant DFT

- Study covariant vs. nonrel. DFT/EFT in controlled expansion
  - Confine system in a Woods-Saxon “trap” with  $V_{\text{ext}}$  and  $S_{\text{ext}}$
  - Choose  $V_{\text{ext}}, S_{\text{ext}}$  so no spin-orbit from external potentials
- First: Consider LO covariant effective Lagrangian

$$\mathcal{L}_{\text{eft}} = \bar{\psi}[i\partial_{\mu}\gamma^{\mu} - M]\psi - \frac{C_s}{2}(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{C_v}{2}(\bar{\psi}\gamma^{\mu}\psi)(\bar{\psi}\gamma_{\mu}\psi)$$

- Compare observables from two DFT functionals
  - Sources coupled to vector  $V^{\mu}\bar{\psi}\gamma_{\mu}\psi$  and scalar  $S\bar{\psi}\psi$  densities  
 $\implies$  two Kohn-Sham potentials, scalar and vector

$$V_0^{\mu}(\mathbf{x}) = \frac{\delta E_{\text{int}}[j^{\mu}, \rho_s]}{\delta j_{\mu}(\mathbf{x})} \quad \text{and} \quad S_0(\mathbf{x}) = \frac{\delta E_{\text{int}}[j^{\mu}, \rho_s]}{\delta \rho_s(\mathbf{x})}$$

- Source coupled to vector  $\tilde{V}^{\mu}\bar{\psi}\gamma_{\mu}\psi$  densities only  
 $\implies$  one (vector) Kohn-Sham potential (plus external fields)

$$\tilde{V}_0^{\mu}(\mathbf{x}) = \frac{\delta \tilde{E}_{\text{int}}[j^{\mu}]}{\delta j_{\mu}(\mathbf{x})}$$

- Consider bowtie diagrams with four-vector and scalar vertices:

$$\Gamma_1 = W_1 = \text{bowtie}_{\gamma_0} + \text{bowtie}_1$$

- Case  $\rho_V, \rho_S$ : Quadratic part of Lagrangian in  $W_0$  diagonalized

$$\int d^4x \bar{\psi} \left[ i\partial^\mu \gamma_\mu - M + S_0(\mathbf{x}) - \gamma_0 V_0^0(\mathbf{x}) \right] \psi$$

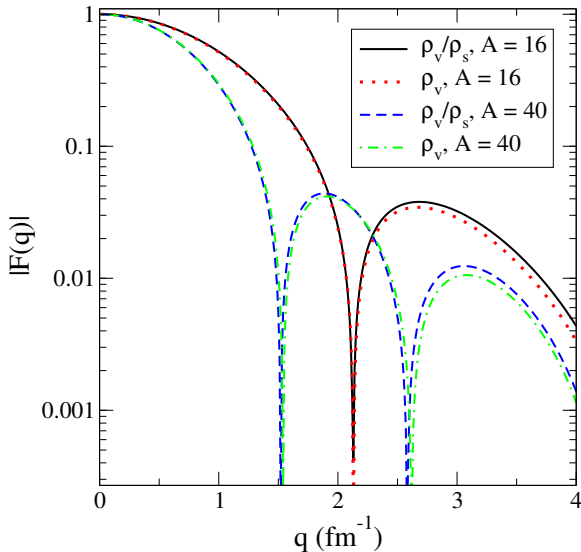
- Kohn-Sham equation  $\implies$  defines  $M^*(\mathbf{x}) \equiv M - S_0(\mathbf{x})$
- Case  $\rho_V$ : Quadratic part of Lagrangian in  $\widetilde{W}_0$  diagonalized

$$\int d^4x \bar{\psi} \left[ i\partial^\mu \gamma_\mu - M - \gamma_0 \widetilde{V}_0^0(\mathbf{x}) \right] \psi$$

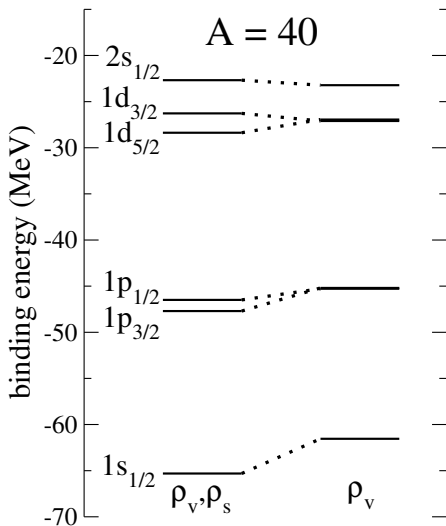
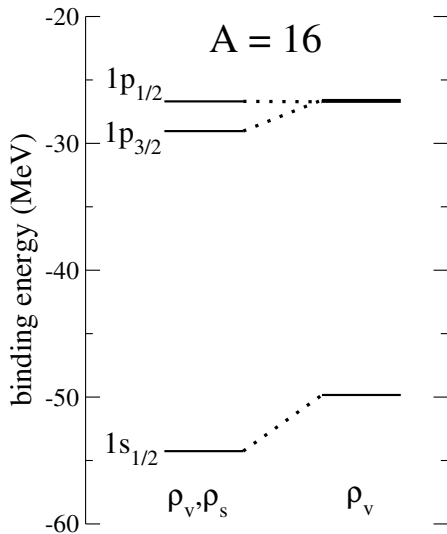
- Scalar diagram evaluated approximately ( $k_F/M$  expansion + LDA)
- How do observables compare?
  - Binding energies, densities (Kohn-Sham observables)
  - What about the single-particle spectra?

# Kohn-Sham LDA $\rho_V$ vs. $\rho_V, \rho_S$ : Comparison

$A = 16$	$BE/A$	$\sqrt{\langle r^2 \rangle}$
$\rho_V$	27.5	1.97
$\rho_V, \rho_S$	27.1	1.99
$A = 40$	$BE/A$	$\sqrt{\langle r^2 \rangle}$
$\rho_V$	29.4	2.57
$\rho_V, \rho_S$	27.8	2.56



# Energy Spectra $\rho_V, \rho_S$ vs. $\rho_V$



# Summary and Future

- Covariant fermions with short-range interactions in trap
  - Laboratory for studying covariant EFT, DFT issues
  - Infrared regularization (IR) restores power counting
  - IR greatly simplifies free space and medium
  - Kohn-Sham Single-particle properties depend on sources
    - ⇒ can also relate to exact Green's function
- Issues under consideration:
  - Matching to free-space scattering
  - Comparison to heavy-baryon expansion
  - Renormalization at NLO
  - Covariant two-body ⇒ non-relativistic three-body forces
  - Time-dependent DFT (cf. RPA)
  - Including pairing
  - ...

# Summary Comments on Vacuum Physics

- Unlike QED DFT, “no sea” for nuclear structure is a misnomer
  - include “vacuum physics” in coefficients through renormalization
- Renormalization versus Renormalizability
  - Renormalization is required to account for short-distance behavior but can be implicit
  - Renormalizability at the hadronic level corresponds to making a model for the short-distance behavior
    - not a good model phenomenologically
  - Fixing short-distance behavior is not the same thing as throwing away negative-energy states
- For a long time, we looked for *unique* “relativistic effects”; these were largely misguided efforts

# Why Use EFT for Energy Functionals

- Similar to conventional “phenomenological” approaches
  - but with a rigorous foundation (DFT from effective action)
  - extendable and can be connected to chiral EFT for NN/NNN
- Eliminating model dependences (cf. “minimal” models)
  - framework for building a “complete” functional
  - more efficient renormalization (e.g., pairing)
- New insight into analytic structure of functional
  - e.g., logs in low-density expansion in  $k_F a_S$  from RG
- Power counting: what to sum at each order in an expansion
  - naturalness  $\implies$  estimates of truncation errors
  - evidence from Skyrme and RMF functionals for hierarchy
  - for covariant EFT, requires special renormalization

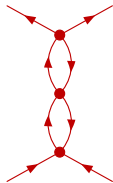
## UV Divergences in Nonrelativistic and Relativistic Effective Actions

- *All low-energy effective theories have incorrect UV behavior*
- Sensitivity to short-distance physics signalled by divergences but finiteness (e.g., with cutoff) doesn't mean not sensitive!  
 $\implies$  must absorb (and correct) sensitivity via renormalization
- Instances of UV divergences

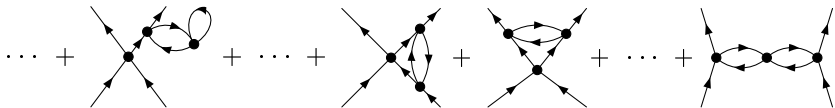
nonrelativistic	covariant
scattering	scattering
pairing	pairing
	anti-nucleons

# Consequences for Free-Space Natural Fermions

- At NNLO, only particle-particle loop diagram survives IR



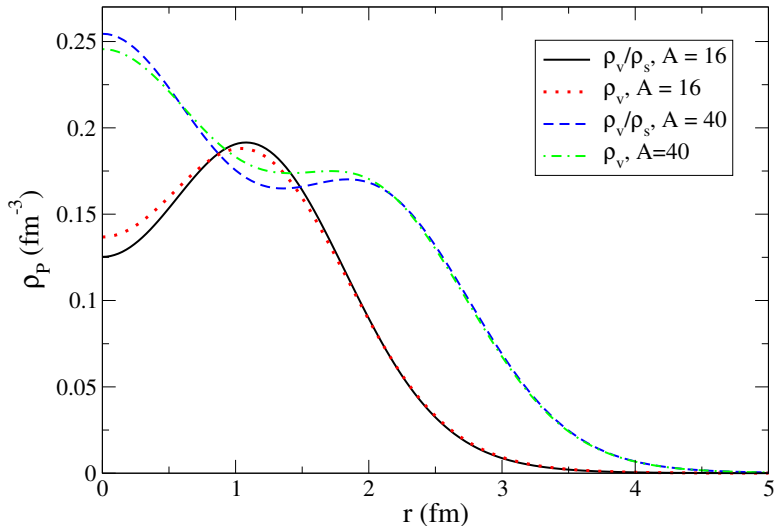
- All other diagrams are zero in IR



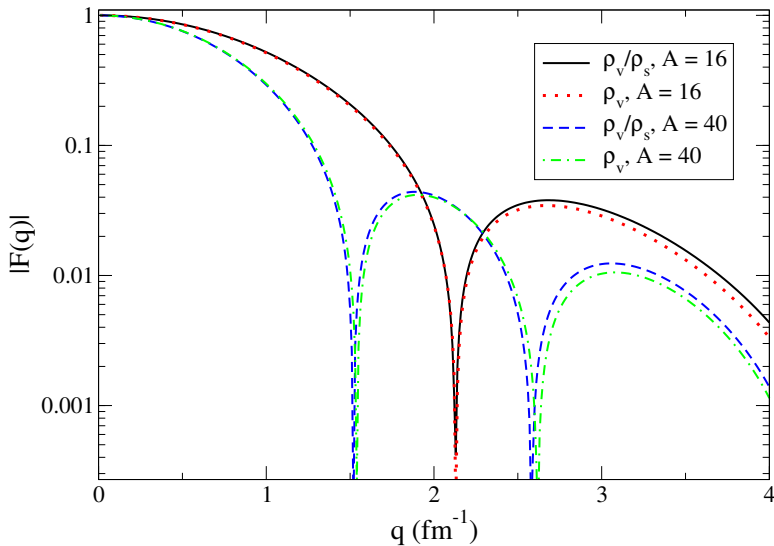
# Moving Dirac Sea Physics into Coefficients

- Absorb the “hard” part of a diagram into parameters,
  - ⇒ the remaining “soft” part satisfies chiral power counting
  - original  $\pi N$  prescription by H.B. Tang (expand, integrate term-by-term, and resum propagators)
  - systematized for  $\pi N$  by Becher and Leutwyler: “infrared regularization” or IR
  - not unique; e.g., Fuchs et al. additional finite subtractions in DR
- Extension of IR to multiple heavy particles [Lehmann and Prézeau]
  - convenient reformulation by Schindler, Gegelia, Scherer
  - tadpoles,  $N\bar{N}$  loops in free space vanish!
  - particle-particle loop reduces to nonrelativistic DR/MS result

# Kohn-Sham LDA $\rho_V$ vs. $\rho_V, \rho_S$



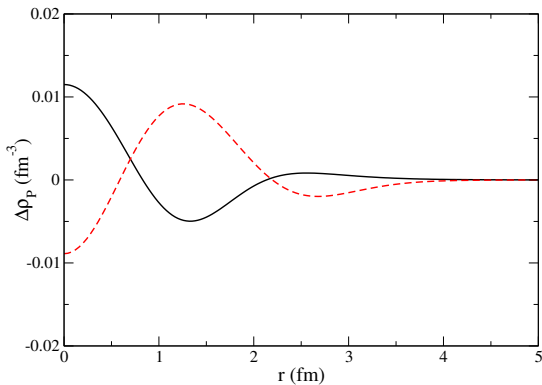
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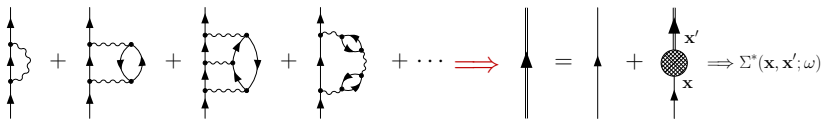
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# How is the Exact $G$ Related to $G_{ks}$ ?

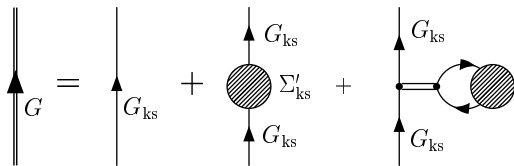


- Add a non-local source  $\xi(x', x)$  coupled to  $\bar{\psi}(x')\psi(x)$ :

$$Z[V, \xi] = e^{iW[V, \xi]} = \int D\psi D\psi^\dagger e^{i \int d^4x [\mathcal{L} + V^\mu(x)\bar{\psi}(x)\gamma_\mu\psi(x) + \int d^4x' \xi(x', x)\bar{\psi}(x')\psi(x)]}$$

- With  $\Gamma[\rho_V, \xi] = \Gamma_0[\rho_V, \xi] + \Gamma_{\text{int}}[\rho_V, \xi]$  (Dirac indices suppressed),

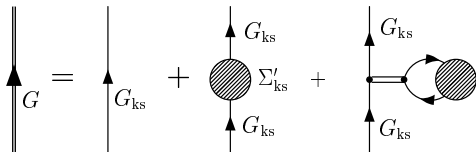
$$G(x, x') = \left. \frac{\delta W}{\delta \xi} \right|_J = \left. \frac{\delta \Gamma}{\delta \xi} \right|_{\rho_V} = G_{ks}(x, x') + G_{ks} \left[ \frac{\delta \Gamma_{\text{int}}}{\delta G_{ks}} - \frac{\delta \Gamma_{\text{int}}}{\delta \rho_V} \right] G_{ks}$$



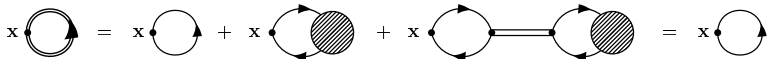
# How Do $G$ and $G_{ks}$ Yield the Same Density?

- Claim:  $\rho_{ks}(\mathbf{x}) = -i\nu G_{KS}^0(x, x^+)$  equals  $\rho(\mathbf{x}) = -i\nu G(x, x^+)$

- Start with



- Simple diagrammatic demonstration:



- Densities agree by construction!
- But other quantities may differ; spectral functions?