From QED to EFT and from there to QMC

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TALENT/INT Course on
Nuclear forces and their impact on structure, reactions and astrophysics
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Basic definitions I

QED = Quantum Electrodynamics

EFT = Effective Field Theory

QMC = Quantum Monte Carlo

Why QED?

- It gives us the opportunity to go over some of the ideas from the other lectures in a different setting
- If you have already taken Quantum Field Theory, you will see familiar results expressed in a slightly unfamiliar manner
- If you haven't taken Quantum Field Theory, you can focus on the essential structures and use this as a set of signposts

Basic definitions II

Regularization Something we do to integrals

Basic definitions II

Regularization	Something we do to integrals
Renormalization	Something we do to parameters

Basic integrals I

A few fundamental results to keep in mind:

$$\int^{\Lambda} k \; dk \propto \Lambda^2$$

Quadratically divergent

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Logarithmically divergent

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Logarithmically divergent

$$\int^{\Lambda} \frac{dk}{k^2} \propto \frac{1}{\Lambda}$$

Convergent

Basic integrals II

Radial measure in *n*-dimensional euclidian space:

$$\int dk = 2\int dq$$

Plus-minus

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$$\int d^2k = 2\pi \int q \; dq$$

Circumference of a circle

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Surface area of a sphere

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You get the picture

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You get the picture

$$\int d^nk = \frac{n(\sqrt{\pi})^n}{\Gamma(1+n/2)} \int q^{n-1} \; dq$$

Handy generalization

QED with external field: traditional

QED Lagrangian: $\mathcal{L} = -\bar{\psi}\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + M\right)\psi - \frac{1}{4}F_{\mu\nu}F_{\mu\nu} + e_0 j_\mu A_\mu$

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Analogous to the non-relativistic $\psi^\dagger$

Dirac 4x4 matrices

Electromagnetic field tensor

$$F_{\mu\nu} \equiv \frac{\partial A_\nu}{\partial x_\mu} - \frac{\partial A_\mu}{\partial x_\nu}$$

Dirac current

$$j_\mu = i\bar{\psi}\gamma_\mu\psi$$

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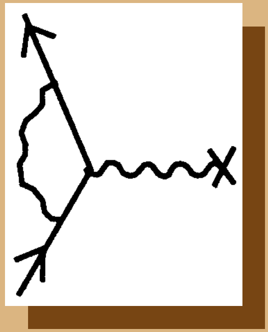
Vertex: (also Dirac spinors, external field, and non-integral terms)



$$\Lambda_\mu(k', k) = \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^2} \gamma_\lambda \frac{1}{i(\not{k}' - \not{q}) + M} \gamma_\mu \frac{1}{i(\not{k} - \not{q}) + M} \gamma_\lambda$$

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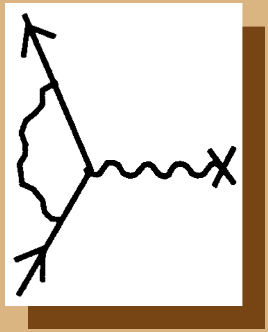

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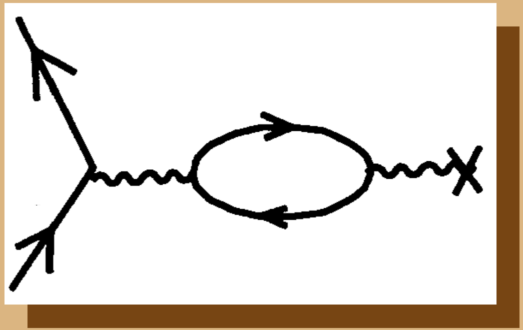
Vacuum polarization:



$$\Pi_{\mu\nu}(q) = \int \frac{d^4k}{(2\pi)^4}\mathrm{Tr}\frac{1}{i(\not{k} - \not{q}/2) + M}\gamma_\mu \frac{1}{i(\not{k} + \not{q}/2) + M}\gamma_\nu$$

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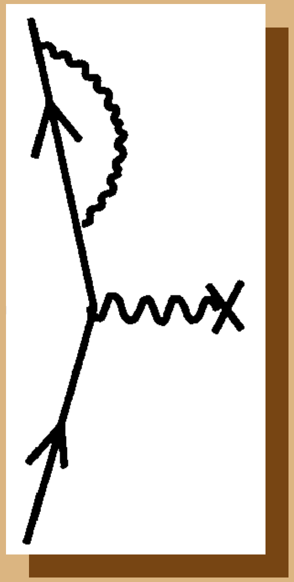
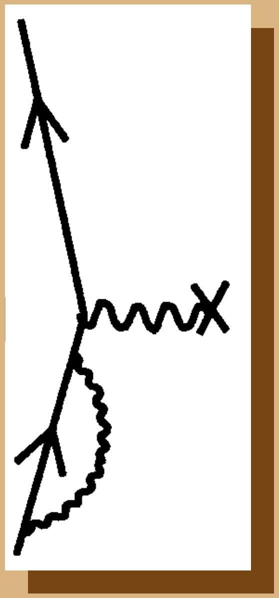
Electron self-energy:



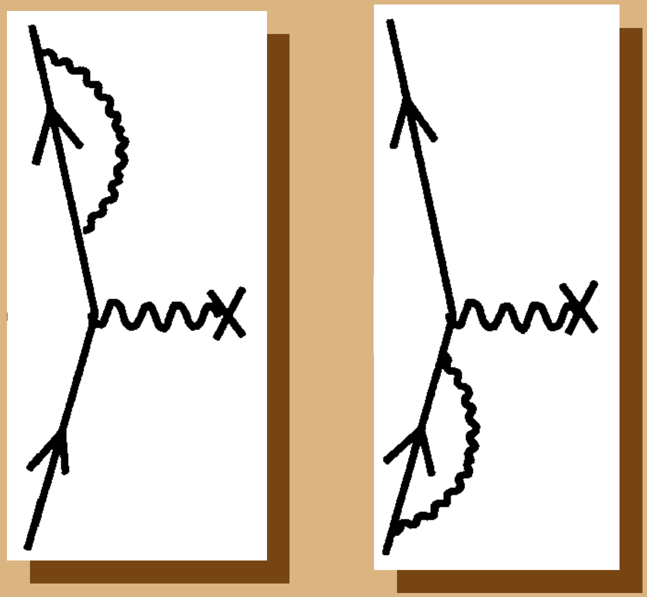


$$\Sigma(k) = \int \frac{d^4 l}{(2\pi)^4}\frac{1}{l^2}\gamma_\lambda \frac{1}{i(\not{k} - \not{l}) + M}\gamma_\lambda$$

QED with external field: traditional

Some divergent parameters, delicate cancellations

Electron self-energy: $\Sigma(k) = \int \frac{d^4 l}{(2\pi)^4} \frac{1}{l^2} \gamma_\lambda \frac{1}{i(\not{k} - \not{l}) + M} \gamma_\lambda$



$$\Sigma(k) = A + (i\not{k} + M)B + (i\not{k} + M)\Sigma_c(k)(i\not{k} + M)$$

A and B divergent

$A = M \frac{3\alpha_0}{2\pi} \ln \frac{\Lambda_0}{M}$ (Logarithmic, not linear as $\Lambda_0 \to \infty$)

A eliminated by mass renormalization

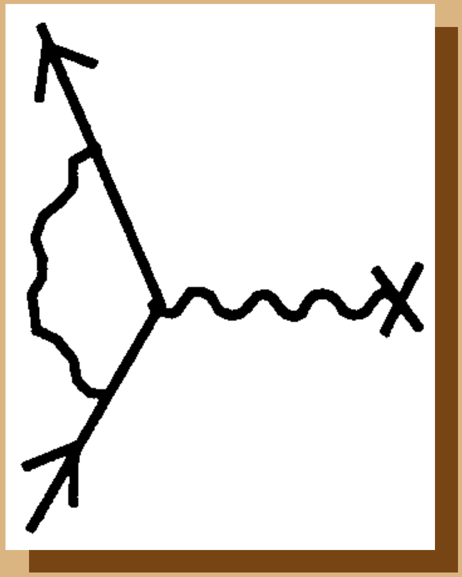
Bare $\alpha_0 = \frac{e_0^2}{4\pi}$

QED with external field: traditional

Ward identity: vertex connected to self-energy

$$\frac{\partial \Sigma(k)}{\partial k_\mu} = i\Lambda_\mu(k,k)$$

Vertex: $\Lambda_\mu(k',k) = \int \frac{d^4q}{(2\pi)^4}\frac{1}{q^2}\gamma_\lambda \frac{1}{i(\not{k}'-\not{q})+M}\gamma_\mu \frac{1}{i(\not{k}-\not{q})+M}\gamma_\lambda$



$$\Lambda_\mu(k',k) = C\gamma_\mu + \Lambda_{c\mu}(k',k)$$

C divergent

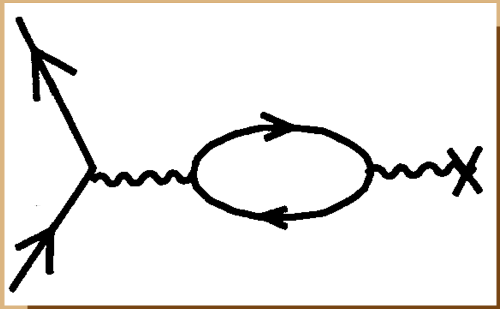
$$C = \frac{\alpha_0}{2\pi}\ln\frac{\Lambda_0}{M} \qquad \Lambda_0 \to \infty$$

$B = C$ from Ward identity

B and C cancel due to wavefn renormalization (½ in front of each self-energy insertion)

QED with external field: traditional

Vacuum polarization:



$$\Pi_{\mu\nu}(q) = \int \frac{d^4k}{(2\pi)^4} \mathrm{Tr} \frac{1}{i(\not{k} - \not{q}/2) + M} \gamma_\mu \frac{1}{i(\not{k} + \not{q}/2) + M} \gamma_\nu$$

$$\Pi_{\mu\nu}(q) = (q_\mu q_\nu - q^2 \delta_{\mu\nu}) D(q^2)$$

$D(0)$ divergent

$$D(0) = \frac{2\alpha_0}{3\pi} \ln \frac{\Lambda_0}{M}$$

(Logarithmic, not quadratic as $\Lambda_0 \to \infty$)

$D(0)$ eliminated by charge renormalization

"The bare charge is infinitely larger than the observed charge"

QED with external field: traditional

QED Lagrangian: $\mathcal{L} = -\bar{\psi}\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + M\right)\psi - \frac{1}{4}F_{\mu\nu}F_{\mu\nu} + e_0 j_\mu A_\mu$

To summarize:

- A series of integrals seemed to be divergent (even quadratically)
- Massaging them we found only logarithmic divergences (equivalently, 1/ε in 4-ε dimensions)
- Some of the divergences were absorbed in parameter redefinitions, while others disappeared from the theory
- In any case, the cutoff dropped out

QED with external field: modern

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Modern approach:

The cutoff really is there: the cutoff dependence implies something important has to happen at the energy scale Λ_0

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Introducing counterterms:

Remove from the theory all states having energies or momenta larger than some new cutoff $\Lambda \ll \Lambda_0$

Pick vertex function as example

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Now rationalize: "Well, we did our best. These things happen."

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$$\Lambda_\mu(k', k) = \int^\Lambda \frac{d^4q}{(2\pi)^4}\frac{1}{q^2}\gamma_\lambda \frac{i(\not{k}' - \not{q}) - M}{(k' - q)^2 + M^2}\gamma_\mu \frac{i(\not{k} - \not{q}) - M}{(k - q)^2 + M^2}\gamma_\lambda$$

The new theory works only for processes at energies much less than Λ, so as a first step we can neglect k' , k , and M

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Contribution amounts to:

$$\Lambda_\mu(k', k; > \Lambda) = \int_\Lambda^{\Lambda_0} \frac{d^4 q}{(2\pi)^4} \frac{1}{(q^2)^2} \gamma_\mu \equiv c_0(\Lambda/\Lambda_0)\gamma_\mu$$

Equivalently re-incorporated as: $\delta\mathcal{L}_1 = e_0 c_0(\Lambda/\Lambda_0) j_\mu A_\mu$

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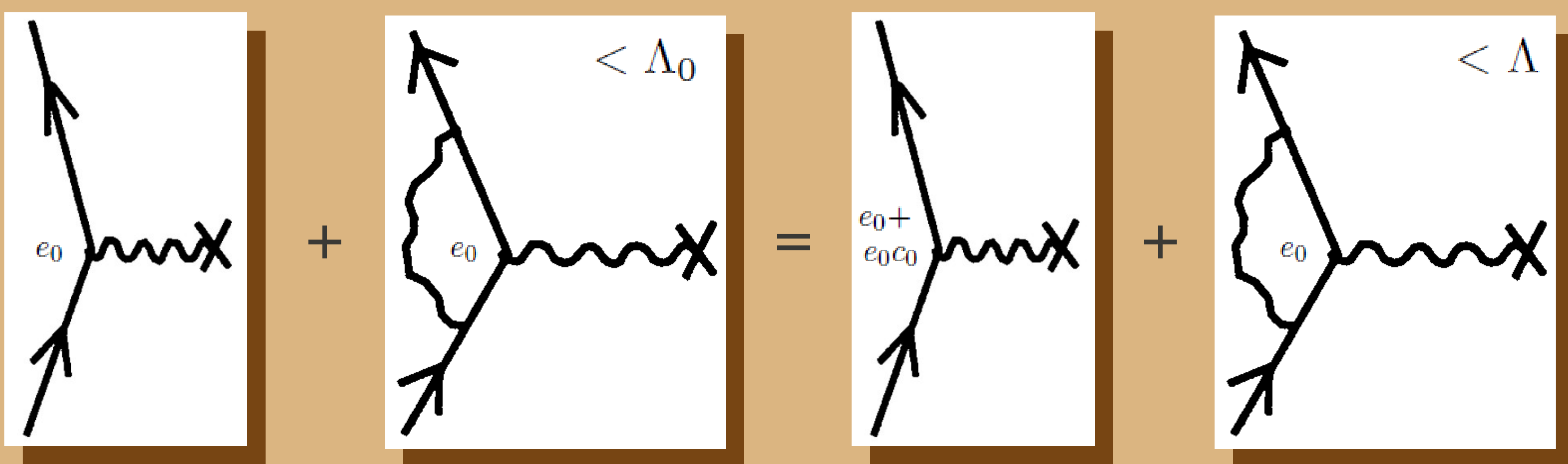

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More generally: Taylor expand in powers of k/Λ , k'/Λ, and M/Λ

getting more counterterms $\delta\mathcal{L}_2 = \frac{e_0 M c_1}{\Lambda^2}\bar{\psi}F_{\mu\nu}\sigma_{\mu\nu}\psi + \frac{e_0 c_2}{\Lambda^2}\bar{\psi}\frac{\partial}{\partial x_\mu}F_{\mu\nu}\gamma_\nu\psi$

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And so it goes: Remove states and re-incorporate by including a *small* number of counterterms

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Note: In the above example we knew the underlying theory, so we could explicitly calculate the low-energy constants.
This is not always the case.

Bibliography

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Chapter 6

(electron vertex function with Pauli-Villars regularization)

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"Advanced Modern Physics"
Chapter 9

(electron vertex function with dimensional regularization)

G. P. Lepage
"What is Renormalization"
arXiv:hep-ph/0506330

(counterterms for QED)

A. Zee
"Quantum Field Theory In A Nutshell"
Chapter III.3

(counterterms for scalar field theory)

And now a brief introduction to chiral EFT

Should we follow the same path for Quantum Chromodynamics?

$$\mathcal{L}_{\rm QCD} = \bar{q}(i\gamma^\mu \mathcal{D}_\mu - \mathcal{M})q - \frac{1}{4}\mathcal{G}_{\mu\nu,a}\mathcal{G}_a^{\mu\nu}$$

Quotes on degrees of freedom

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Quotes on degrees of freedom

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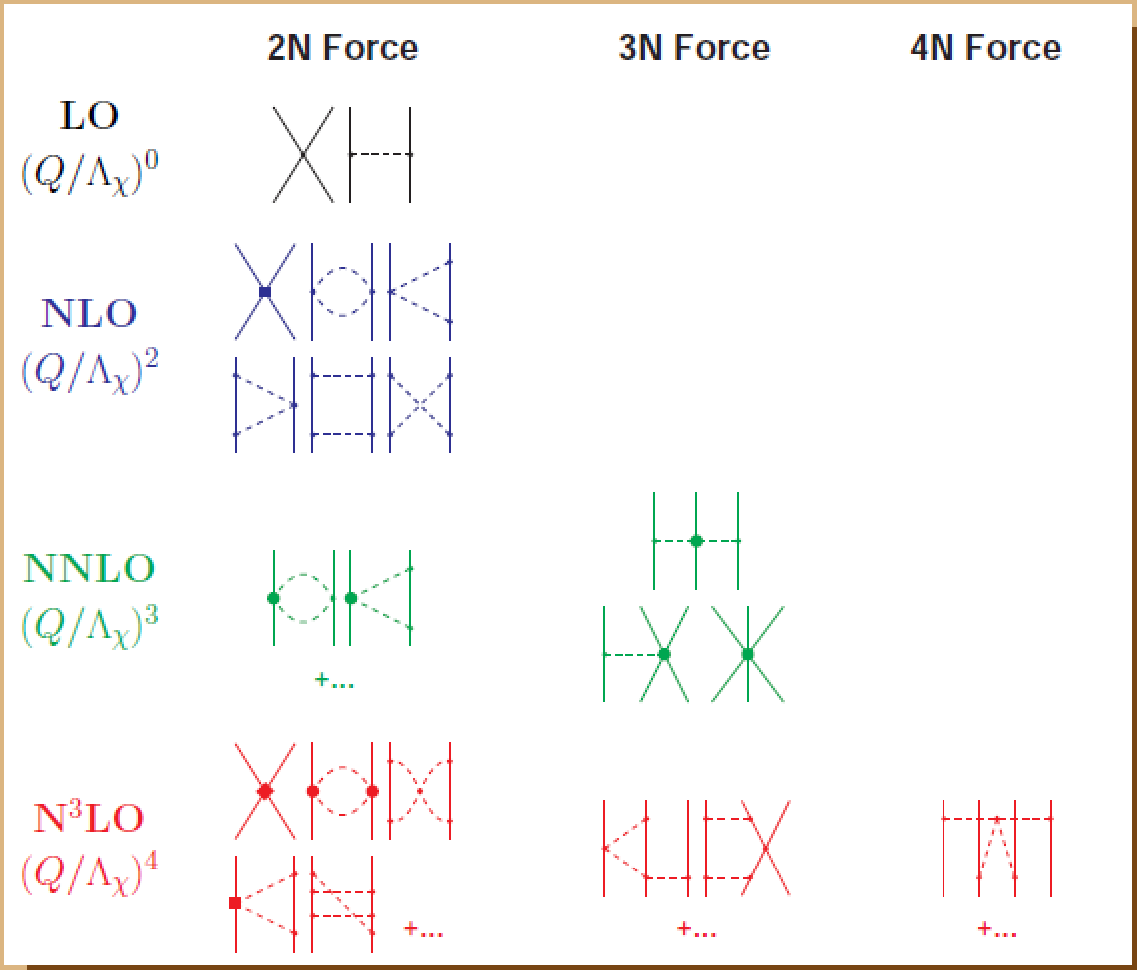
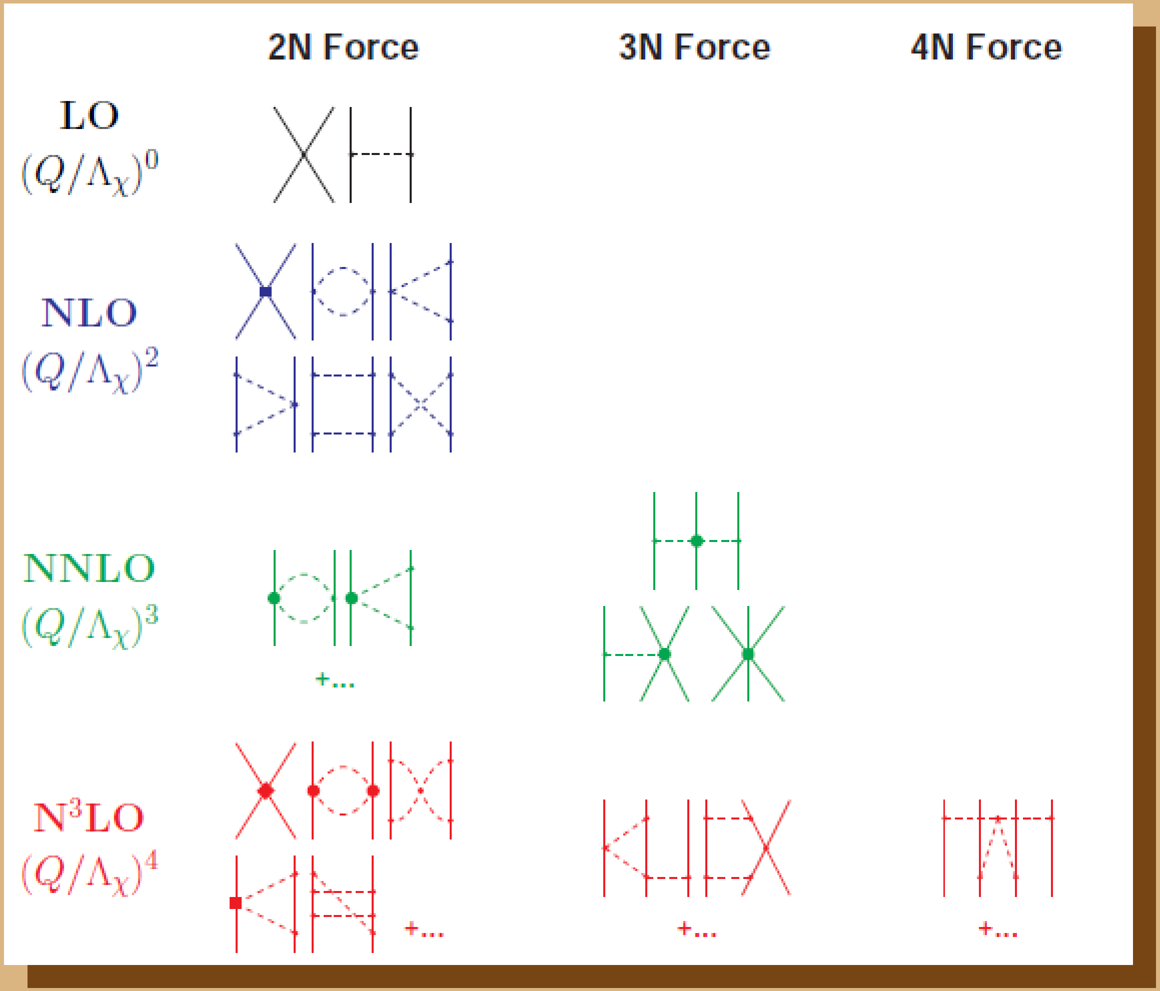
Nuclear Hamiltonian: chiral EFT



- Attempts to connect with underlying theory (QCD)
- Systematic low-momentum expansion
- Consistent many-body forces
- Low-energy constants from experiment or lattice QCD
- Until now non-local in coordinate space, so unused in continuum QMC
- Power counting's relation to renormalization still an open question

Nuclear Hamiltonian: chiral EFT



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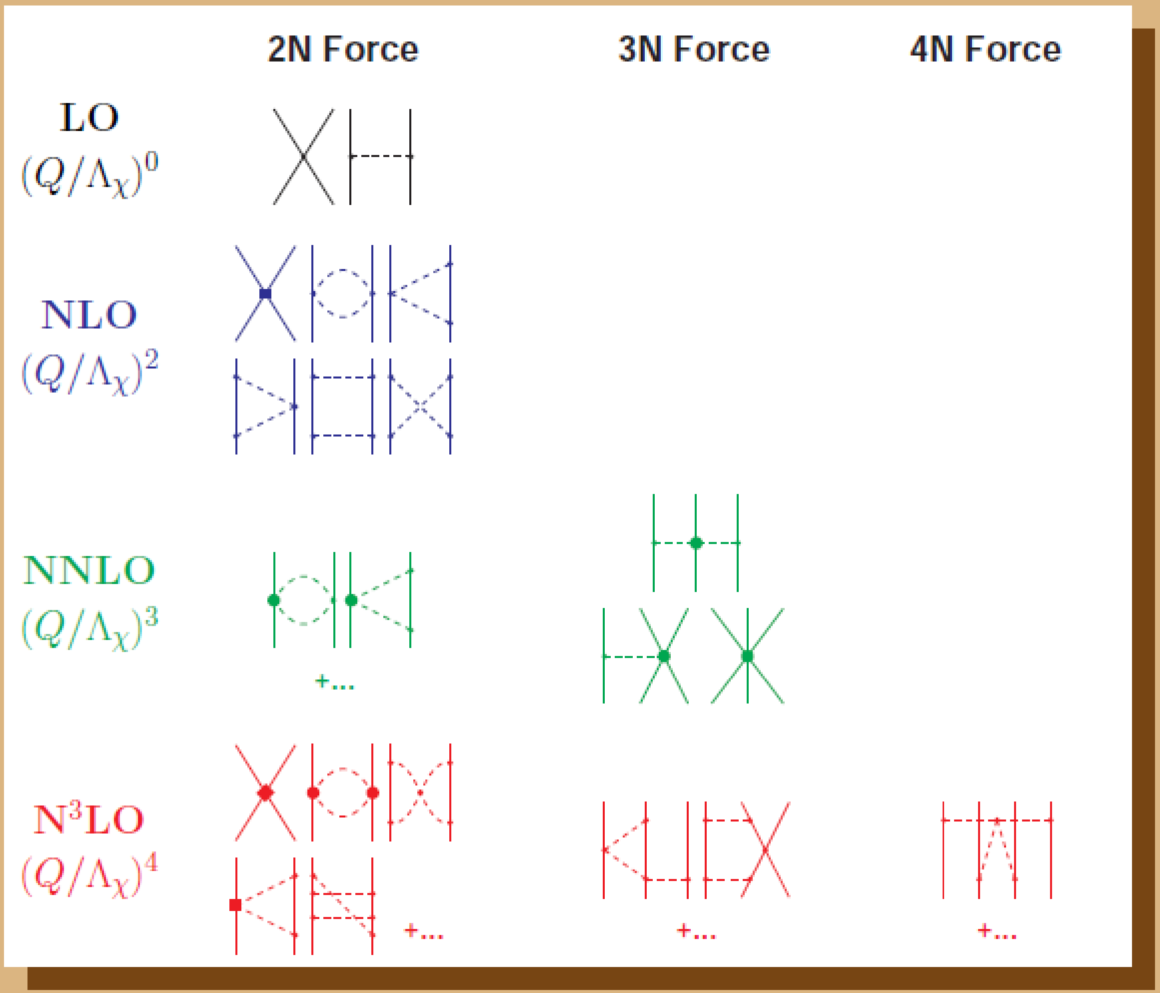

Regulator and dictionary:

$$f(p,p') = e^{-(p/\Lambda)^{2n}} e^{-(p'/\Lambda)^{2n}}$$

$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2 \qquad \mathbf{k} = (\mathbf{p}' + \mathbf{p})/2$$

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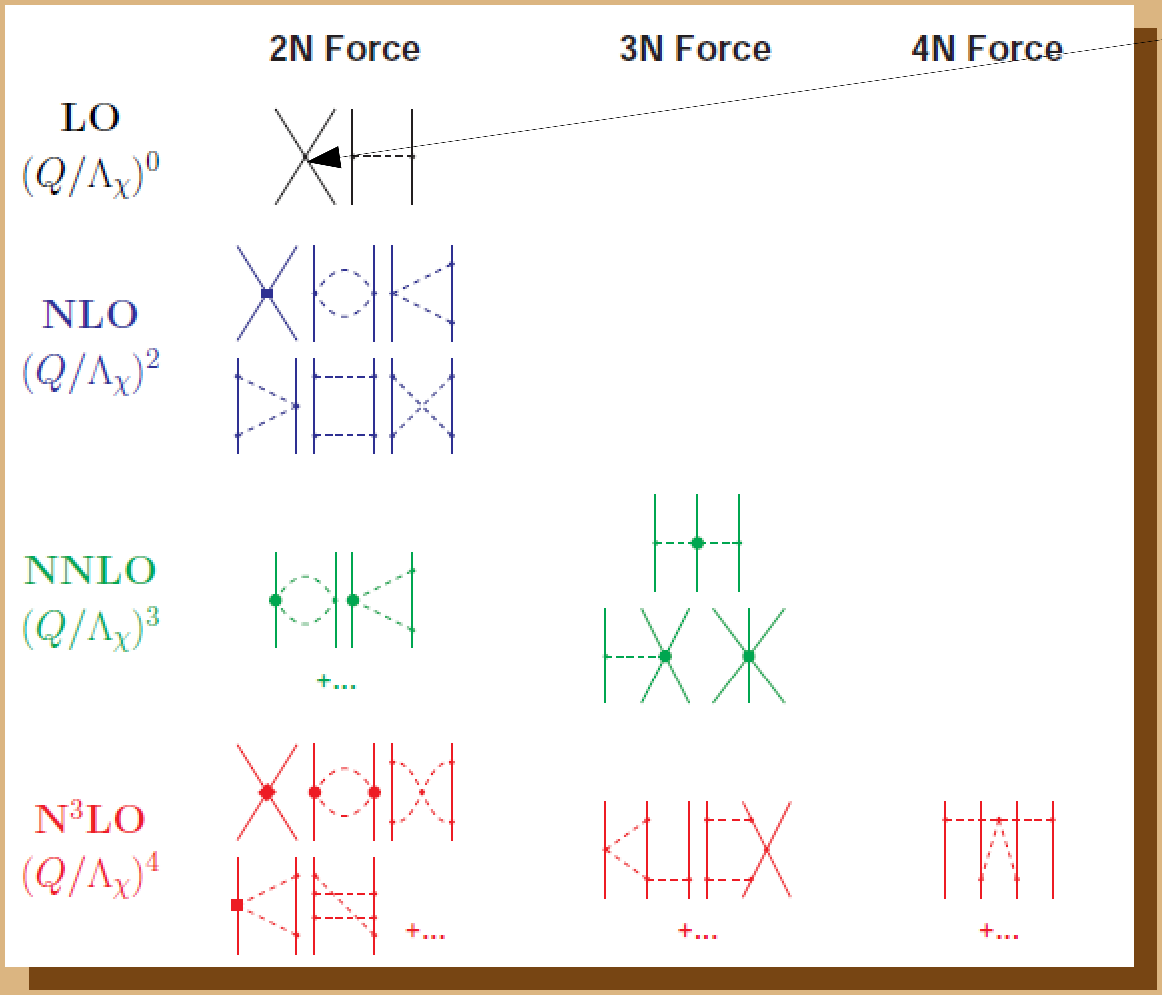
Nuclear Hamiltonian: chiral EFT

$$V_{ct}^{(0)} = C_S + C_T\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$



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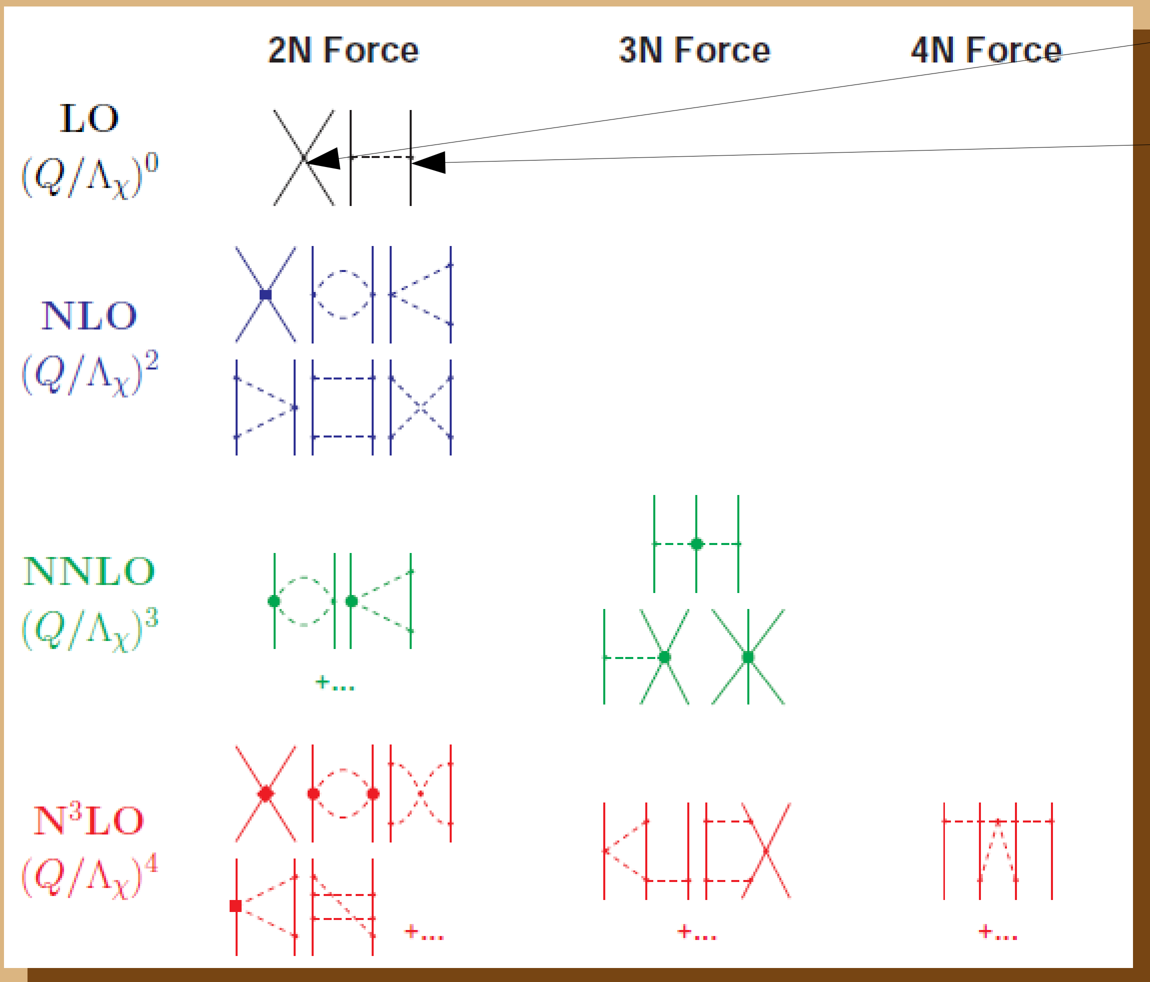

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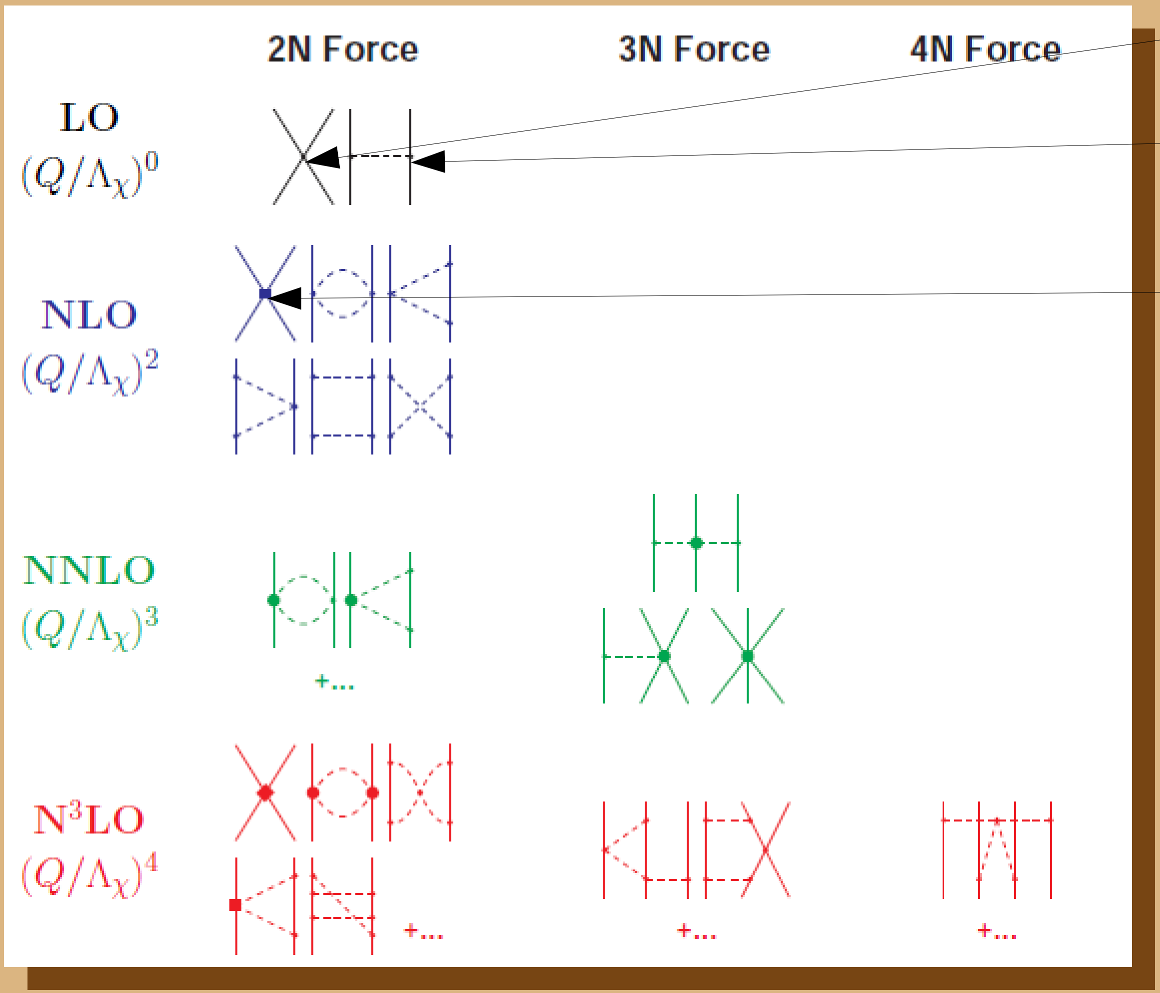

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$$\begin{aligned} V_{\rm ct}^{(2)} &= C_1 \, q^2 + C_2 \, k^2 \\ &+ \left(C_3 \, q^2 + C_4 \, k^2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\ &+ i \frac{C_5}{2} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{q} \times \mathbf{k}) \\ &+ C_6 (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\ &+ C_7 (\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) \end{aligned}$$

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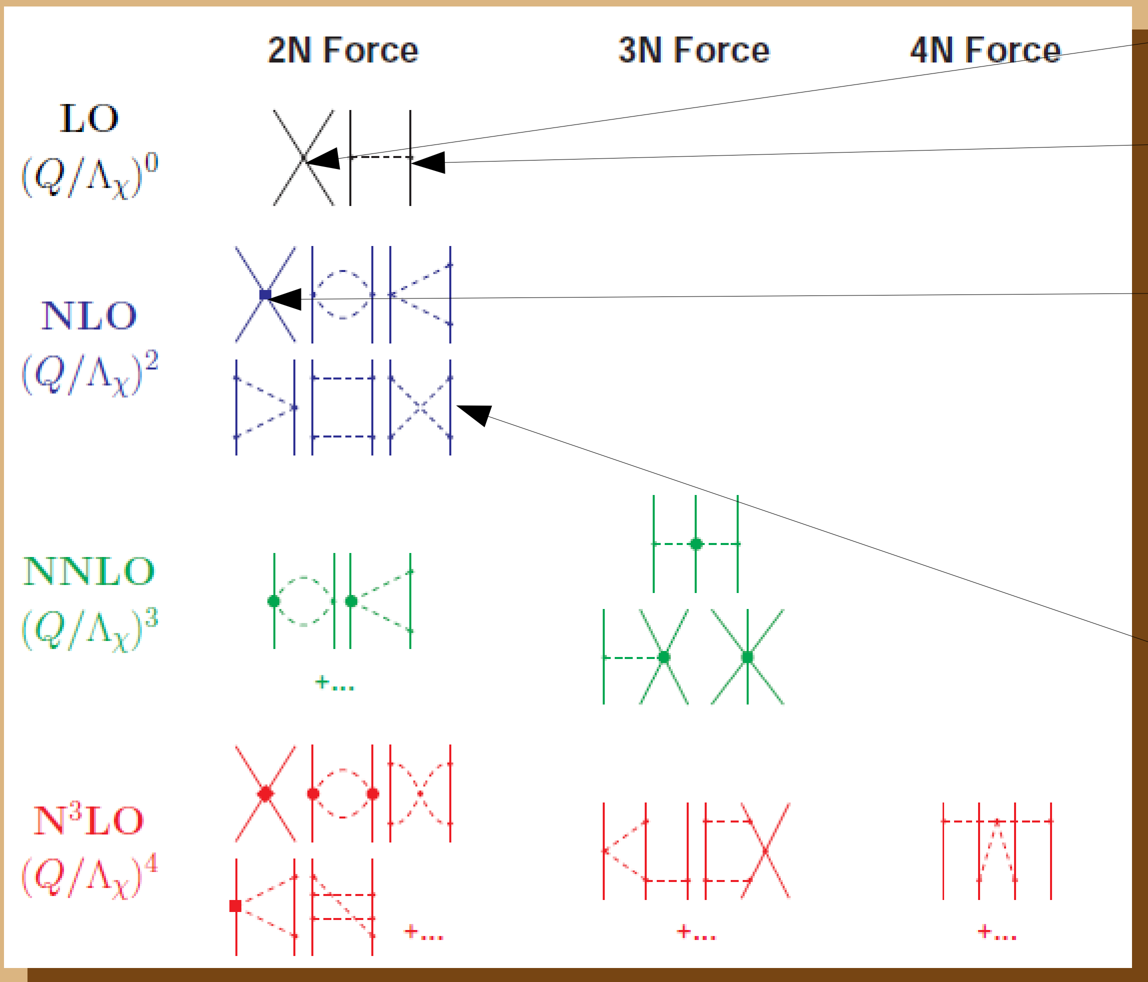

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Long-studied
two-pion exchange

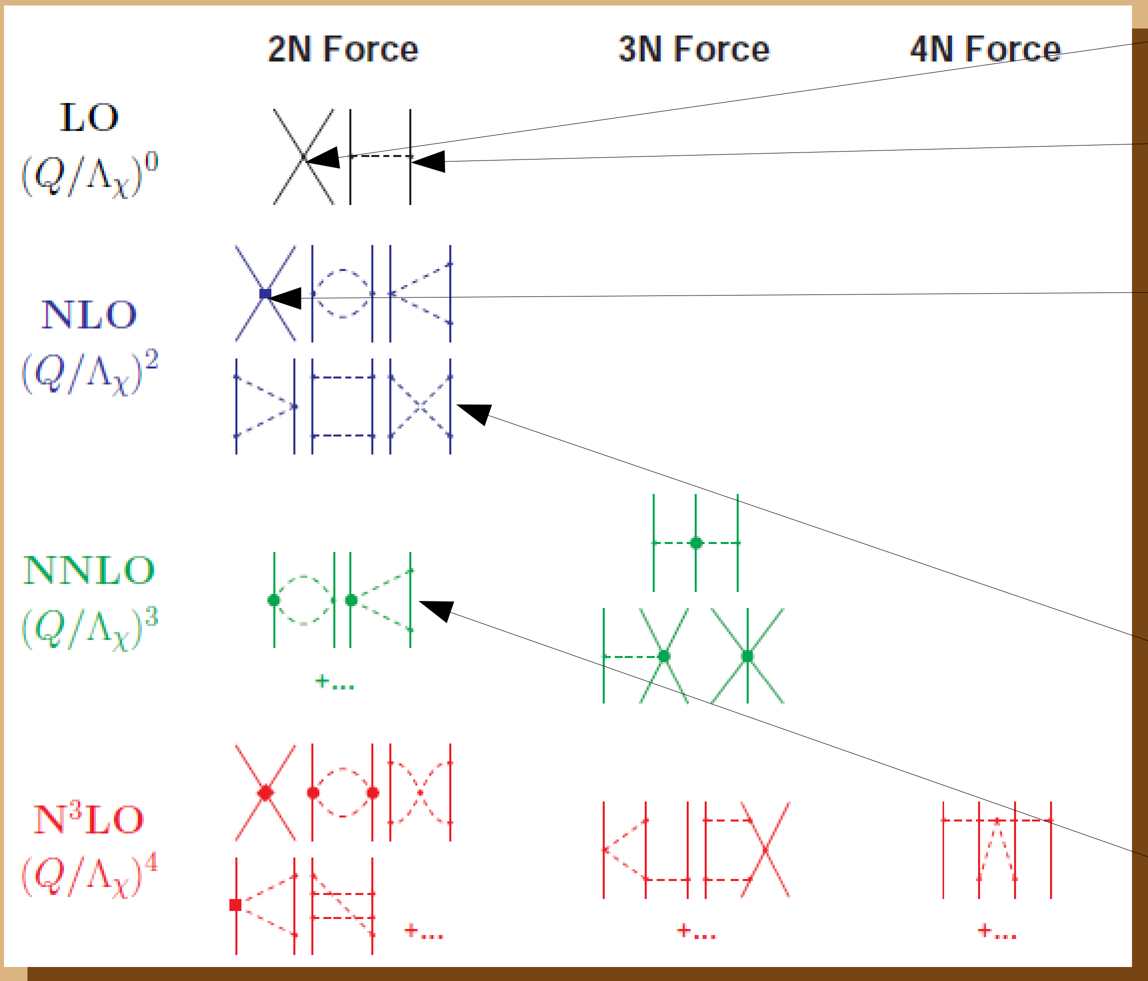
Regulator and dictionary:

$$f(p, p') = e^{-(p/\Lambda)^{2n}} e^{-(p'/\Lambda)^{2n}}$$

$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2 \qquad \mathbf{k} = (\mathbf{p}' + \mathbf{p})/2$$

$$\mathbf{p}' = (\mathbf{p}_1' - \mathbf{p}_2')/2 \qquad \mathbf{q} = \mathbf{p}' - \mathbf{p}$$

Nuclear Hamiltonian: chiral EFT



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Long-studied
two-pion exchange

Contains couplings
from πN scattering

Regulator and dictionary:

$$f(p, p') = e^{-(p/\Lambda)^{2n}} e^{-(p'/\Lambda)^{2n}}$$

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Turning to Quantum Monte Carlo

Continuum Quantum Monte Carlo

Rudiments of Diffusion Monte Carlo:

$$\Psi(\tau \to \infty) = \lim_{\tau \to \infty} e^{-(\mathcal{H}-E_T)\tau} \Psi_V$$
$$\to \alpha_0 e^{-(E_0-E_T)\tau} \Psi_0$$

How to do? Start somewhere and evolve

$$\psi(\mathbf{R}, \tau) = \int G(\mathbf{R}, \mathbf{R}', \tau) \psi(\mathbf{R}', 0) d\mathbf{R}'$$

With a standard propagator

$$G(\mathbf{R}, \mathbf{R}', \tau) = \langle \mathbf{R} | e^{-(H-E_0)\tau} | \mathbf{R}' \rangle$$

Cut up into many time slices

$$G(\mathbf{R}, \mathbf{R}', \Delta\tau) \approx e^{-\frac{V(\mathbf{R})+V(\mathbf{R}')}{2}\Delta\tau} \left(\frac{m}{2\pi\hbar^2\tau}\right)^{\frac{3A}{2}} e^{-\frac{m|\mathbf{R}-\mathbf{R}'|^2}{2\hbar^2\tau}}$$

Quantum Monte Carlo

What about more general Hamiltonians?

$$H \quad = \quad -\frac{\hbar^2}{2m}\sum_{j=1,N}\nabla_j^2 + \sum_{j<k} v_{jk} + \sum_{j<k<l} V_{jkl}$$

Focus on the two-body interactions for now

$$V_2 = \sum_{j<k} v_{jk} = \sum_{j<k}\sum_{p=1}^{8} v_p(r_{jk}) O^{(p)}(j,k)$$

Quantum Monte Carlo

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Eight channels often enough (e.g. Argonne v8')

$$O^{p=1,8}(j,k) = (1, \sigma_j \cdot \sigma_k, S_{jk}, \mathbf{L}_{jk}\cdot\mathbf{S}_{jk}) \otimes (1, \tau_j \cdot \tau_k)$$

With tensor: $S_{jk} = 3(\hat{r}_{jk}\cdot\sigma_j)(\hat{r}_{jk}\cdot\sigma_k) - \sigma_j\cdot\sigma_k$

And spin, orbit:

$$\mathbf{S}_{jk} = \frac{\hbar}{2}(\sigma_j + \sigma_k)$$

$$\mathbf{L}_{jk} = \frac{\hbar}{2\imath}(\mathbf{r}_j - \mathbf{r}_k) \times (\nabla_j - \nabla_k)$$

Continuum Quantum Monte Carlo

Rudiments of wave functions from yesterday's lecture

Normal gas for frozen spins

Two Slater determinants, written either using the antisymmetrizer:

$$\Phi_S(\mathbf{R}) = \mathcal{A}[\phi_n(r_1)\phi_n(r_2)\ldots\phi_n(r_{\frac{N}{2}})]\ \ \mathcal{A}[\phi_n(r_{1'})\phi_n(r_{2'})\ldots\phi_n(r_{\frac{N}{2}'})]$$

or actual determinants (e.g. 7 + 7 particles):

$$\Phi_S(\mathbf{R}) = \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) & \ldots & \phi_1(r_7) \\ \phi_2(r_1) & \phi_2(r_2) & \ldots & \phi_2(r_7) \\ \phi_3(r_1) & \phi_3(r_2) & \ldots & \phi_3(r_7) \\ \phi_4(r_1) & \phi_4(r_2) & \ldots & \phi_4(r_7) \\ \phi_5(r_1) & \phi_5(r_2) & \ldots & \phi_5(r_7) \\ \phi_6(r_1) & \phi_6(r_2) & \ldots & \phi_6(r_7) \\ \phi_7(r_1) & \phi_7(r_2) & \ldots & \phi_7(r_7) \end{vmatrix} \begin{vmatrix} \phi_1(r'_1) & \phi_1(r'_2) & \ldots & \phi_1(r'_7) \\ \phi_2(r'_1) & \phi_2(r'_2) & \ldots & \phi_2(r'_7) \\ \phi_3(r'_1) & \phi_3(r'_2) & \ldots & \phi_3(r'_7) \\ \phi_4(r'_1) & \phi_4(r'_2) & \ldots & \phi_4(r'_7) \\ \phi_5(r'_1) & \phi_5(r'_2) & \ldots & \phi_5(r'_7) \\ \phi_6(r'_1) & \phi_6(r'_2) & \ldots & \phi_6(r'_7) \\ \phi_7(r'_1) & \phi_7(r'_2) & \ldots & \phi_7(r'_7) \end{vmatrix}$$

Continuum Quantum Monte Carlo

More generally, we keep track of the spins-isospins

For A particles we have 2^A ways of arranging the spins.
Take A=3 as an example ($2^3 = 8$):

$$|\uparrow\uparrow\uparrow\rangle,\ |\uparrow\uparrow\downarrow\rangle,\ |\uparrow\downarrow\uparrow\rangle,\ |\uparrow\downarrow\downarrow\rangle,\ |\downarrow\uparrow\uparrow\rangle,\ |\downarrow\uparrow\downarrow\rangle,\ |\downarrow\downarrow\uparrow\rangle,\ |\downarrow\downarrow\downarrow\rangle$$

Continuum Quantum Monte Carlo

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$$|pnn\rangle,\ |npn\rangle,\ |nnp\rangle$$

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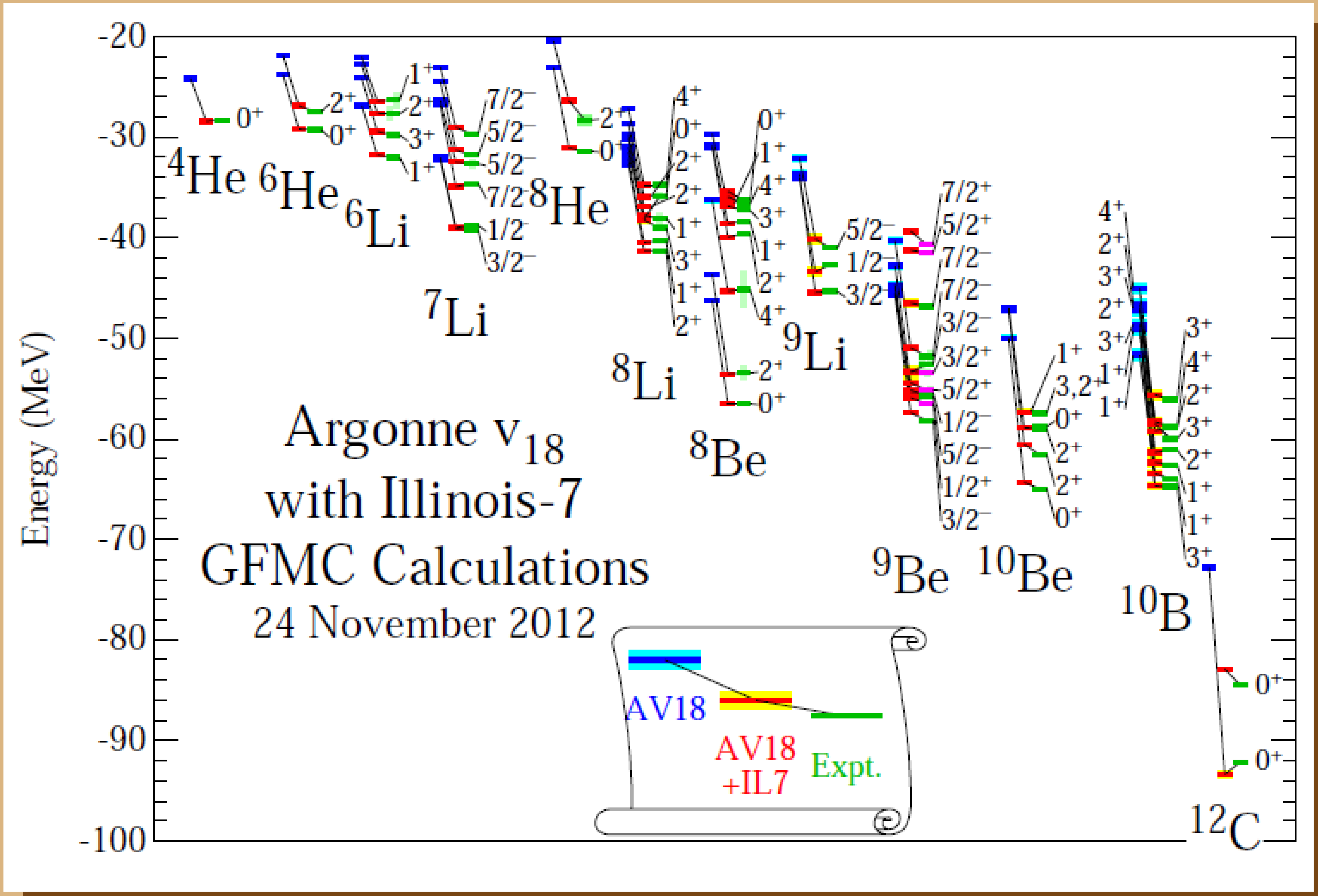
A general nucleus needs $2^A \dfrac{A!}{Z!(A-Z)!}$ states

Phenomenological Hamiltonian

Green's Function Monte Carlo is very accurate and very expensive



Credit: Steve Pieper

Quantum Monte Carlo

Auxiliary Field Diffusion Monte Carlo (Schmidt-Fantoni 1999)

GFMC needs $2^A \dfrac{A!}{Z!(A-Z)!}$ numbers, AFDMC would like only $4A$

Goal: To tackle larger nuclei and infinite matter

Quantum Monte Carlo

Auxiliary Field Diffusion Monte Carlo

Take $V_2 = \sum_{j<k} v_{jk} = V_{\mathrm{SI}} + V_{\mathrm{SD}}$ and split

Spin-independent: $V_{\mathrm{SI}} = \sum_{j<k} [v_1(r_{jk}) + v_2(r_{jk})]$

Spin-dependent: $V_{\mathrm{SD}} = \frac{1}{2} \sum_{j,\alpha,k,\beta} \sigma_{j,\alpha} \; A_{j,\alpha;k,\beta} \; \sigma_{k,\beta}$

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For neutrons: 3N by 3N *A* matrix knows about spin-spin and tensor:

$$\begin{aligned} A_{j,\alpha;k,\beta} \quad = \quad & (v_3(r_{jk}) + v_4(r_{jk}))\delta_{\alpha\beta} + \\ & [v_5(r_{jk}) + v_6(r_{jk})]\,[3\hat{r}_{jk}\cdot\hat{x}_\alpha\,\hat{r}_{jk}\cdot\hat{x}_\beta - \delta_{\alpha\beta}] \end{aligned}$$

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\end{aligned}
$$

Now diagonalize. Use eigendecomposition to create squares:

$V_2 \quad = \quad V_{\rm SI} + \frac{1}{2} \sum_{n=1}^{3N} (O_n)^2 \lambda_n$ This will end up in an exponent.

Quantum Monte Carlo

Auxiliary Field Diffusion Monte Carlo (continued)

Handle squares through a Hubbard-Stratonovich transformation:

$$e^{-\frac{1}{2}\lambda O^2 \Delta\tau} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2}} e^{x\sqrt{-\lambda\Delta\tau}O}$$

Quantum Monte Carlo

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This leads to the following short-time Green's function:

$$G(\mathbf{R}, \mathbf{R}', \Delta\tau) = \left(\frac{m}{2\pi\hbar^2\Delta\tau}\right)^{3N/2} \exp\left(-\frac{m(\mathbf{R}-\mathbf{R}')^2}{2\hbar^2\Delta\tau}\right) e^{-V_{\mathrm{SI}}(R)\Delta\tau}$$

$$\prod_{n=1}^{3N} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx_n e^{-\frac{x_n^2}{2}} e^{x_n\sqrt{-\lambda_n\Delta\tau}O_n}$$

Quantum Monte Carlo

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Use importance function (phase of walkers):

$$\psi_I(\mathbf{R}, S) = \prod_{i<j} f(r_{ij})\, \mathcal{A}\left[\prod_{i=1}^{N} \phi_\alpha(\mathbf{r}_i, s_i)\right] \qquad |s_i\rangle = a_i|\uparrow\rangle + b_i|\downarrow\rangle$$

How to go beyond?

Combine power of Quantum Monte Carlo with consistency of chiral Effective Field Theory

Write down a local energy-independent NN potential

- Use local pion-exchange regulator $f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4}$

cf. $f(p, p') = e^{-(p/\Lambda)^{2n}} e^{-(p'/\Lambda)^{2n}}$

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- Use local pion-exchange regulator $f_{\text{long}}(r) = 1 - e^{-(r/R_0)^4}$
- Pick 7 different contacts at NLO, just make sure that when antisymmetrized they lead to a set obeying the required symmetry principles

$$\begin{aligned} V_{\text{ct}}^{(2)} &= C_1\, q^2 + C_2\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ &+ \left(C_3\, q^2 + C_4\, q^2\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \\ &+ i\, \frac{C_5}{2}\, (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{q} \times \mathbf{k} \\ &+ C_6\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}) \\ &+ C_7\, (\boldsymbol{\sigma}_1 \cdot \mathbf{q})(\boldsymbol{\sigma}_2 \cdot \mathbf{q})\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \end{aligned}$$

cf.

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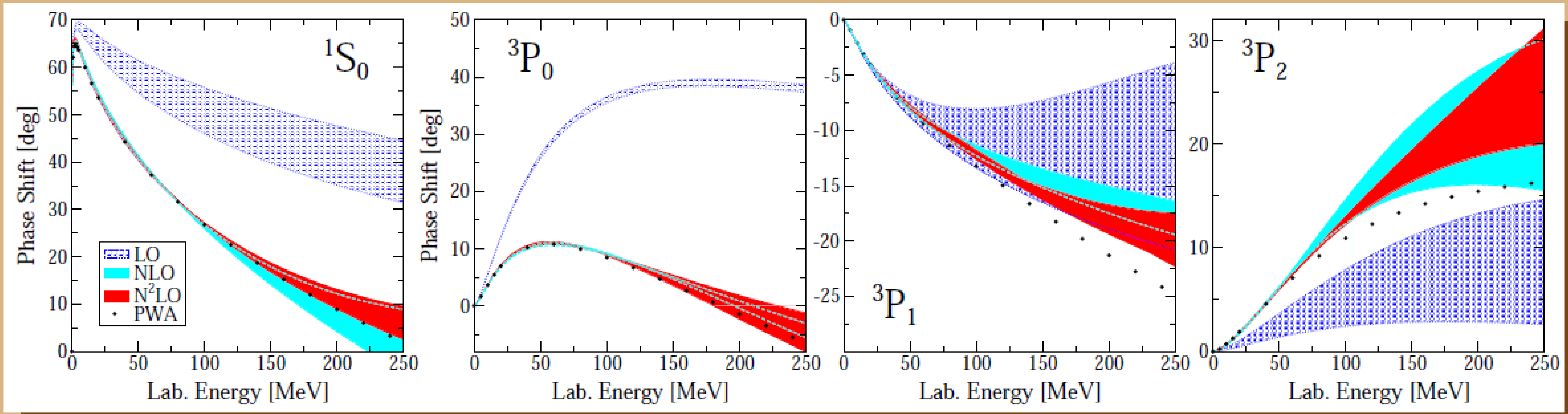
How to go beyond?

Combine power of Quantum Monte Carlo with consistency of chiral Effective Field Theory

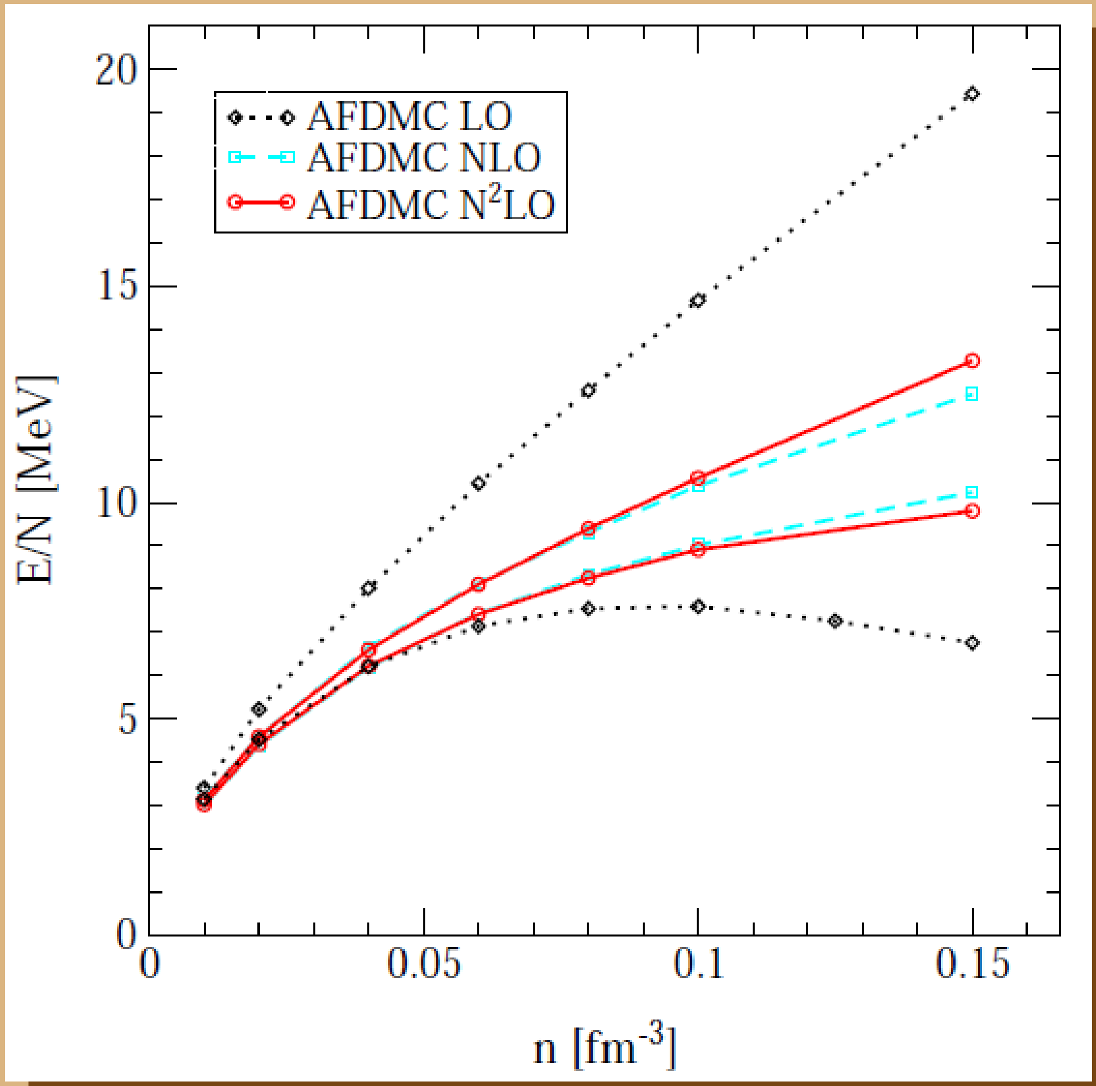
- Write down a local energy-independent NN potential

- Before doing many-body calculations, fit to NN phase shifts



A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, arXiv:1303.6243

Chiral EFT in QMC

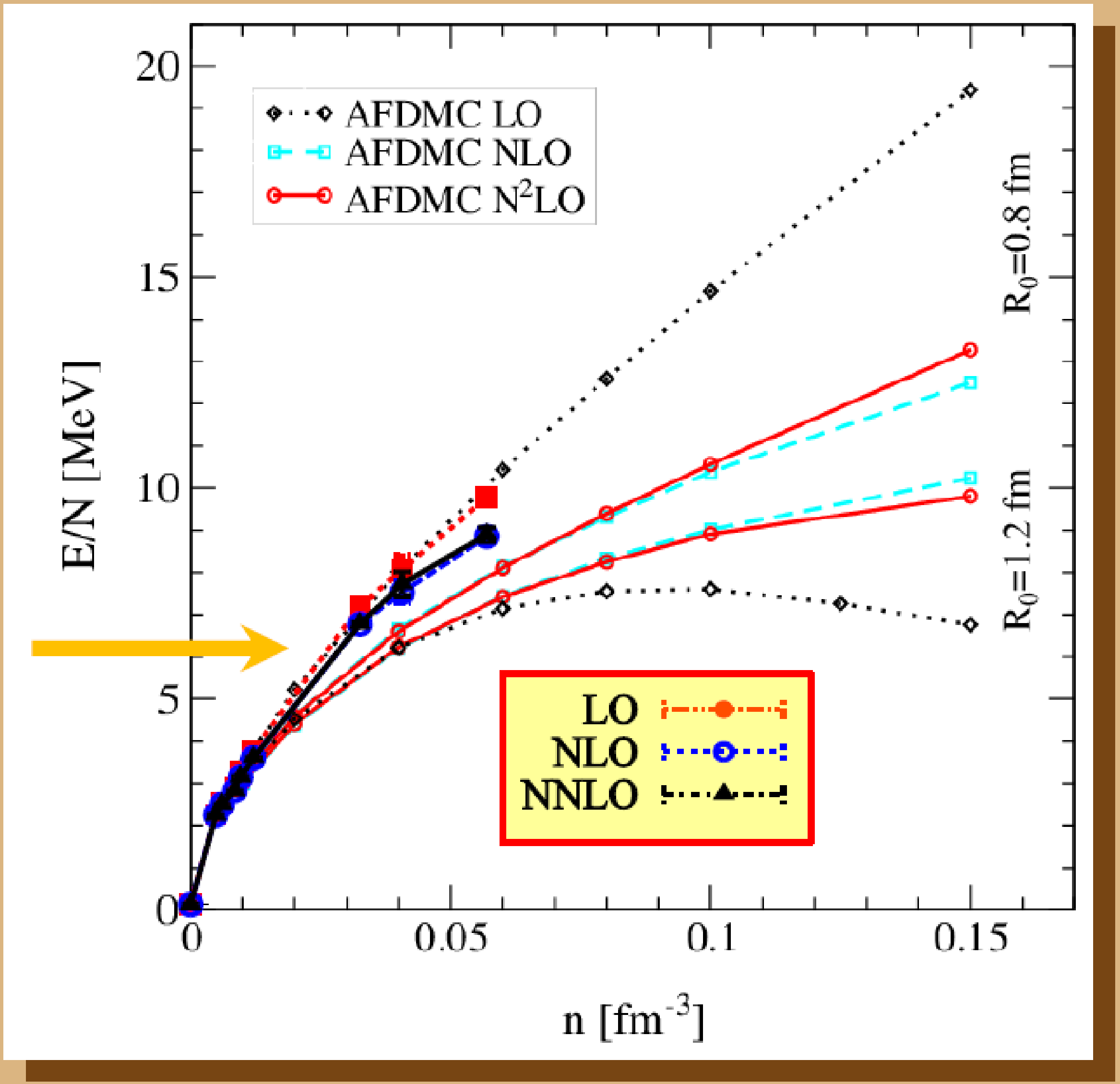


- Use Auxiliary-Field Diffusion Monte Carlo to handle the full interaction
- First ever non-perturbative systematic error bands
- Band sizes to be expected
- Many-body forces will emerge systematically

NEUTRONS

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, arXiv:1303.6243

Chiral EFT in lattice QMC

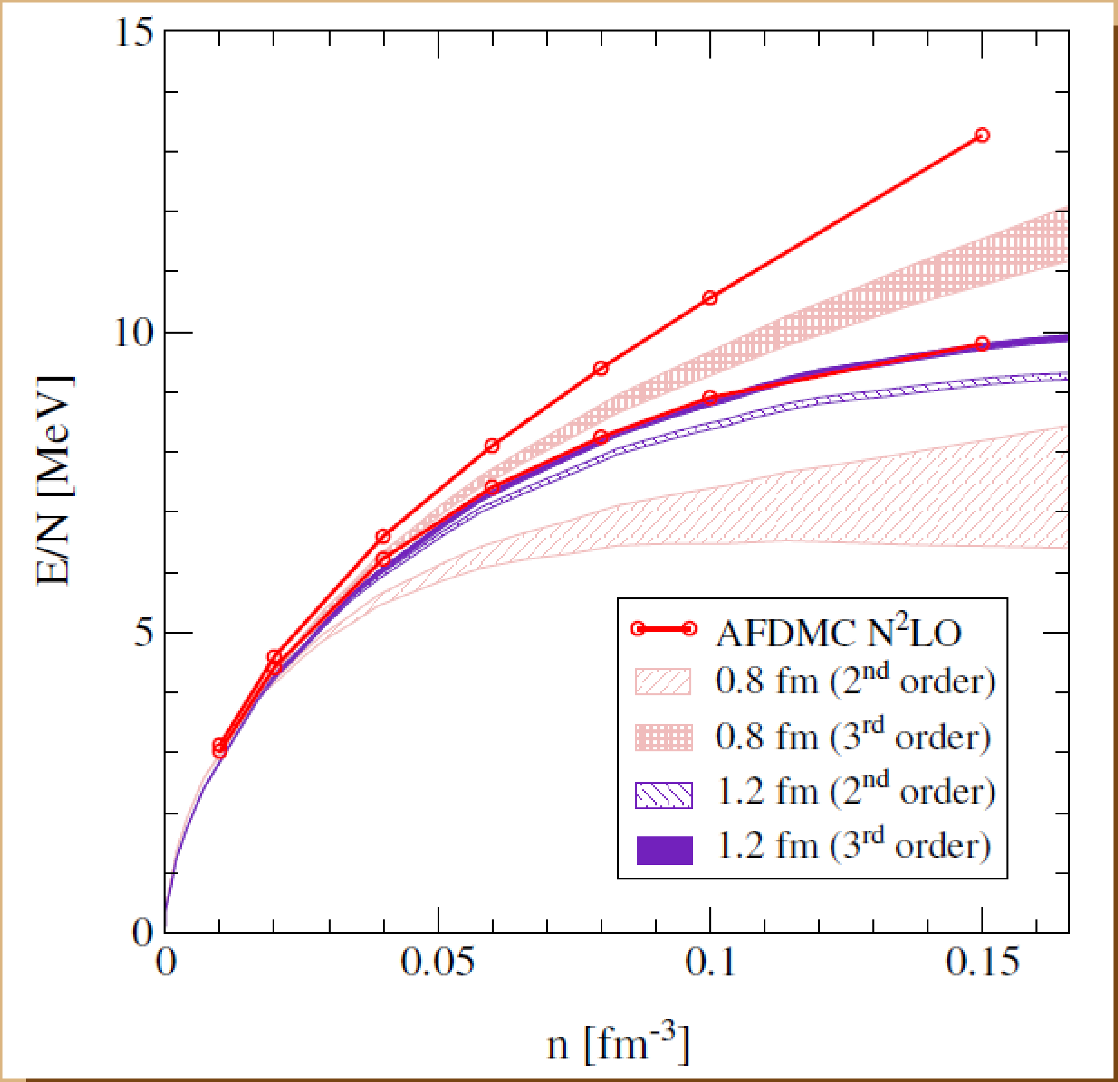


- Complementary Quantum Monte Carlo approach that has already been using chiral EFT forces
- Formalism to be discussed in later lecture
- Preliminary results

NEUTRONS

Dean Lee/nuclear lattice EFT collaboration

QMC vs MBPT



- Comparison with many-body perturbation approach
- MBPT bands come from diff. single-particle spectra
- Soft potential in excellent agreement with AFDMC
- Hard potential slower to converge

NEUTRONS

A. Gezerlis, I. Tews, E. Epelbaum, S. Gandolfi, K. Hebeler, A. Nogga, A. Schwenk, arXiv:1303.6243

Conclusions

- Chiral EFT can now be used in continuum Quantum Monte Carlo methods
- The perturbativeness of different orders can be directly tested
- Non-perturbative systematic error bands can be produced

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