High-Order Nuclear Matter Calculations
with
Chiral EFT Interactions

Corbinian Wellenhofer
(TU Darmstadt)

Progress in *Ab Initio* Techniques in Nuclear Physics

TRIUMF Vancouver BC Canada

March 1, 2019

TECHNISCHE
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SFB 1245

(Towards)

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Drischler, Hebeler, Schwenk: PRL 122 (2019)

Wellenhofer, Drischler, Schwenk: arXiv 1812.08444

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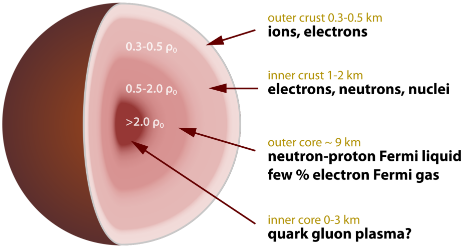
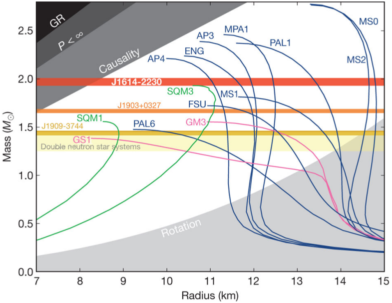
The Nuclear-Many-Body Problem





Demorest *et al.*; "... two solar mass neutron star", Nature (2010)

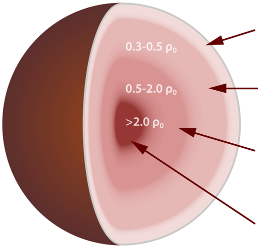
Nuclear saturation density: $\rho_0 \approx 0.16\,\mathrm{fm}^{-3}$, $k_{\mathrm{F},0} \approx 1.33\,\mathrm{fm}^{-1} = 262\,\mathrm{MeV}$

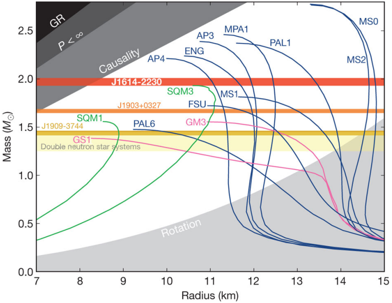
TOV equation:

$$\frac{\mathrm{d}P(r)}{\mathrm{d}r} = -\frac{\mathcal{G}}{r^2c^2}\left[E(r) + P(r)\right]\left[M(r) + 4\pi r^3\frac{P(r)}{c^2}\right] \times \left[1 - \frac{2\mathcal{G}M(r)}{c^2 r}\right]^{-1} .$$

EOS $P(E)$ determines mass-radius relation of neutron star ($T = 0$)

The Nuclear-Many-Body Problem





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Task: Compute Nuclear Matter Properties with Controlled Uncertainties

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

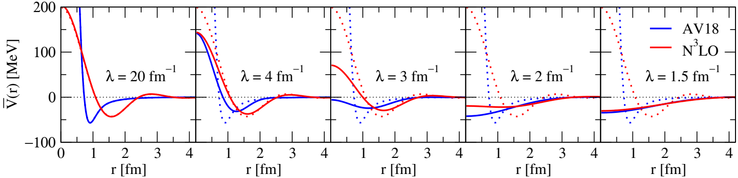
Uncertainties governed by:

many-body method (→ **MBPT**), effective description of nuclear interactions

Nuclear Interactions

Modern methods: **effective field theory**, **RG methods**

$\rightsquigarrow$ many-body problem *not* intrinsically nonperturbative, MBPT applicable ?



Furnstahl; "The renormalization group in nuclear physics", Nucl. Phys. B Proc. Suppl. (2012)

Hard core not observable! → can generate 'perturbative' nuclear potentials

Unitary transformation (SRG): $H_\lambda = U_\lambda H U_\lambda^\dagger$

$$\frac{dV_\lambda}{d\lambda} = [[\underbrace{T_{\text{kin}}}_{\sim a^\dagger a}, \underbrace{H_\lambda}_{\sim a^\dagger a^\dagger aa}], H_\lambda] = \sum a^\dagger a^\dagger aa + \sum a^\dagger a^\dagger a^\dagger aaa \quad \rightarrow \text{induced 3N forces}$$

Weinberg eigenvalue analysis with V_λ → MBPT ladders convergent!

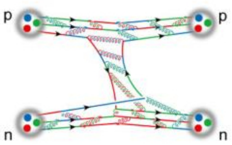
Bogner, Furnstahl, Schwenk; "From low-momentum interactions to nuclear structure", Prog.Part.Nucl.Phys.65 (2010)

But: MBPT much more than ladders; → test order-by-order convergence!

Modern Theory of Nuclear Interactions

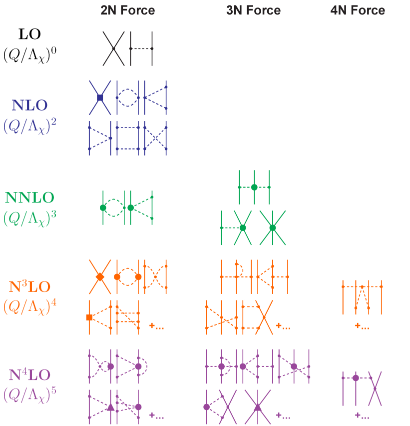
Low-Energy Quantum Chromodynamics

- Strongly-coupled, confinement
- Nonlinear realization of $SU(2)_L \times SU(2)_R$



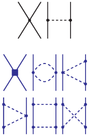
Chiral EFT of Nuclear Interactions

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 effective degrees of freedom:
   nucleons N, pions π, $(\ldots)$
3. General Lagrangian consistent with symmetries: $\mathscr{L}_{\mathrm{EFT}}(N, \pi)$
   → 'Low-Energy Constants' $\{c_i\}$
4. **Renormalization, LEC Fixing, Power Counting, Uncertainty Analysis**



Machleidt; "Chiral symmetry and the NN interaction, Symm. 8 (2016)

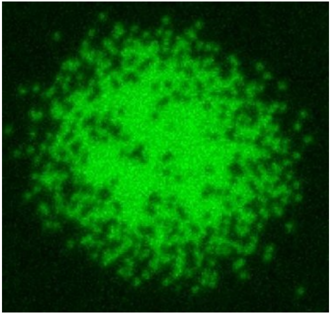
Part 1: Short-Ranged EFT & Dilute Fermi Gas

	2N Force			2N Force
LO $(Q/\Lambda_\chi)^0$		$\longrightarrow$	LO $(Q/\Lambda_\chi)^0$	
NLO $(Q/\Lambda_\chi)^2$			NLO $(Q/\Lambda_\chi)^2$	

Part 2: Chiral EFT & Nuclear Matter

Fermion Scattering at Very Low Energies: ERE

Goal: calculate ground-state energy $E(k_F)$ of dilute gas of interacting fermions



Two-Body Interactions at Very Low Energies → Effective-Range Expansion (ERE)

$$T(p, \cos\theta) = \frac{4\pi}{M} \sum_L \frac{2L+1}{p\cot\delta_L - ip} P_L(\cos\theta)$$

$p\cot\delta_0 = -\frac{1}{a_s} + \frac{1}{2} r_s p^2 + \ldots$ $\qquad$ $p\cot\delta_1 = -\frac{3}{p^2 {a_p}^3} + \ldots$ $\qquad$ scattering lengths $a_{s,p}$

effective range r_s

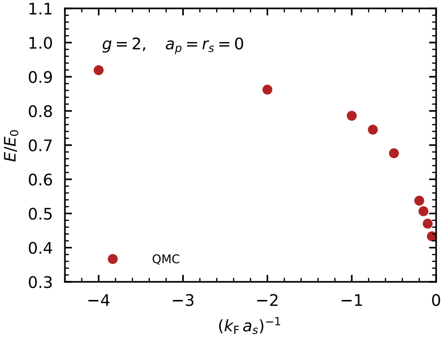
- e.g., hard-sphere potential $V(r) = \infty$ for $r > R$: $\quad a_s = 3r_s/2 = a_p = 3R/2$

Dilute Fermi Gas from QMC

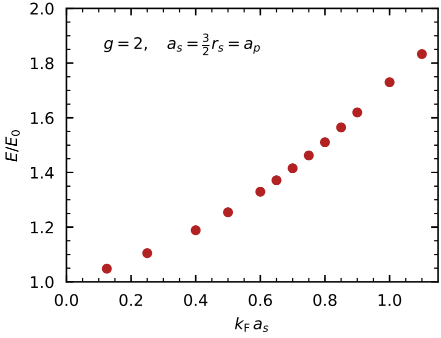
Goal: calculate ground-state energy $E(k_\mathrm{F})$ of dilute gas of interacting fermions

Quantum Monte-Carlo (QMC) Computations with Potential $V(r)$

- start with trial many-body wave function $\psi = \sum_i a_i \phi_i$
- imaginary-time evolution $\psi(\tau) = \sum_i e^{-E_i\tau}\, a_i\phi_i \longrightarrow e^{-E_0\tau}\, a_0\phi_0$
- compute $\psi(R, \tau_0 + \Delta\tau) = \int_R \langle R|\, e^{-H\Delta\tau}\, |R'\rangle\, \psi(R, \tau_0)$ stochastically



Gandolfi, Gezerlis, Carlson; Ann. Rev. Nucl. Part. Sci. 65 (2015)



Pilati, Bertaina, Giorgini, Troyer, PRL 105 (2010).

Unitary Fermi Gas $a_s \to \infty$: $E(k_\mathrm{F}) = \xi E_0(k_\mathrm{F})$, Bertsch parameter $\xi \approx 0.38$

EFT for Dilute Fermi Gas (I): Lagrangian, Renormalization

Goal (EFT): derive expression for $E(k_{\rm F}; a_s, r_s, a_p, \ldots)$

Lagrangian

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

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Renormalization

- divergent loop integrals (NN): $\mathcal{I}_{\psi\psi} = \frac{1}{2\pi}\int_0^\Lambda d^3q \, \frac{q^0}{q^2 - p^2 - i\epsilon} = 2\Lambda + i\pi p + \mathcal{O}(\Lambda^{-1})$
- particle-particle ladders (MBPT): $\mathcal{I}_{\mathrm{MBPT}} = \frac{1}{2\pi}\fint_{k_\mathrm{F}}^{\Lambda} d^3q \, \frac{q^0}{q^2 - p^2} =$

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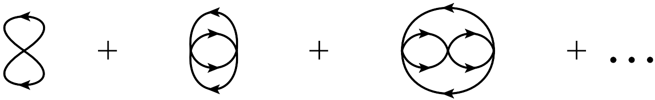

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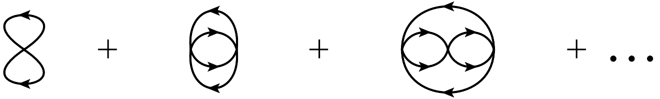

Renormalization

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- particle-particle bubbles (MBPT): $\mathcal{I}_{\rm MBPT} = \mathcal{I}_{\rm fin} + \frac{1}{2\pi}⨍_0^\Lambda d^3q \, \frac{q^0}{q^2 - p^2} = 2\Lambda + \mathcal{I}_{\rm fin} + \mathcal{O}(\Lambda^{-1})$

$\Rightarrow$ same counterterms renormalize NN scattering and MBPT! ($\sim$ medium is non-UV effect)

EFT for Dilute Fermi Gas (II): LEC Fixing & Power Counting, k_{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) $\sim k_\mathrm{F}^n$

Fermi-momentum expansion for ground-state energy density $E(k_\mathrm{F})$

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

T.D. Lee, C.N. Yang; Phys. Rev 105 (1957)
C. de Dominicis, P.C. Martin; Phys. Rev 105 (1957)
V.N. Efimov; Sov. Phys. JETP 22(1966)
H.-W. Hammer,R.J. Furnstahl; NPA 678 (2000)
N. Kaiser; NPA 860 (2011), EPJA 53 (2017)

C_0 contributions: MBPT(1,2): 1 diag, MBPT(3): 3 diags, MPT(4): 33 diags, MBPT(5): 668

Calculation of $E_4(k_\mathrm{F})$

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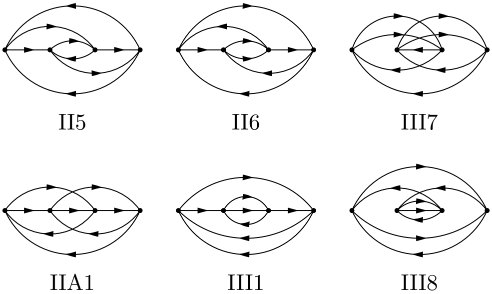


- I(1,2,4,5), II(1,2,6), III(1,8): UV power divergences: subladders, NN counterterms

- II(5,6), IIA1, III1: logarithmic UV divergences: 3N counterterm $g > 2$, cancel $g = 2$

  $\rightsquigarrow$ logarithmic term at fourth order $(g-2)(k_\mathrm{F} a_s)^4 \ln k_\mathrm{F}/\Lambda_0$

  V. N. Efimov, Phys. Lett. 15, (1965)

- III(1,2,8,10): infrared divergences: cancel in III(1+8) and III(2+10)

Calculation of $E_4(k_F)$

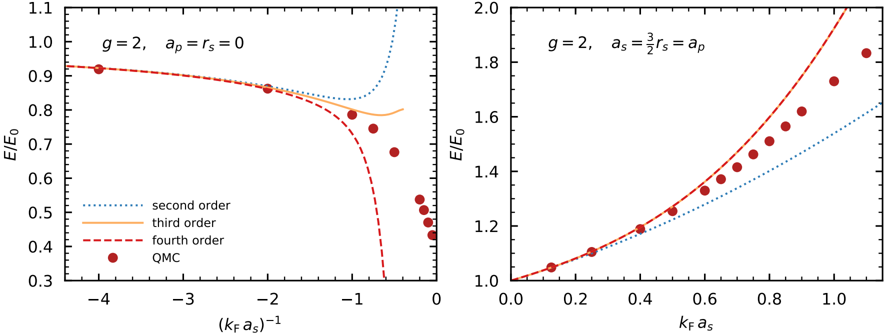
Table : Diagrams with $*$ ($**$) have power (logarithmic) divergences.
Diagrams with $***$ have infrared divergences.

diagram	g factor	value
I1*	1	$+0.0383115(0)$
I2*+I3+I4*+I5*	1	$+0.0148549(0)$
I6	1	$-0.0006851(0)$
IA1	$g(g-3)+4$	$-0.003623(1)$
IA2	$g(g-3)+4$	$-0.001672(1)$
IA3	$g(g-3)+4$	$-0.003343(1)$
II1*+II2*	$g-3$	$+0.058359(1)$
II3+II4	$g-3$	$-0.003358(1)$
II5**	$g-3$	$+0.0645(1)$
II6**,*	$g-3$	$-0.0265(2)$
II7+II12	$g-3$	$+0.003923(1)$
II8+II11	$g-3$	$+0.007667(1)$
II9	$g-3$	$-0.000981(1)$
II10	$g-3$	$-0.000347(1)$
IIA1**	$3g-5$	$+0.0647(1)$
IIA2+IIA4	$3g-5$	$+0.004122(1)$
IIA3	$3g-5$	$-0.000461(1)$
IIA5	$3g-5$	$+0.003542(1)$
IIA6	$3g-5$	$+0.003331(1)$
III1***,**,*+III7+III8***,*	$g-1$	$-0.0513(2)$
III2***+III9+III10***	$g-1$	$+0.001650(1)$
$(\text{II5+IIA1})_{g=2}$	1	$+0.00018(1)$
$(\text{II6+III1+III7+III8})^*_{g=2}$	1	$-0.0248(1)$
$\sum_{\text{diagrams},g=2}$	1	$-0.0425(1)$

I1-I6: pp-hh ladder diagrams

IA1-IA3: ring diagrams

k_F Expansion Results (I): Order-By-Order



k_F expansion for spin one-half fermions ($g = 2$)

$$g = 2: \qquad \frac{E(k_F)}{E_0} = 1 + \sum_{\nu=1}^{N} X_\nu \delta^\nu + o(\delta^N),$$

where X_n are determined by the ERE parameters. For $r_s = a_p = 0$ we have

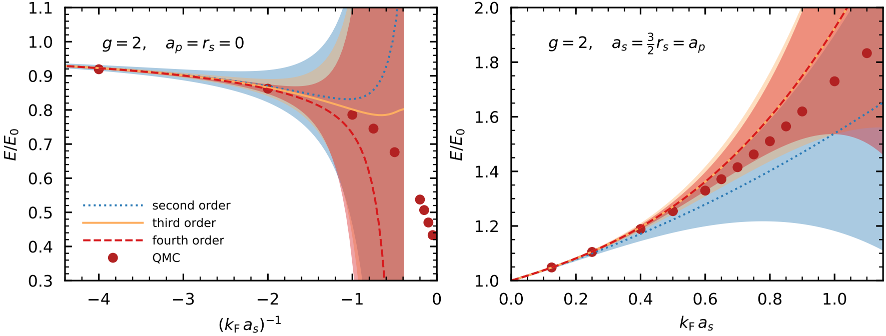
$$(X_1, X_2, X_3, X_4) = (+0.354, +0.186, +0.030, -0.071)$$

and for the hard-sphere gas (HS) with $a_s = 3r_s/2 = a_p$ we obtain

$$(X_1, X_2, X_3, X_4) = (+0.354, +0.186, +0.384, +0.001)$$

Uncertainties?

k_F Expansion Results (II): Uncertainty Systematics



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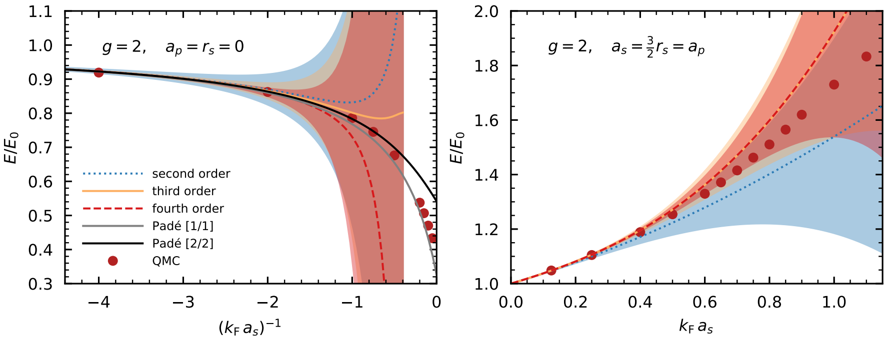
Uncertainty bands by setting $X_{N+1} = \pm \max[X_{\nu \le N}]$

k_F Expansion Results (III): Padé Approximants



k_F expansion for spin one-half fermions ($g = 2$)

$$\text{Padé}[N, M] = \frac{a_0 + a_1 x + a_2 x^2 + \ldots + a_N x^N}{1 + b_1 x + b_2 x^2 + \ldots b_m x^M}$$

Unitary Fermi Gas $a_s \to \infty$: $E(k_F) = \xi E_0(k_F)$, Bertsch parameter $\xi \approx 0.38$

→ diagonal Padé approximants

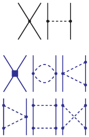
Padé$[1,1]$, $[2,2] \to \xi_n \in [0.33, 0.54]$, is consistent with the value $\xi_n = 0.45$ extracted from experiments with cold atomic gases Ku, Sommer, Cheuk, Zwierlein; Science 335 (2012)

Part 1: Short-Ranged EFT & Dilute Fermi Gas

2N Force

LO $(Q/\Lambda_\chi)^0$

NLO $(Q/\Lambda_\chi)^2$



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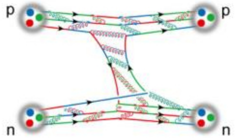

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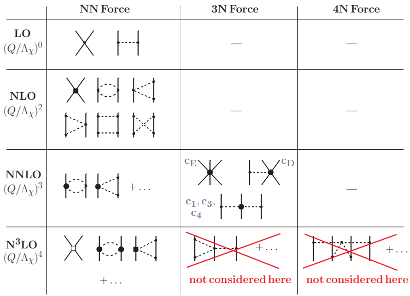

Renormalization, LEC Fixing, Power Counting

Perturbative EFT for Dilute Fermi Gas

- Perturbative renormalization: counterterms, $\Lambda \to \infty$
- LEC Fixing: 'bare' LECs c_i matched to ERE
- Power Counting: $\sim (Q/\Lambda_\chi)^n$ for observables (requires natural c_i's)

Uncertainties via: EFT orders

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

χEFT for Nuclear Matter: Chiral Nuclear Potentials (Standard Approach)

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

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

} nuclear potentials:

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

MBPT → low-momentum potentials: $\Lambda \lesssim 500$ MeV

Uncertainties via: EFT orders, cutoff variation, fit ambiguities

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- Perturbative renormalization: counterterms, $\Lambda \to \infty$
- LEC Fixing: 'bare' LECs c_i matched to ERE
- Power Counting: $\sim (Q/\Lambda_\chi)^n$ for observables (requires natural c_i's)

Uncertainties via: EFT orders

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

χEFT for Nuclear Matter: Chiral Nuclear Potentials (Standard Approach)

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

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

} nuclear potentials:

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

MBPT $\to$ low-momentum potentials: $\Lambda \lesssim 500$ MeV

Uncertainties via: EFT orders, cutoff variation, fit ambiguities

- Other approaches suggested; $\sim$ LO beyond NDA, NLO perturbatively

  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

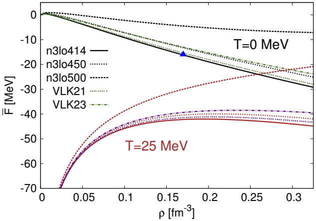
  Entem, Machleidt; PRC 68 (2003), Gazit; Phys.Lett.B 666 (2008), Coraggio, Holt *et al.*; PRC 87 (2013) + PRC 89 (2014)

- **"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

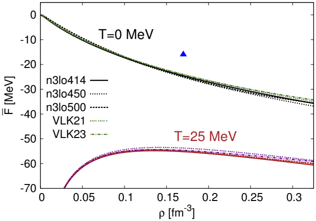
  Bogner, Furnstahl, Schwenk, Nogga; NPA 763 (2005), Nogga, Bogner, Schwenk; PRC 70 (2004)

	Λ (fm^{-1})	ν	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	∞	-0.625	-2.062	-0.76	-4.78	3.96
VLK23	2.3	∞	-0.822	-2.785	-0.76	-4.78	3.96

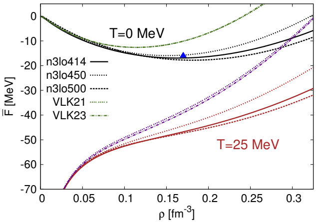
Free Energy of Symmetric Nuclear Matter, Free Spectrum $\varepsilon = k^2/(2M)$



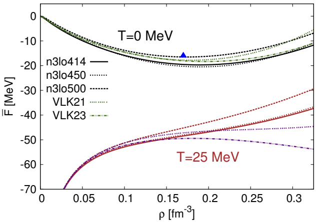
(a) NN first order, no 3N



(b) NN second order, no 3N



(c) NN second order, 3N first order



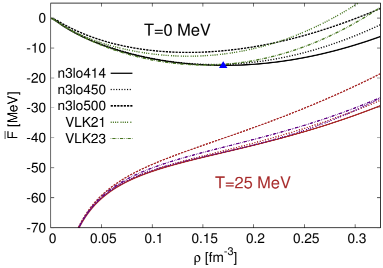
(d) NN second order, 3N second order

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

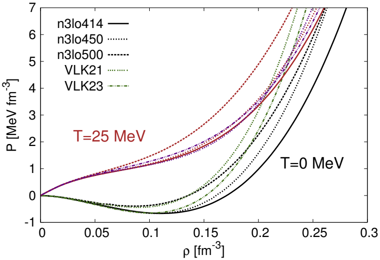
Wellenhofer, Holt, Kaiser; PRC 92 (2015)

Nuclear Matter EOS & 3N Forces

Free Energy + Pressure of Symmetric Nuclear Matter, HF Spectrum $\varepsilon = k^2/(2M) + U_{1,k}$



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



Wellenhofer, Holt, Kaiser; PRC 92 (2015)

- saturation point $(E_0, \rho_0) \approx (16\,\text{MeV}, 0.16\,\text{fm}^{-3})$ improved by U_1
  n3lo414, n3lo450, ~~n3lo500~~, ~~VLK21~~, VLK23 (n3lo500 nonperturbative?)
- VLK21 & VLK23: pressure isotherm crossing
  → negative thermal expansion coefficient $\alpha = \kappa_T \frac{dP}{dT}$ (~ water below 4°C)
  → thermal index $\Gamma = 1 + \frac{P(T)-P(0)}{\epsilon(T)-\epsilon(0)} < 1$, Free Fermi Gas: $\Gamma = 1.66$

Reference Hamiltonian beyond Hartree-Fock

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

with 'mean-field' $\mathcal{U} = \sum_{\boldsymbol{k}} U_{\boldsymbol{k}}\, a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} \rightarrow$

usually: Hartree-Fock mean-field: $U_{\boldsymbol{k}} = \dfrac{\delta \Omega_1}{\delta n_{\boldsymbol{k}}}$

Generalization: order-by-order renormalization of mean-field: $U_{\boldsymbol{k}} = \sum_{n=1}^{N} \dfrac{\delta \Omega^{*,**,***}_{n,\text{normal}}}{\delta n_{\boldsymbol{k}}}$

- thermodynamic relations of Fermi-liquid theory ($\sim$ Landau), valid $\forall T$

  $\varrho = \sum_{\boldsymbol{k}} n_{\boldsymbol{k}}, \quad S = -\sum_{\boldsymbol{k}} \big(n_{\boldsymbol{k}} \ln n_{\boldsymbol{k}} + \bar{n}_{\boldsymbol{k}} \ln \bar{n}_{\boldsymbol{k}} \big), \quad \frac{\delta E}{\delta n_{\boldsymbol{k}}} = \epsilon_{\boldsymbol{k}}$

- finite-T and $T = 0$ MBPT consistent: $F(T,\mu) \xrightarrow{T\to 0} E(k_{\mathrm{F}})$

- “*at each new order, not only is new information about interaction effects included, but this information automatically improves the reference point*”

  Wellenhofer; arXiv:1804.03040

- Fermi-liquid relations: $\rightsquigarrow$ phenomenological parametrizations, Sommerfeld
- Second-order contribution $U_{2,k}$ has significant effects! Holt, Kaiser; PRC 95 (2017)

- **But**: convergence rate with higher-order $\mathcal{U}$? $\rightarrow$ Current Work!

Summary

Part 1: Short-Ranged EFT & Dilute Fermi Systems

- Perturbative renormalization, two-body LECs c_i matched to scattering parameters, EFT power counting for observables
- **Uncertainties: EFT orders**
- Perturbation series for $E(k_{\mathrm{F}})$ evaluated up to fourth order, convergence for $k_{\mathrm{F}} a_s \lesssim 0.5$

Part 2: Chiral EFT & Nuclear Matter

(Standard Weinberg Approach)

- Finite cutoff Λ, $c_i(n, \Lambda)$ via fits to (few-body) data, EFT power counting for potentials
- Few-body systems nonperturbative, soft potentials → MBPT for nuclear matter
- **Uncertainties: (U1) EFT orders, (U2) cutoff variation, (U3) fit ambiguities**
  → 3N contributions appear to dominate uncertainties
- Temperature dependence of EOS sensitive to **3N contributions**
- **Current work: Towards UQ for Nuclear Matter Calculations**
  - Higher orders, test MBPT convergence
  - **3N contributions** beyond N2LO at MBPT(2)
  - MBPT with improved mean-field

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