INT Program INT-16-2a Bayesian Methods in Nuclear Physics June 24, 2016

Bayes Identifying and quantifying theoretical uncertainties.

Doron Gazit Racah Institute of Physics Hebrew University of Jerusalem



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Outline

- In the talk I will present a few recent problems where theoretical uncertainty assessment has become a main part of the challenge:
 - *Nuclear physics of light nuclei*: tale of two effective field theory descriptions of light nuclei
 - Nuclear fusion rates: predicting the proton-proton fusion rate in the Sun.
 - Atomic physics of in extreme density and temperature: the solar abundance problem.
- In all these problems, my feeling is that I've used the "chi-by-eye" version of theoretical uncertainty assessment:
 - Is there a better, more systematic, approach?

Bayesian Methods in Nuclear Physics June 24, 2016 Bayes this, please.

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CORRELATIONS IN NUCLEAR PHYSICS AND FINE TUNING.

• Interaction is assessed using the "cross-section":





• Interaction is assessed using the "cross-section":



a – "scattering length" – extent of the wave function (layman term)

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• Interaction is assessed using the "cross-section":



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 $\sigma = 4\pi a^2 >> 4\pi r^2$

 $a \approx 10 \text{ fm} >> r \approx 1 \text{ fm}$

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 $\sigma = 4\pi a^2 >> 4\pi r^2$ $a \approx 10 \, fm >> r \approx 1 \, fm$

1. Nucleon-nucleon scattering experiments,

n

2. deuteron (bound state of neutron and proton) "vanishing" binding energy >>> from dimensional analysis in the presence of one dominant length scale.

$$E = -\frac{\hbar^2}{2ma^2} \to 0$$

1. "Size" of the nucleus.

 $\sigma = 4\pi a^2 >> 4\pi r^2$

 $a \approx 10 \text{ fm} >> r \approx 1 \text{ fm}$

- 1. Nucleon-nucleon scattering experiments,
- 2. deuteron (bound state of neutron and proton) "vanishing" binding energy >>from dimensional analysis in the presence of one dominant length scale.
- 1. "Size" of the nucleus.

"Pionless" effective field theory of nuclear physics:

- 1. Leading order $r/a \rightarrow 0$; Next to leading order r/a linear corrections
- 2. The EFT is applicable at low energies, in which only nucleons are valid degrees of freedom. Most general interaction consistent with power counting.
- 3. If Lagrangian consistent with QCD symmetries: a QCD prediction.
- 4. Renormalization group invariance: given the EFT Lagrangian, low energy observables are insensitive to details at high energies: introduce a cutoff Λ , and verify that observables are independent of Λ .

πEFT @ LO: 3 particles ground state

Bedaque, Hammer, van-Kolck: (1999) What is the binding energy of triton?



$\pi \pi EFT$ – and Correlations in light nuclei

- No 4 body parameter at LO.
- The binding energy of the 4-body ground state should be correlated to 3-body ground state.
- Phenomenological "Tjon" correlation (1975) originates in Pionless EFT!



Platter (2006), Platter, Hammer, Meissner (2005), Kirscher, Griesshammer, Hofmann (2007)



Finite range of the interaction indicates the existence of a massive particle that intermediates the strong force: The pion!

$$m_{\pi} \approx 135 \text{MeV/c}^2 \sim \frac{1}{r} \frac{\hbar c}{c^2}$$

$$r \approx 1 fm$$

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"Chiral" effective field theory of nuclear physics:

- 1. Expansion about zero momentum and zero pion mass of a theory of nucleons interacting via contacts and pion exchanges.
- 2. The EFT is applicable at energies up to few hundered MeV/c.
- 3. The Lagrangian is intimately related to QCD fundamental symmetries: a QCD prediction!
- 4. The common approach is NOT renormalization group invariant.

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28 total parameters @ NNLO, Fitted to hundreds of data points!

PHYSICAL REVIEW X 6, 011019 (2016)

Uncertainty Analysis and Order-by-Order Optimization of Chiral Nuclear Interactions

B. D. Carlsson,^{1,*} A. Ekström,^{2,3,†} C. Forssén,^{1,2,3,‡} D. Fahlin Strömberg,¹ G. R. Jansen,^{3,4} O. Lilja,¹ M. Lindby,¹ B. A. Mattsson,¹ and K. A. Wendt^{2,3}

¹Department of Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

²Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA

³Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

⁴National Center for Computational Sciences, Oak Ridge National Laboratory,

Oak Ridge, Tennessee 37831, USA

(Received 18 June 2015; revised manuscript received 6 November 2015; published 24 February 2016)

χ EFT potential



28 total parameters @ NNLO, Fitted to hundreds of data points!

Power counting leads to 3-body forces at Next-to-next-to-leading order.

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Two QCD EFTs



χ χ EFT – three body problem in the (c_D, c_E) plane. $\mathsf{NNLO}_{opt} \Lambda {=} 500 \ \mathrm{MeV}$ 3H 3He -0.2 ^{3}H -0.40.0- ^E -0.8 ³He -1.019 -0.3 -0.6 -0.5 -0.4-0.2 -0.1 0.0 C_D Lupu, Barnea, DG, arXiv: arXiv: 1508.05654

χ χ EFT – three body problem in the (c_D, c_E) plane.



Lupu, Barnea, DG, arXiv: arXiv: 1508.05654

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λ χ EFT – a Tjon line representation



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χ EFT – a Tjon line representation



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χ EFT – a Tjon line representation



NUCLEAR FUSION REACTION RATES IN THE SUN: ASSESSING THE ACCURACY OF NUCLEAR PHYSICS PREDICTIONS

 ^{2}H

 $^{1}\mathsf{H}$

³He

 ^{1}H

γ Gamma Ray

Neutrino

 ^{1}H

³He

 ^{1}H

Proton

Neutron

Positron

Proton-proton fusion in the Sun cannot be measured terrestrially.

Reliable theoretical prediction needed.

 ^{2}H

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Widely believed:



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\checkmark Weak proton-proton fusion in the Sun – theory standards

SFII – Adelberger et al., Rev. Mod. Phys. 83, 195 (2011)

 $3.99(1 \pm 0.030) \times 10^{-25}$ MeV b pionless EFT.

SFII recommended value (2011): $S_{11}(0) = 4.01(1 \pm 0.009) \times 10^{-25}$ MeV b.

<u>" χ EFT" calculation by Marcucci et al., Phys. Rev. Lett. (2013)</u>: Use consistent ³H decay-rate to constrain consistently axial MEC (DG, Quaglioni, Navratil, PRL 2009), and predict pp-fusion rate.

$$S(0) = (4.030 \pm 0.006) \times 10^{-23} \text{ MeV fm}^2$$

Including: p-wave contribution (+0.5%), full EM (-0.25-(-0.75)%), difference between 500 and 600 MeV cutoff and potential models.

Recently Archaya et al (1603.01593) χ EFT: $S(0) = (4.081^{+0.024}_{-0.032}) \times 10^{-23} \text{ MeV fm}^2$

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Can we reach precision physics with πEFT ?





Role of π EFT: Coherent and sysytematic (theoretical) uncertainty quantification. Big question: is precision physics a possible frontier of π EFT?

We revisit the pp-fusion problem within pionless EFT, fixing the unknown LEC using triton decay.

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Advantages of π EFT for proton-proton fusion:

Small number of parameters.
Two NLO π EFT arrangements.
A "cheat-sheet" in the electromagnetic sector.
Cutoff independence up to infinity.

De-Leon, Gazit, in preparation (2016)

A fully perturbative pionless EFT A=2, 3 calculation @NLO

- LO Parameters:
 - nn and 2-np Scattering lengths: ³S₁, ¹S₀.
 - pp scattering length.
 - Fine structure constant.
 - Three body force.
- NLO parameters:
 - 2 effective ranges.
 - Renormalizations of pp and 3NF.
 - (isospin dependent NLO 3NF to prevent logarithmic divergence in the binding energy of ³He).

Weak Interaction: LO (g_A – 1 body), NLO (L_{1A} – 2 body)

From neutron decay These parameters fixed using nuclear data

De-Leon, Gazit, in preparation (2016)

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Weak observables in two and three body nuclear systems:

е

 $n \rightarrow p + e^- + \overline{V}_e$

 \overline{V}_e

neutron decay: measured

$^{3}\text{H} \rightarrow ^{3}\text{He} + e^{-} + \overline{V}_{e}$

triton decay: measured

$p + p \rightarrow d + v_e + e^+$

е

Ve

Proton-proton fusion – needs to be predicted

A fully perturbative pionless EFT A=2, 3 calculation @NLO

- LO Parameters:
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De-Leon, Gazit, in preparation (2016)

The role of the deuteron tail

Many low energy reactions depend on deuteron normalization.

$$Z_d^{-1} = i \frac{\partial}{\partial_{p_0}} \frac{1}{i \mathcal{D}_t(p_0, p)} \Big|_{p_0 = \frac{\gamma_t^2}{M_N}, p = 0}$$

- One has a choice of rearranging the expansion:
 - rho-parameterization: $Z_d = \frac{1}{1 \gamma \rho} \approx 1 + \gamma \rho + (\gamma \rho)$ $Z_{d} = \frac{1}{1 - \gamma \rho} \approx 1 - (Z_{d} - 1) + 0 + \dots$
 - Z-parameterization:

Both are valid rearrangements! Z-parameterization has quicker convergence, especially for observables sensitive to the deuteron tail.

> Phillips, Rupak, Savage, Phys. Lett. **B473**, 209 (2000) Grießhammer, Nucl. Phys. A744, 192 (2004)

De-Leon, Gazit, in preparation (2016)
Advantages of π EFT for proton-proton fusion:

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Analogy between weak and EM:



Advantages of π EFT for proton-proton fusion:

Small number of parameters.
 Two NLO π EFT arrangements.
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De-Leon, Gazit, in preparation (2016)



Rho-parameterization





Adding the NLO 1-body contributions

De-Leon, Gazit, in preparation (2016)



Adding all contribution, but L_{1A}

1st estimate of theoretical uncertainty: All NLO contributions are of the same order (1-2%), one can estimate higher order effects as the NLO contribution.

1.8

1.65

1.6

 $\langle GT \rangle$



Adding all contributic

Translates to $\pm 2\%$ difference in pp fusion

1st estimate of theoretical uncertainty: All NLO contributions are of the same order (1-2%), one can estimate highe De-Leon, Gazit, in preparation (2016)



2nd estimate of theoretical uncertainty: difference between Zed and Rho Paramerizations.

De-Leon, Gazit, in preparation (2016)



Translates to $\pm 2\%$ difference in pp fusion

2nd estimate of theoretical uncertainty: difference between Zed and Rho Paramerizations.

De-Leon, Gazit, in preparation (2016)

So... is 3% too big to be called precision physics?

i.e., theoretical uncertainty of the same order of systematic experimental error due to g_A and ³H half life (2% total).



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- Pionless EFT reproduces low-energy <u>electromagnetic</u> observables to a very good precision (~1%), even at NLO.
- Theoretical uncertainty estimated from:
 - (Natural) Size of NLO contribution (all NLO contributions are of the same order of magnitude).
 - Difference between different arrangements of perturbative expansion.
 - Both error estimates lead to about 2% uncertainty.
- Proton-proton fusion NLO prediction and error assessment reliable!
- Uncertainty quantification challenges:

Is there a way to assign some confidence level to the theoretical uncertainty?

Is there a better way to incorporate experimental systematic uncertainties?



ATOMIC PHYSICS AT THE SOLAR INTERIOR: HOW WELL DO WE KNOW OUR SUN?

The Solar Interior

• Radiative zone: energy transport by photon diffusion.



A solar recipe



A solar recipe



Helioseismology: outer constraint

Neutrinos:





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differential probing of solar structure
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Metals are a major source of opacity in the Sun



- 98% H+He
- Other ~2% "<u>Metals</u>"
- A **Hot**-**Dense** Plasma (@R_{cz}: 180 eV, 0.5 g/cc; @center: 1.5 keV, 150 g/cc)
- Pressure is not affected by these "metals".
- However "metals" have many bound electrons: contribute to opacity!

M. Krief, A. Feigel, and D. Gazit, "Line broadening and the solar opacity problem", ApJ 2016

The Rosseland Opacity

Photon mean-free-path

$$l_v = \frac{1}{k_v} = \frac{1}{\rho \kappa_v}$$

Rosseland Mean

Energy
Flux

$$\mathbf{S}_{v} = -\frac{cl_{v}}{3} \nabla U_{P,v} = -\frac{c}{3k_{v}} \frac{dU_{P,v}}{dT} \nabla T$$

Planck Energy Density
 $\mathbf{S} = -\frac{cl_{R}}{3} \nabla U_{P}$
 $l_{R} = \frac{1}{k_{R}} = \frac{\int_{0}^{\infty} dv \frac{1}{k_{v}} \frac{dU_{P}}{dT}}{\int_{0}^{\infty} dv \frac{dU_{P}}{dT}}$





The Bound-Bound Opacity Spectra



Two major difficulties:

 For mid-Z and high-Z elements - a <u>HUGE</u> number of lines for each pair of configurations
 For hot plasmas - a <u>HUGE</u> number of atomic configurations must be included June 24, 2016

A Huge Number of Configurations In The Solar Interior





Unresolved Transition Arrays (UTA)

- In a hot plasma, the large number of lines between pairs of configurations often overlap and can be approximated by a single "effective" line
- Calculate only the moments of the effective lines







M. Krief, A. Feigel, and D. Gazit, *"Line broadening and the solar opacity problem"*, ApJ 2016 Blancard, et. Al ApJ 745.1 (2011): 10 & Iglesias et al. ApJ 464 (1996): 943.

A solar recipe



- Solar atmosphere spectra (1D\3D)
- Meteorites



- Hydrostatic
- 1D
- Opacities

.

- Eqs. of state (EOS)
- Nuclear rates
- •



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A solar recipe



Solar atmosphere spectra (1D\3D)

• Meteorites



- Hydrostatic
- 1D
- **Opacities**

.

- Eqs. of state (EOS)
- Nuclear rates
- •





- 20%~ less metals in new abundance determination
- Metals determine most of the opacity, but not EOS
- Solar opacities are exclusively theoretical
- Opacities are believed to be the "source" of the problem
- Other ideas <u>revised solar models</u> (magnetic fields, rotation, dark matter... etc.) no satisfactory model exists

- 2. F.L. Villante APJ 2010
- 3. Bergemann, and A Serenelli. 2014



Solar abundance problem opacity

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M. Krief, A. Feigel, and D. Gazit, *"Line broadening and the solar opacity problem"*, ApJ 2016 Blancard, et. Al ApJ 745.1 (2011): 10 & Iglesias et al. ApJ 464 (1996): 943.

Steps Towards Solution

- Point out and check physics "beyond" current state of the art atomic models
- Alternatively, point out and quantify <u>sources of</u> <u>uncertainty</u> in atomic models and check sensitivities
- We have developed state of the art atomic models in order to <u>investigate the source</u> of the solar opacity problem
- 1. M. Krief, A. Feigel, and D. Gazit, "Line broadening and the solar opacity problem", ApJ 2016
- 2. M. Krief, A. Feigel, and D. Gazit, "Solar opacity calculations using the super-transition-array method" ApJ, 2016
- 3. M. Krief, A. Feigel "Variance and shift of transition arrays for electric and magnetic multipole transitions", HEDP 2015
- 4. M. Krief, A. Feigel "The effect of first order superconfiguration energies on the opacity of hot dense matter", HEDP 2015 68



M. Krief, A. Feigel, and D. Gazit, *"Line broadening and the solar opacity problem"*, ApJ 2016 Blancard, et. Al ApJ 745.1 (2011): 10 & Iglesias et al. ApJ 464 (1996): 943.

Possible explanations?



Possible explanations?



Possible explanations?


Effect of heavy elements?

Calculation is possible only with STA



M. Krief, A. Feigel, and D. Gazit, *"Solar opacity calculations using the super-transition-array method"* ApJ, 821:45, 2016
Iglesias, C. A., Wilson, B. G., Rogers, F. J., Goldstein, W. H., Bar-Shalom, A., & Oreg, J. (1995). APJ, 445, 855-860.

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Possible explanations?

- Effect of the Plasma environment? Atchic calculation from gh-Z (i.e., c. aion of sper en a potentia, Source of problem T_H
- Line Shapes
- Level populations
- Line-Shifts (screening)



Photons Escape Through Opacity "Windows"



'5

Marcel Klapisch, APIP, April 2016

Uncertainties in collisional line broadening: enormous differences between models



Uncertainties in collisional line broadening: enormous differences between models





• No experimental data - what is the actual uncertainty of current models?

M. Krief, A. Feigel, and D. Gazit, "Line broadening and the solar opacity problem", ApJ 2016

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A factor of ~100 is needed to solve the problem quantitatively and qualitatively Sun (LSM) 40 widths $\times 50$ widths ×100 widths ×200 30 8 $\kappa_R/\kappa_R^{STAR}\!-\!1$ The sun 20 Helioseismology, neutrinos x200 x100 10 x50 -10L 0.0 0.1 0.2 0.4 0.5 0.7 0.3 0.6 R/R_{\odot}

The uncertainty may depend on the line, atomic number, temperature and density

A factor of ~100 is needed to solve the problem **quantitatively** and **qualitatively** $40 \xrightarrow[widths \times 50]{}$



The uncertainty may depend on the line, atomic number, temperature and density

M. Krief, A. Feigel, and D. Gazit, "Line broadening and the solar opacity problem", ApJ 2016

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A Rumsfeld type of summary 😳

Well, there are known knowns... and known unknowns... and of course, unknown unknowns... June 24, 2016

Summary...

I showed a few "qualitative" approaches to "quantitatively" assess theoretical uncertainties:



[•]The Ion-Sphere model

- The plasma is divided into <u>spherical cells</u>
- The density dictates the size of the "Wigner-Seitz" cell, in which neutrality is imposed
- The surrounding plasma of each cell is considered a heat bath

