# Uncertainty Quantification

for

# Nuclear Many-Body Calculations

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(Technical University Darmstadt)

with: C. Drischler, J.W. Holt, N. Kaiser, A. Schwenk, W. Weise

**ECT* workshop**

"New ideas for constraining nuclear forces"

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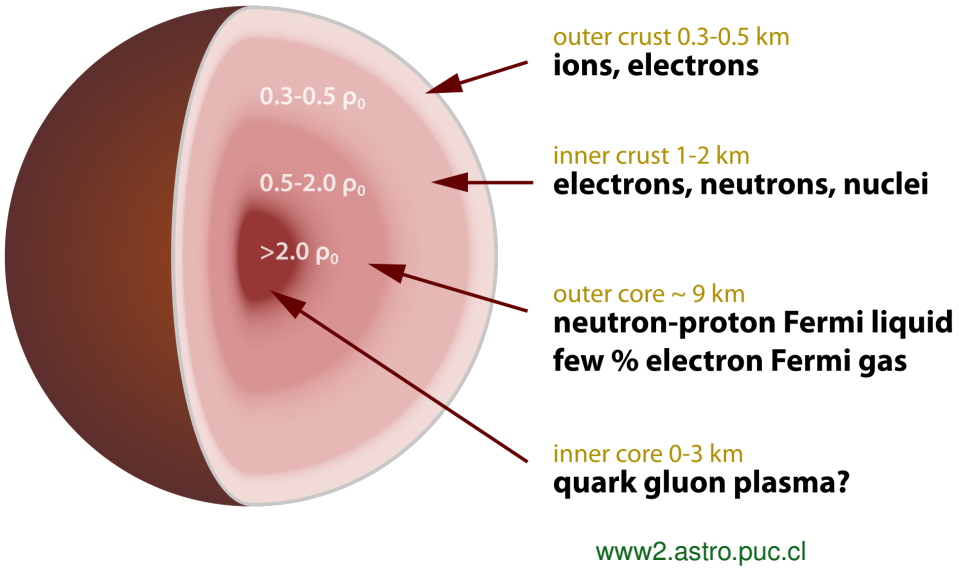
TECHNISCHE UNIVERSITÄT DARMSTADT

SFB 1245

# The Nuclear-Many-Body Problem

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| origin | core-collapse supernova |
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| mass | $\sim 10^{30}\,\mathrm{kg}$ |
| $\rho_0$ | $0.16\,\mathrm{fm}^{-3} \simeq 3 \times 10^{14}\mathrm{g/cm}^3$ |

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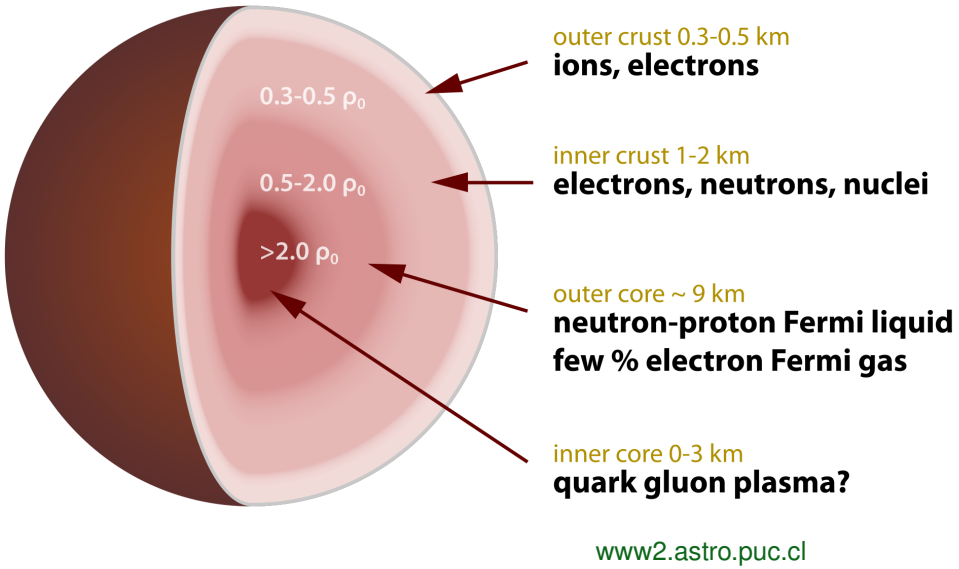


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- ground-state properties (neutron star structure)
- thermodynamic potentials (supernovae, neutron star mergers)
- transport properties (supernovae, neutron star mergers)

MBPT + chiral EFT provides a consistent and systematic framework for this

**Uncertainties governed by:**
many-body truncations → MBPT order-by-order convergence

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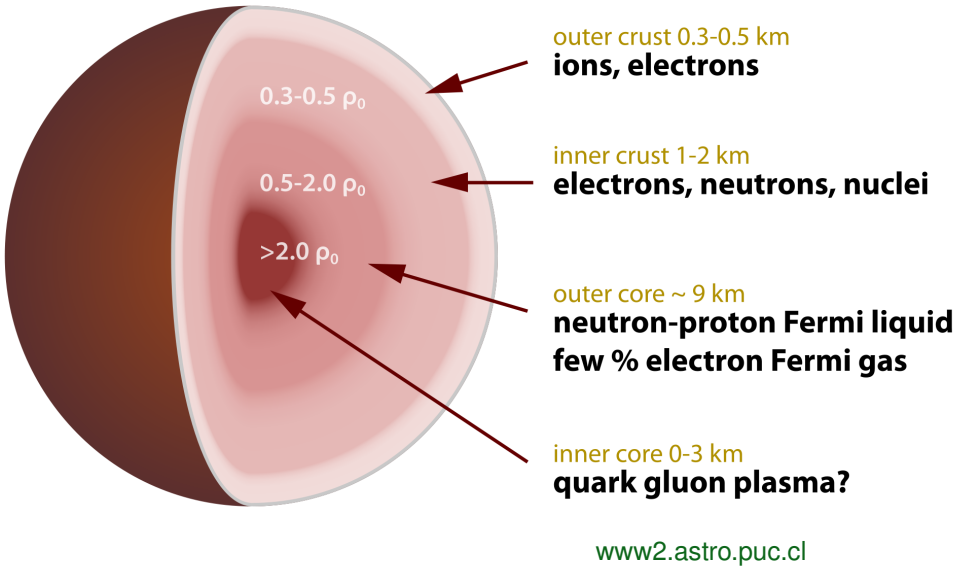


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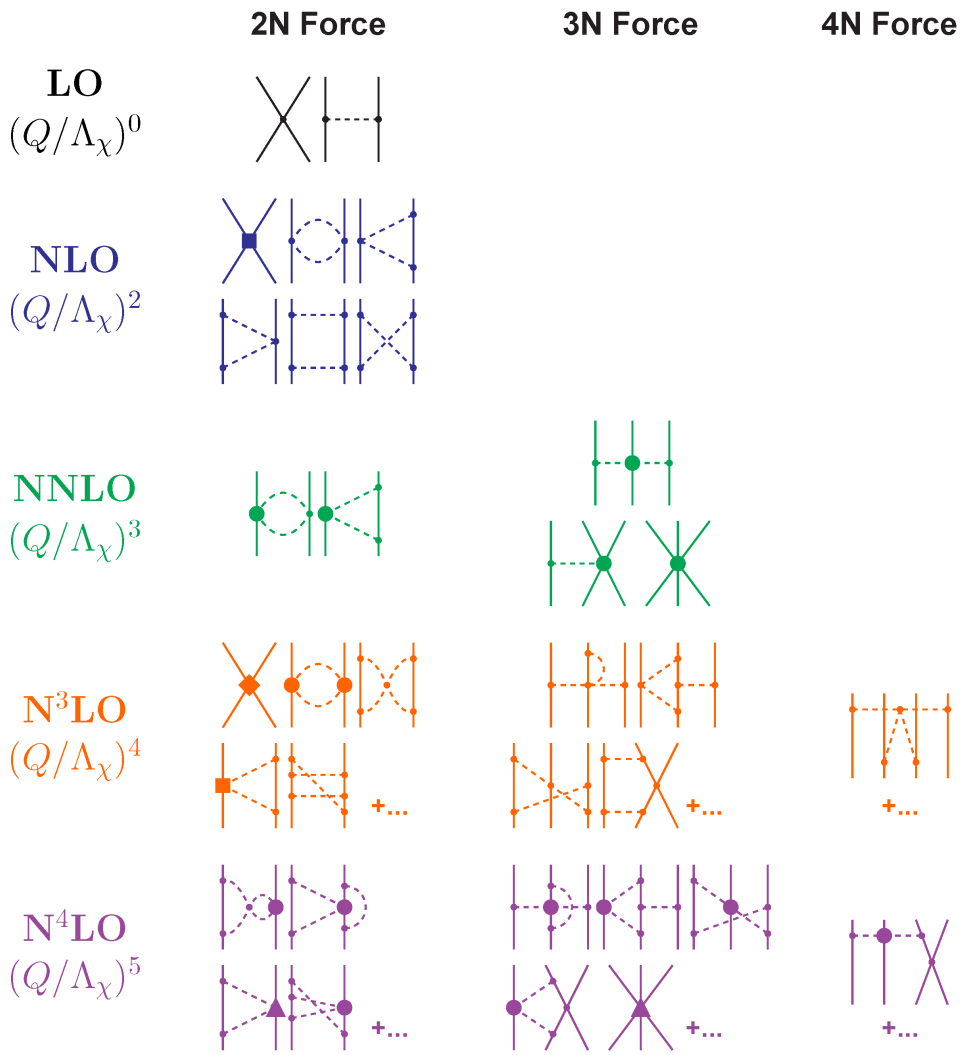
effective description of nuclear interactions → EFT power counting

# Chiral EFT of Nuclear Interactions

## Effective Field Theory (EFT)

1. Identify energy scales:
   'breakdown scale' $\Lambda_\chi \sim 1$ GeV
   'soft scale' $Q < \Lambda_\chi$,
2. Identify symmetries:
   $SU(2)_L \times SU(2)_R \supset SU(2)_V$
   Identify relevant degrees of freedom:
   nucleons $N$, pions $\pi$, (...)
3. General Lagrangian consistent with symmetries: $\mathscr{L}_{\text{EFT}}(N, \pi)$
   $\rightarrow$ 'Low-Energy Constants' $\{c_i\}$
4. **Renormalization, LEC Fixing, Power Counting**

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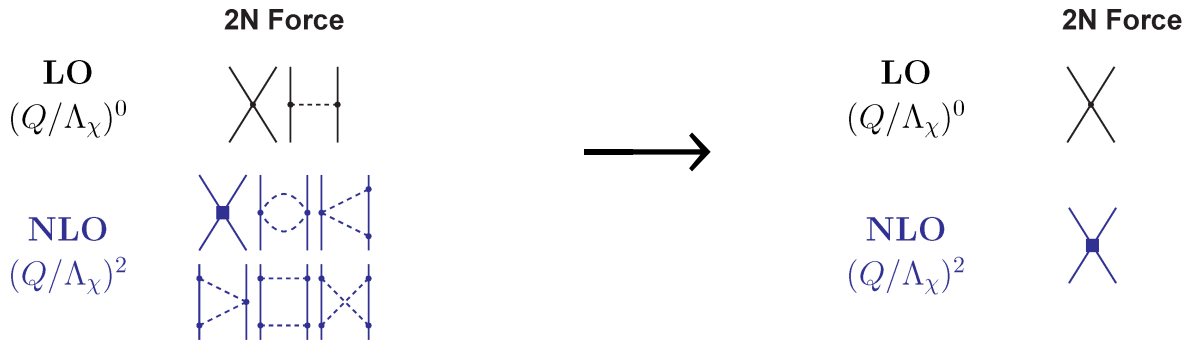
**Part 1: Dilute Fermi Gas**

EFT without pions

Higher-order many-body calculations in pionless EFT




**Part 2: Nuclear Matter**

Chiral EFT and nuclear potentials

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# Pionless EFT (I): Lagrangian, Renormalization

## Lagrangian

$$\mathscr{L}_{\text{EFT}}[\psi] = \psi^\dagger \left[ i\partial_t + \frac{\vec{\nabla}^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 + \frac{C_2}{16} \left[ (\psi\psi)^\dagger (\psi \overleftrightarrow{\nabla}^2 \psi) + h.c. \right]$$
$$+ \frac{C_2'}{8} (\psi \overleftrightarrow{\nabla} \psi)^\dagger \cdot (\psi \overleftrightarrow{\nabla} \psi) - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \ldots$$

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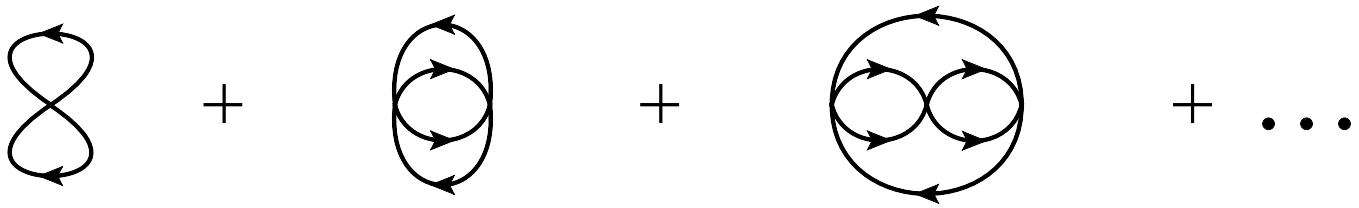

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- particle-particle bubbles (MBPT): $\mathcal{I}_{\text{MBPT}} = \frac{1}{2\pi} \fint_{k_F}^\Lambda d^3q \, \frac{q^0}{q^2 - p^2} =$

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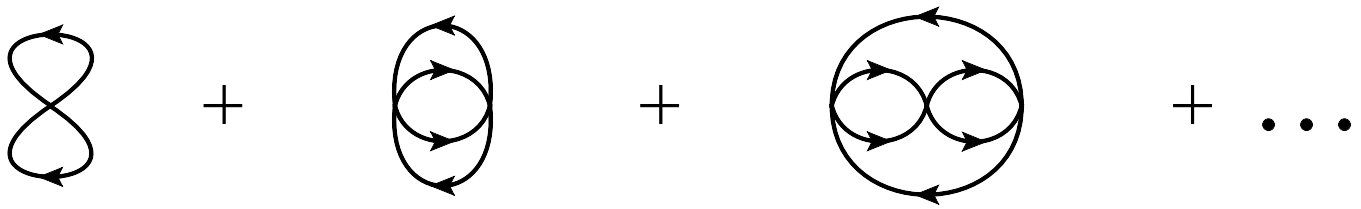

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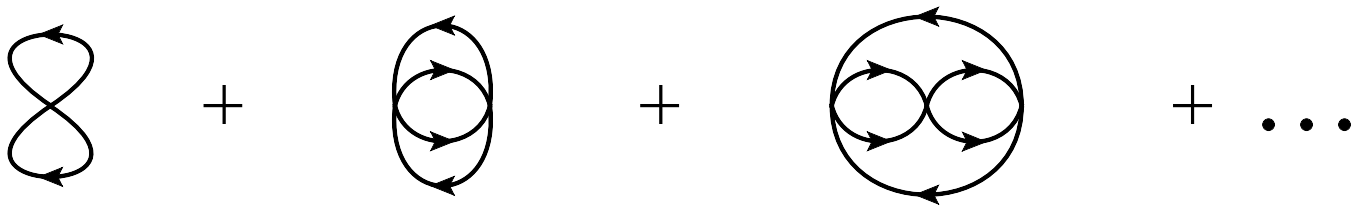

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$\Rightarrow$ same counterterms regularize NN and MBPT! Cutoff independent results for $\Lambda \to \infty$

# Pionless EFT (II): LEC Fixing & Power Counting, $k_{\mathrm{F}}$ Expansion

**LEC Fixing:** match two-body LECs to effective-range expansion

$$C_0 = \frac{4\pi a_s}{M}, \qquad C_2 = C_0 \frac{a_s r_s}{2}, \qquad C_2' = \frac{4\pi a_p^3}{M}$$

- **Power counting** for natural LECs: $|C_0| \sim 1/\Lambda_\chi$, $|C_2| \sim |C_2'| \sim 1/(\Lambda_\chi)^3$

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- EFT power counting and MBPT($n$) in direct correspondence, $T = 0$: MBPT($n$) $\sim k_F^n$

Fermi-momentum expansion for ground-state energy density $E(k_F)$

$$E(k_F) \simeq \varrho \frac{k_F^2}{2M}\Bigg[\frac{3}{5} + (g-1)\Bigg\{\frac{2}{3\pi}k_F a_s + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a_s)^2 + \Big(0.0755732 + 0.0573879(g-3)\Big)(k_F a_s)^3\Bigg\} + \frac{1}{10\pi}(g-1)(k_F a_s)^2 k_F r_s + \frac{1}{5\pi}(g+1)(k_F a_p)^3 + E_4(k_F) + \mathcal{O}(k_F^5 \ln|k_F|)\Bigg]$$

H.-W. Hammer,R.J. Furnstahl; NPA 678 (2000)

N. Kaiser; NPA 860 (2011), EPJA 53 (2017)

- MBPT(1): 1 diag, MBPT(2)=1(2), MBPT(3)=3(15), MBPT(4)=33(..), MBPT(5)=668(..)

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- Logarithmic divergences, first in MBPT(4): $\sim (g-2)\,(k_F a_s)^4 \ln|k_F a_s|$
  $\rightarrow$ Pauli blocked for $g = 2$
  $\rightarrow$ $g \geq 2$: $D_0(\Lambda)$ counterterm, $D_0(\Lambda_0)$ needs to be fixed by 3N (or many-body) data

# Pionless EFT (IV): Contributions to $(k_F a_s)^4$ Term

Numerical calculations carried out using novel Monte-Carlo Framework for MBPT

Drischler, Hebeler, Schwenk; "Chiral interactions up to N3LO and nuclear saturation ", arXiv:1710.08220 (2017)

Table : Diagrams with $*$ ($**$) have power (logarithmic) divergencies.

| diagram | type | $g$ factor | *value* |
|---|---|---|---|
| I1$^*$ | *pp* ladder | 1 | +0.0383 |
| I2$^*$+I5$^*$ | *pp-hh* ladder | 1 | +0.0099 |
| I3+I4$^*$ | *pp-hh* ladder | 1 | +0.0050 |
| I6 | *hh* ladder | 1 | -0.0007 |
| IA1 | *ph* ladder (ring) | $g(g-3)+4$ | -0.0037 |
| IA2 | *ph* ladder | $g(g-3)+4$ | -0.0033 |
| IA3 | *ph* ladder | $g(g-3)+4$ | -0.0017 |
| II1$^*$+II2$^*$ | skeleton | $g-3$ | +0.0292 |
| II3+II4 | skeleton | $g-3$ | -0.0034 |
| II5$^{**}$ | skeleton | $g-3$ | +0.0617 |
| II6$^{**,*}$ | skeleton | $g-3$ | -0.0080 |
| II7+II12 | skeleton | $g-3$ | +0.0039 |
| II8+II11 | skeleton | $g-3$ | +0.0077 |
| II9 | skeleton | $g-3$ | -0.0010 |
| II10 | skeleton | $g-3$ | -0.0003 |
| IIA1$^{**}$ | skeleton | $3g-5$ | +0.0619 |
| IIA2+IIA4 | skeleton | $3g-5$ | +0.0041 |
| IIA3 | skeleton | $3g-5$ | -0.0005 |
| IIA5 | skeleton | $3g-5$ | +0.0035 |
| IIA6 | skeleton | $3g-5$ | +0.0033 |
| III1$^{**,*}$ | 2-2 non-skeleton | $g-1$ | -0.0123 |
| III2 | 2-2 non-skeleton | $g-1$ | -0.0032 |
| III7+III8$^*$ | 2-2 non-skeleton | $g-1$ | -0.0357 |
| III9+III10 | 2-2 non-skeleton | $g-1$ | +0.0049 |

I1-I6: N. Kaiser; "Resummation of fermionic in-medium ladders to all orders", NPA 860 (2011)

Regular diagrams: G.A. Baker; "Singularity Structure of the Perturbation Series for the Ground-State Energy of a Many-Fermion System", RMP 43 (1971)

# Pionless EFT (V): Convergence of the Fermi-Momentum Expansion

**$g = 2$, set $a_p = r_s = 0$**

$$E/E_0 \simeq 1 + 0.35368 k_F a_s + 0.18554 (k_F a_s)^2 + 0.03031 (k_F a_s)^3 - 0.0476(5)(k_F a_s)^4$$

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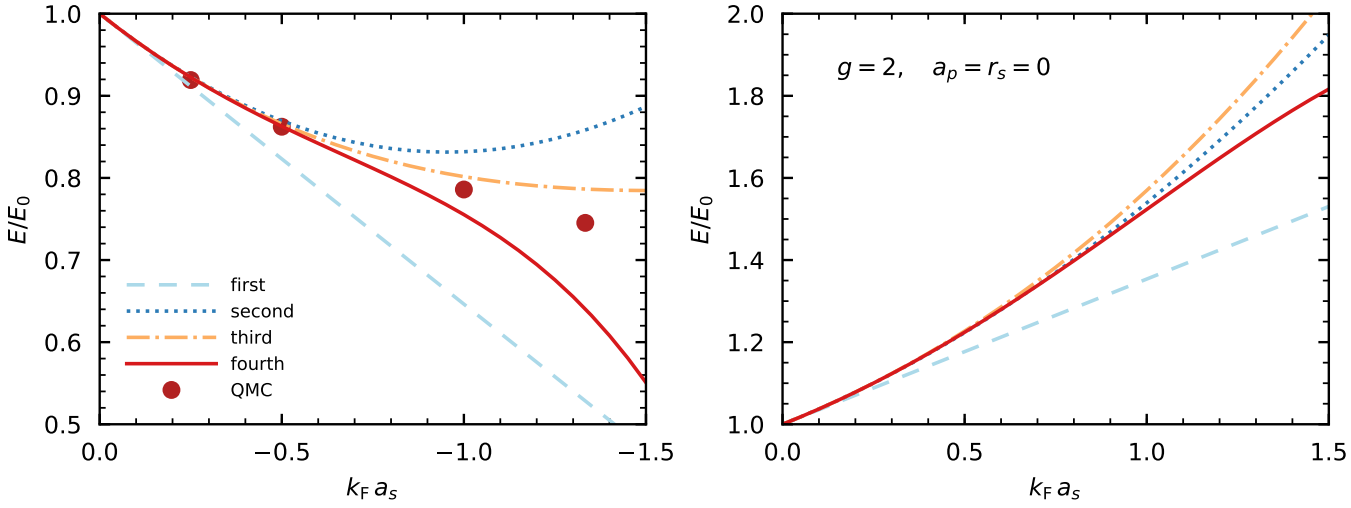


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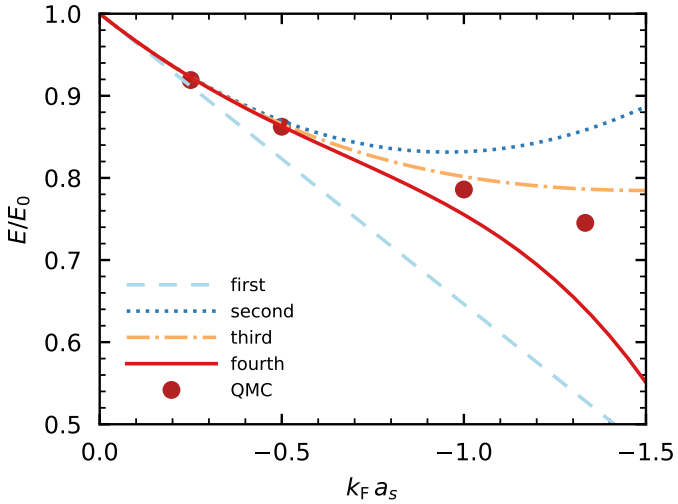


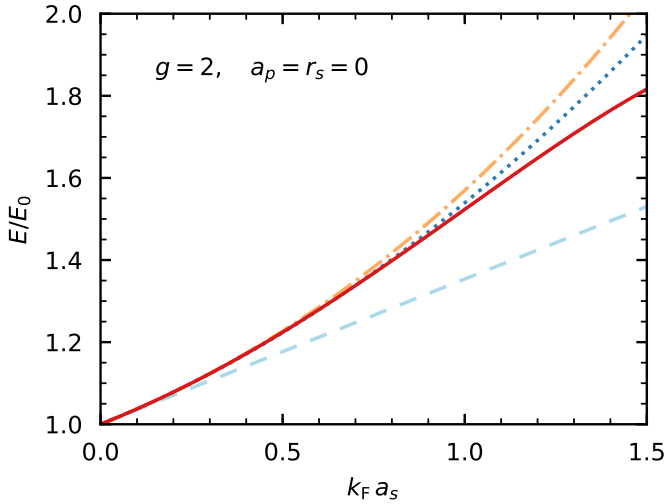


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**$k_F a_s$ expansion constitutes unique MBPT series — but in general MBPT series not unique!**

$$\textbf{MBPT:} \quad \mathcal{H} = \mathcal{T}_{\text{kin}} + \mathcal{V} = \underbrace{(\mathcal{T}_{\text{kin}} + \mathcal{U}_{\text{HF}})}_{\substack{\text{reference system} \\ \text{“mean-field theory”}}} + \underbrace{(\mathcal{V} - \mathcal{U}_{\text{HF}})}_{\substack{\text{perturbation} \\ \text{“correlations”}}}$$

- momentum independent interaction ($\sim a_s$) $\rightarrow U_{\text{HF}} =$ const., no effect
- chiral EFT interactions $\rightarrow$ perturbation series depends on reference Hamiltonian!

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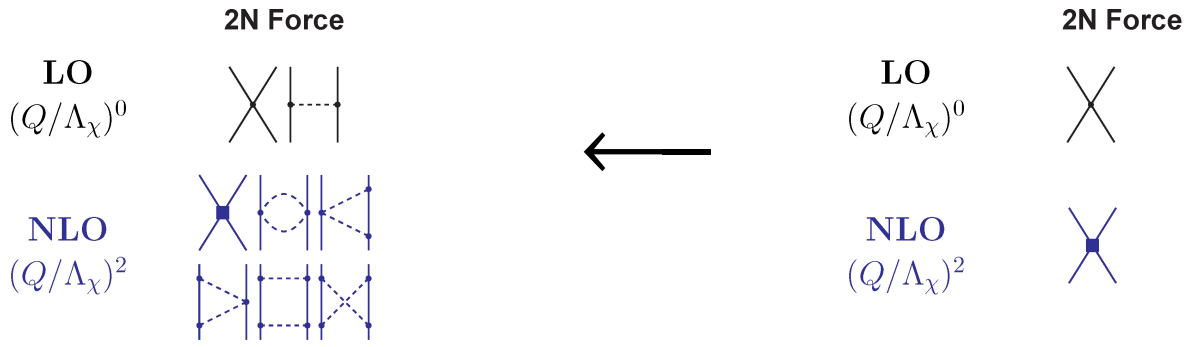


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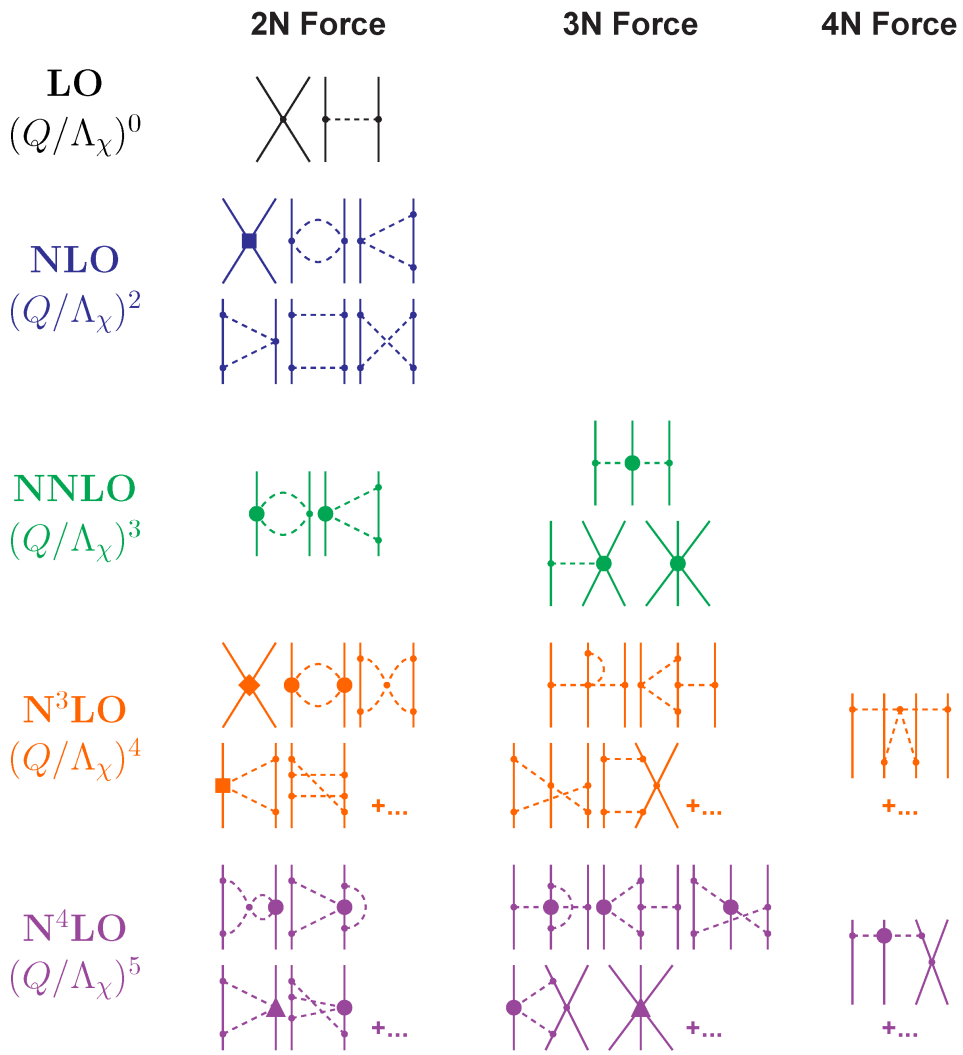


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nuclear potentials:

$V_{NN}(n,\Lambda,c_i(n,\Lambda))$,
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**Uncertainties via**: EFT orders, cutoff variation, fit ambiguities

# Renormalization, LEC Fixing, Power Counting

**Simplest Case** (e.g., EFT for Photon-Photon Scattering)

- Renormalization; e.g., subtraction of divergencies in perturbation theory, $\Lambda \to \infty$
- LEC Fixing: 'bare' LECs $c_i$ matched to fundamental theory
- Power Counting: $\sim (Q/\Lambda_\chi)^n$ for observables (requires natural $c_i$'s)

**Nuclear physics:** bound states + large scattering lengths $\to T_{NN,3N,\ldots}$ nonperturbatively!

**'Potential EFT'** (Standard Approach)

Weinberg; "Nuclear forces from chiral lagrangians" Phys.Lett.B (1990)

- Regularization; e.g., sharp cutoff $\Lambda$
- $c_i(n,\Lambda)$ fit to data
- Power Counting: $\sim (Q/\Lambda_\chi)^n$ for potentials

nuclear potentials:

$V_{NN}(n,\Lambda,c_i(n,\Lambda))$,
$V_{3N}(n \geq 3,\Lambda,c_i(n,\Lambda)),\ldots$

**Uncertainties via**: EFT orders, cutoff variation, fit ambiguities

- **KSW approach:** PDS scheme, $C_0$ to all orders, otherwise perturbative
  Kaplan, Savage, Wise; "Two-nucleon systems from effective field theory" NPB 534 (1998)
- **NTvK approach:** renormalize 'potential EFT' via additional contacts at each order
  Nogga, Timmermans, van Kolck; "Renormalization of one-pion exchange and power counting", PRC 72 (2005)

# Chiral Potentials: Cutoff Variation and Fit Ambiguities

## N3LO two-nucleon + N2LO three-nucleon potential

- nonlocal regulator $f(p,p') = \exp[-(p/\Lambda)^{2\nu}] - (p'/\Lambda)^{2\nu}]$
- low-momentum potentials ($\Lambda \lesssim 500$ MeV) required for MBPT convergence
- **"n3lo"**: $c_i$'s from fits to phase shifts, $c_D$ & $c_E$ from fits to $^3$H binding energy and $^3$H-$^3$He Gamow-Teller matrix element ($\rightarrow c_D$ issue!)

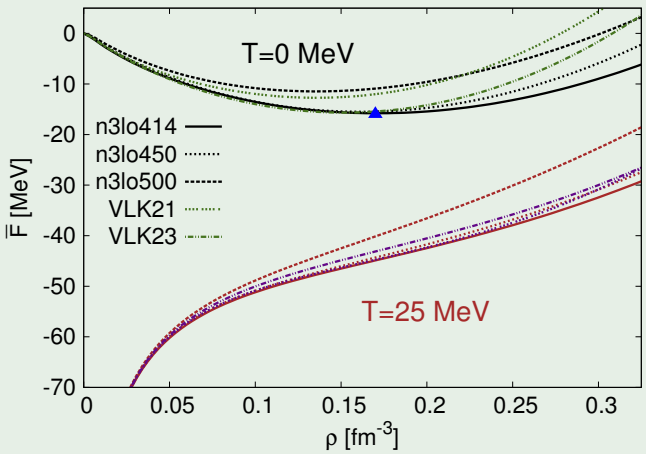
  Entem, Machleidt; PRC 68 (2003), Gazit; Phys.Lett.B 666 (2008), Coraggio, Holt *et al.*; PRC 87 (2013) + PRC 89 (2014)
- **"VLK"**: NN potential from RG evolution of n3lo500, Nijmegen values for 3N $c_i$'s, $c_D$ & $c_E$ from fits to $^3$H, $^3$He, $^4$He binding energies

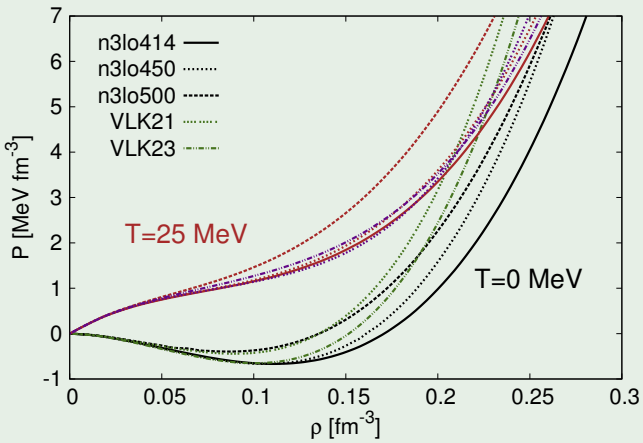
  Bogner, Furnstahl, Schwenk, Nogga; NPA 763 (2005), Nogga, Bogner, Schwenk; PRC 70 (2004)

| | $\Lambda$ (fm$^{-1}$) | $\nu$ | $c_E$ | $c_D$ | $c_1$ (GeV$^{-1}$) | $c_3$ (GeV$^{-1}$) | $c_4$ (GeV$^{-1}$) |
|---|---|---|---|---|---|---|---|
| n3lo414 | 2.1 | 10 | -0.072 | -0.4 | -0.81 | -3.0 | 3.4 |
| n3lo450 | 2.3 | 3 | -0.106 | -0.24 | -0.81 | -3.4 | 3.4 |
| n3lo500 | 2.5 | 2 | -0.205 | -0.20 | -0.81 | -3.2 | 5.4 |
| VLK21 | 2.1 | $\infty$ | -0.625 | -2.062 | -0.76 | -4.78 | 3.96 |
| VLK23 | 2.3 | $\infty$ | -0.822 | -2.785 | -0.76 | -4.78 | 3.96 |

# Second-Order MBPT with “n3lo” and “VLK” Potentials

## Isospin-symmetric nuclear matter: $\delta := (\rho_n - \rho_p)/\rho = 0$, $Y := \rho_p/\rho = 1/2$




- saturation point: n3lo414, n3lo450, ~~n3lo500~~, ~~VLK21~~, VLK23 (n3lo500 nonperturbative?)
- VLK21 & VLK23: pressure isotherm crossing (large $c_3$ artifact?)

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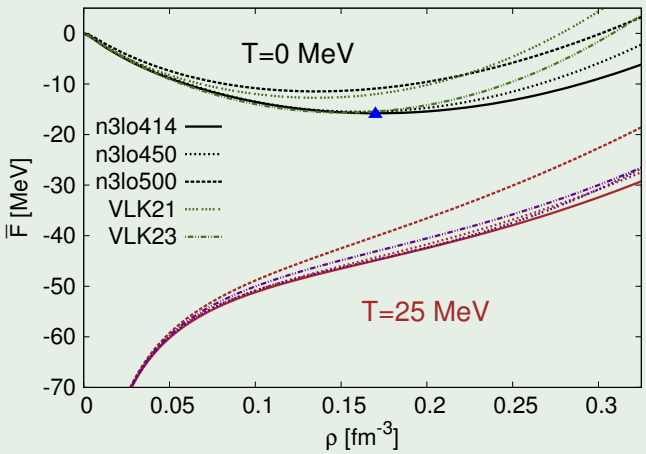


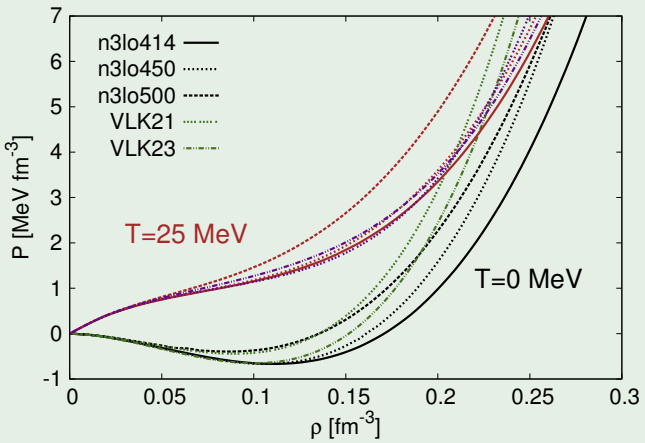


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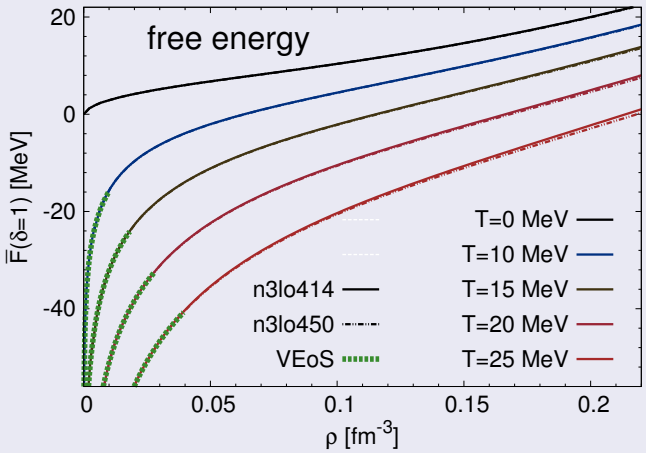
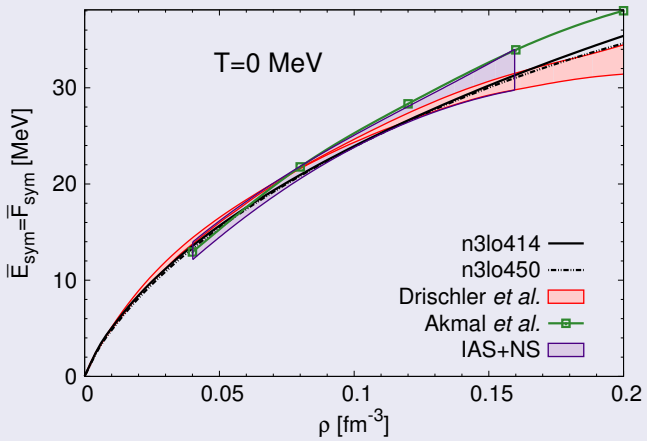
## Pure neutron matter ($\delta = 1$, $Y = 0$) $\bar{E}_{\text{sym}} := \bar{E}(\delta = 1) - \bar{E}(\delta = 0)$



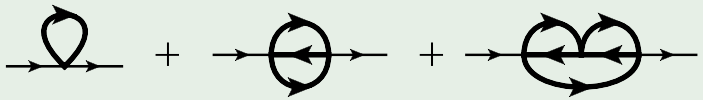

Wellenhofer, Holt, Kaiser, Weise; PRC 89 (2014)

Wellenhofer, Holt, Kaiser; PRC 92 (2015)

# Formalism for Improved MBPT Calculations

Two formalisms in MBPT: **Feynman** (Fourier/Matsubara space) vs. **Goldstone** ("direct")

## Self-consistent propagators in Feynman formalism

$\Sigma(\zeta_\ell) =$  $\equiv \mathcal{G}_r(\zeta_{\ell'}) = \int \frac{d\omega}{2\pi} \frac{A_r(\omega)}{\zeta_{\ell'} - \omega}$

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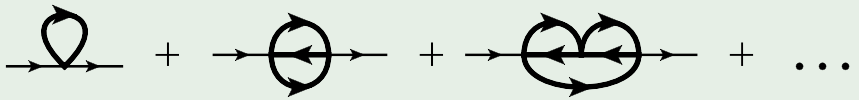
$\Sigma(\zeta_\ell) =$  $\equiv \mathcal{G}_r(\zeta_{\ell'}) = \int \frac{d\omega}{2\pi} \frac{A_r(\omega)}{\zeta_{\ell'} - \omega}$

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## Self-consistent SP potential $\mathcal{U} = \sum_r U_r(\{\varepsilon_i\})\, a_r^\dagger a_r$ in Goldstone formalism

$$\mathcal{H} = \underbrace{(\mathcal{T}_{\text{kin}} + \mathcal{U})}_{\substack{\text{reference system } \mathcal{T} \\ \text{"mean-field theory"}}} + \underbrace{(\mathcal{V} - \mathcal{U})}_{\substack{\text{perturbation} \\ \text{"correlations"}}}, \quad \text{with } \varepsilon_k = k^2/(2M) + U_r(\{\varepsilon_i\}) \text{ self-consistently}$$

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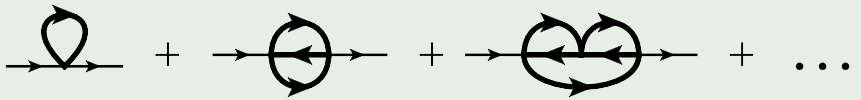
$\Sigma(\zeta_\ell) =$  $\equiv \mathcal{G}_r(\zeta_{\ell'}) = \int \frac{d\omega}{2\pi} \frac{A_r(\omega)}{\zeta_{\ell'} - \omega}$

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- usual choice: $U_r = \dfrac{\delta \Omega_1}{\delta n_r}$, MBPT(n) with fixed spectrum
- (suggested) generalization: MBPT(n) with $U_{n;r} = \dfrac{\delta \tilde{\Omega}^{*,**,***}_{n,\text{normal}}}{\delta n_r}$

  $\rightarrow$ cancellation of certain classes of diagrams to all orders

  $\rightarrow$ statistical-quasiparticle relations, $F(T,\mu) \xrightarrow{T\to 0} E(k_{\text{F}})$

"At each new order, not only is new information about 'correlations' included, but this information automatically improves the reference point."

Wellenhofer; arXiv:1804.03040

# Summary

## Pionless EFT (Natural LECs) and Dilute Fermi Systems

- Exact cutoff independence for $\Lambda \to \infty$, two-body LECs $c_i$ matched to scattering parameters, EFT power counting for observables
- **Uncertainties: EFT orders**
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## Chiral EFT Potentials and Nuclear Matter

- Finite cutoff $\Lambda$, $c_i(n, \Lambda)$ via fits to (few-body) data, EFT power counting for potentials
- Few-body systems nonperturbative, MBPT for nuclear matter
- MBPT convergence studies require self-consistent renormalization!
- **Uncertainties: (U1) EFT orders, (U2) cutoff variation, (U3) fit ambiguities**

# Questions

**Uncertainties: (U1) EFT orders, (U2) cutoff variation, (U3) fit ambiguities**

- Expectation for uncertainties, should **U3,U2 < U1** ?
- What is the status/prospect on U3 ?

**Treatment of many-body constraints (saturation point, binding energies, . . .)**

- Postselection of EFT potentials vs. LECs fit to many-body observables
- Conceptual issues, impact of postselection/fit on extrapolation error-bands?

**Assessment of 'nonstandard' organization schemes for many-body calculations**

- KSW approach → in-medium $\chi$PT, but how fix LECs?
- NTvK approach(es) → what is the benefit/relevance of this for MBPT?

Thank you for your attention!

Special thanks to:

My collaborators: Christian Drischler, Kai Hebeler, Jeremy Holt, Norbert Kaiser, Achim Schwenk, Wolfram Weise

The organizers: Andreas Ekström, Jason Holt, Joel Lynn, Ingo Tews

# Backup: Leading Logarithmic Divergencies in Pionless EFT

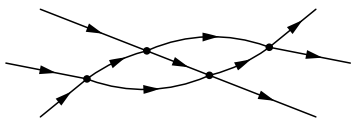
**To extract divergent part, set bounded integration variables to zero**

$$\mathrm{D1}^{\mathrm{div}} = (C_0)^4 \xi' \int_{\eta}^{\Lambda/k_F} d^3\alpha \frac{1}{\alpha^2} \int_{\eta}^{\Lambda/k_F} d^3\gamma \frac{1}{(\alpha^2+\gamma^2)^2} = \frac{(C_0)^4 \xi'}{2} \mathrm{Ti}_2(\Lambda/(k_F\eta)) + \mathcal{O}(1)$$

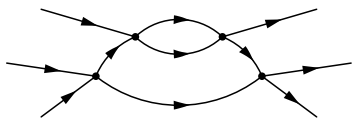
$$= -(C_0)^4 \xi \ln(\Lambda/k_F) + \mathcal{O}(1)$$

$$\mathrm{Ti}_2(x) = \int_0^x dy \frac{\arctan y}{y} = \mathrm{Ti}_2(1/x) + (\pi/2)\mathrm{sgn}(x) \ln|x|$$

$$\mathrm{Ti}_2(0) = 0$$



D1



D2

**Renormalization via three-body coupling $D_0$**

$$\text{RGE:} \quad \frac{\partial}{\partial \Lambda}\left[-(C_0)^4 \xi_{3N} \ln \Lambda + D_0(\Lambda)\right] = 0$$

$$\Rightarrow \quad D_0(\Lambda) = D_0(\Lambda_0) + (C_0)^4 \xi_{3N} \ln|\Lambda/\Lambda_0|$$

$$\Rightarrow \quad E_4^{\mathrm{reg}} = \overbrace{E_4 + (C_0)^4 \xi \ln(\Lambda/k_F)}^{\text{finite,}} + E_1^{D_0(\Lambda_0)} + (C_0)^4 \xi \ln|k_F/\Lambda_0|$$

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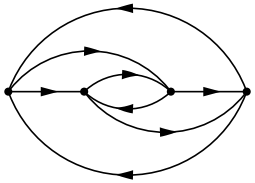
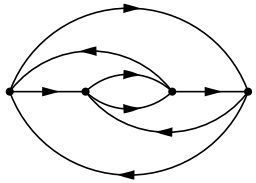
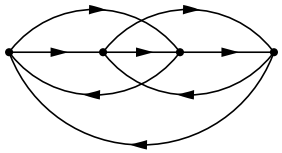


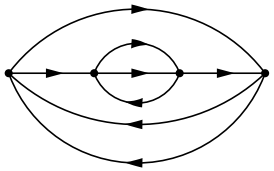
II5



II6



IIA1



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