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Ab Initio Nuclear Theory for Precision Electroweak Physics

Electroweak Physics InterseCtions — EPIC 2024 Calaserena Resort, Geremeas, Sardinia September 22-27, 2024

Petr Navratil

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Discovery, accelerated

Outline

- Introduction Ab initio nuclear theory no-core shell model (NCSM)
- *Ab initio* calculations of parity-violating moments
- ⁶He β-decay
- ⁷Li(p,e⁺e⁻)⁸Be internal pair creation and the X17 anomaly
- Conclusions & topics for discussion
- Backup slides muon capture on light nuclei, ¹⁶N beta decay

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Ab initio nuclear theory no-core shell model (NCSM)



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First principles or ab initio nuclear theory







Review Ab initio no core shell model Bruce R. Barrett^a, Petr Navrátil^b, James P. Vary^{C.}





- Basis expansion method
 - Harmonic oscillator (HO) basis truncated in a particular way (N_{max})

Conceptually simplest ab initio method: No-Core Shell Model (NCSM)

- Why HO basis?
 - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 – ⁴He, ¹⁶O, ⁴⁰Ca)
 - Equivalent description in relative(Jacobi)-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances

$$\Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi^{HO}_{Ni}(\vec{\eta}_{1}, \vec{\eta}_{2}, ..., \vec{\eta}_{A-1})$$

$$\Psi_{SD}^{A} = \sum_{N=0}^{N_{max}} \sum_{j} c_{Nj}^{SD} \Phi_{SDNj}^{HO}(\vec{r}_{1}, \vec{r}_{2}, ..., \vec{r}_{A}) = \Psi^{A} \varphi_{000}(\vec{R}_{CM})$$



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 $E = (2n + l + \frac{3}{2})\mathfrak{h}\Omega$



Novel chiral Hamiltonian and observables in light and medium-mass nuclei

V. Somà,^{1,*} P. Navrátil⁽⁰⁾,^{2,†} F. Raimondi,^{3,4,‡} C. Barbieri⁽⁶⁾,^{4,§} and T. Duguet^{1,5,||}

Binding energies of atomic nuclei with NN+3N forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
 - The Hamiltonian fully determined in A=2 and A=3,4 systems
 - Nucleon–nucleon scattering, deuteron properties, ³H and ⁴He binding energy, ³H half life
 - Light nuclei NCSM

Egs [MeV]

Medium mass nuclei – Self-Consistent Green's Function method

NN N³LO (Entem-Machleidt 2003) 3N N²LO w local/non-local regulator





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-10

-20 -30

-40

-50

-60

-70

-80

-90

-100

-110 -120

-130

Egs [MeV]

³He

Ή

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Ab initio calculations of parity-violating moments



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Why investigate the anapole moment and the EDM?

- Parity violation in atomic and molecular systems sensitive to a variety of "new physics"
 - Probes electron-quark electroweak interaction
 - Best limits on the Z' boson parity violating interaction with electrons and nucleons
- The EDM is a promising probe for CP violation beyond the standard model as well as CP violating QCD $\bar{\theta}$ parameter
 - Nuclear structure can enhance the EDM
 - Nuclear EDMs can be measured in storage rings (CERN feasibility study: arXiv:1912.07881)

Nuclear spin dependent parity violating effects in light polyatomic molecules

- Experiments proposed for ⁹BeNC, ²⁵MgNC
- To extract the underlying physics, atomic, molecular and nuclear structure effects must be understood
 - Ab initio calculations

- Spin dependent PV
 - Z-boson exchange between nucleon axialvector and electron-vector currents (b)
 - Electromagnetic interaction of atomic electrons with the nuclear anapole moment (c)



Parity violating nucleon-nucleon interaction

- Meson exchange approach
- Chiral EFT
- Unknown parameters (LECs)
 - DDH (1980) estimates based on the quark model
 - Experiments give conflicting limits on the weak couplings



AND BARRY R. HOLSTEIN Physics Division, National Science Foundation, Washington, D. C. 20550 $V_{12}^{\text{p.v.}} = \frac{f_{\pi}g_{\pi NN}}{2^{1/2}} i\left(\frac{\vec{\tau}_1 \times \vec{\tau}_2}{2}\right)^z (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \left[\frac{\vec{p}_1 - \vec{p}_2}{2M}, f_{\pi}(r)\right]$ $-g_{\rho}\left(h_{\rho}^{0}\vec{\tau}_{1}\cdot\vec{\tau}_{2}+h_{\rho}^{1}\left(\frac{\vec{\tau}_{1}+\vec{\tau}_{2}}{2}\right)^{z}+h_{\rho}^{2}\frac{(3\tau_{1}^{z}\tau_{2}^{z}-\vec{\tau}_{1}\cdot\vec{\tau}_{2})}{2(6)^{1/2}}\right)$ $\times \left((\vec{\sigma}_1 - \vec{\sigma}_2) \cdot \left\{ \frac{\vec{p}_1 - \vec{p}_2}{2M}, f_{\rho}(r) \right\} + i(1 + \chi_{v}) \, \vec{\sigma}_1 \times \vec{\sigma}_2 \cdot \left[\frac{\vec{p}_1 - \vec{p}_2}{2M}, f_{\rho}(r) \right]$ $-g_{\omega}\left(h_{\omega}^{0}+h_{\omega}^{1}\left(\frac{\check{\tau}_{1}+\check{\tau}_{2}}{2}\right)^{z}\right)$ $X \left(\left(ec{\sigma}_1 - ec{\sigma}_2
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annals of physics **124**, 449–495 (1980)

Unified Treatment of the Parity Violating Nuclear Force

BERTRAND DESPLANQUES*

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JOHN F. DONOGHUE[†]

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Center for Theoretical Physics, Laboratory for Nuclear Science and Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

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$$\begin{aligned} \mathscr{H}_{MNN}^{\mathbf{p}.\mathbf{v}.} &= (2)^{-1/2} f_{\pi} \overline{N} (\vec{\tau} \times \hat{\phi}^{\pi})^{3} N \\ &+ \overline{N} \left[h_{\rho}^{0} \vec{\tau} \cdot \hat{\phi}_{\mu}^{\rho} + h_{\rho}^{1} \phi_{\mu}^{\rho3} + h_{\rho}^{2} \frac{(3\tau^{3} \phi_{\mu}^{\rho3} - \vec{\tau} \cdot \hat{\phi}_{\mu}^{\rho})}{2(6)^{1/2}} \right] \gamma^{\mu} \gamma_{5} N \\ &+ \overline{N} [h_{\omega}^{0} \phi_{\mu}^{\omega} + h_{\omega}^{1} \tau^{3} \phi_{\mu}^{\omega}] \gamma^{\mu} \gamma_{5} N \\ &- h_{\rho}^{\prime 1} \overline{N} (\vec{\tau} \times \hat{\phi}_{\mu}^{\rho})^{3} \frac{\sigma^{\mu\nu} k_{\nu}}{2M} \gamma_{5} N. \end{aligned}$$
$$\begin{aligned} \mathscr{H}_{MNN}^{\mathbf{p}.\mathbf{c}.} &= i g_{\pi NN} \overline{N} \gamma_{5} \vec{\tau} \cdot \hat{\phi}^{\pi} N + g_{\rho} \overline{N} \left(\gamma_{\mu} + \frac{i \chi_{\nu}}{2M} \sigma_{\mu\nu} k^{\nu} \right) \vec{\tau} \cdot \hat{\phi}^{\mu\rho} N \end{aligned}$$

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Parity violating nucleon-nucleon interaction and the nuclear anapole moment

- Parity violating (non-conserving) V_{NN}^{PNC} interaction
 - Conserves total angular momentum I
 - Mixes opposite parities
 - Has isoscalar, isovector and isotensor components
 - Admixes unnatural parity states in the ground state

$$\begin{aligned} |\psi_{\rm gs} I\rangle &= |\psi_{\rm gs} I^{\pi}\rangle + \sum_{j} |\psi_{j} I^{-\pi}\rangle \\ &\times \frac{1}{E_{\rm gs} - E_{j}} \langle \psi_{j} I^{-\pi} | V_{\rm NN}^{\rm PNC} | \psi_{\rm gs} I^{\pi} \rangle \end{aligned}$$

$$\begin{split} V_{12}^{\mathbf{p},\mathbf{v}} &= \frac{f_{\pi}g_{\pi NN}}{2^{1/2}} i\left(\frac{\dot{\tau}_{1} \times \dot{\tau}_{2}}{2}\right)^{z} (\ddot{\sigma}_{1} + \ddot{\sigma}_{2}) \cdot \left[\frac{\vec{p}_{1} - \vec{p}_{2}}{2M}, f_{\pi}(r)\right] \\ \text{nts} &= g_{\rho} \left(h_{\rho}^{0} \dot{\tau}_{1} \cdot \dot{\tau}_{2} + h_{\rho}^{1} \left(\frac{\dot{\tau}_{1} + \dot{\tau}_{2}}{2}\right)^{z} + h_{\rho}^{2} \frac{(3\tau_{1}^{z}\tau_{2}^{z} - \dot{\tau}_{1} \cdot \dot{\tau}_{2})}{2(6)^{1/2}}\right) \\ \text{ate} &\times \left((\ddot{\sigma}_{1} - \ddot{\sigma}_{2}) \cdot \left\{\frac{\vec{p}_{1} - \vec{p}_{2}}{2M}, f_{\rho}(r)\right\} + i(1 + \chi_{v}) \, \ddot{\sigma}_{1} \times \ddot{\sigma}_{2} \cdot \left[\frac{\vec{p}_{1} - \vec{p}_{2}}{2M}, f_{\rho}(r)\right] \\ &- g_{\omega} \left(h_{\omega}^{0} + h_{\omega}^{1} \left(\frac{\dot{\tau}_{1} + \dot{\tau}_{2}}{2}\right)^{z}\right) \\ &\times \left((\ddot{\sigma}_{1} - \ddot{\sigma}_{2}) \cdot \left\{\frac{\vec{p}_{1} - \vec{p}_{2}}{2M}, f_{\omega}(r)\right\} + i(1 + \chi_{S}) \, \ddot{\sigma}_{1} \times \ddot{\sigma}_{2} \cdot \left[\frac{\vec{p}_{1} - \vec{p}_{2}}{2M}, f_{\omega}(r)\right] \\ &- (g_{\omega}h_{\omega}^{1} - g_{\rho}h_{\rho}^{1}) \left(\frac{\dot{\tau}_{1} - \dot{\tau}_{2}}{2}\right)^{z} \left(\ddot{\sigma}_{1} + \dot{\sigma}_{2}\right) \cdot \left\{\frac{\vec{p}_{1} - \vec{p}_{2}}{2M}, f_{\rho}(r)\right], \end{split}$$

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$$\times \frac{1}{E_{\rm gs} - E_{j}} \langle \psi_{j} I^{-\pi} | V_{\rm NN}^{\rm PNC} | \psi_{\rm gs} I^{\pi} \rangle$$

Anapole moment operator dominated by spin contribution

$$oldsymbol{a} = -\pi \int d^3 r \, r^2 \, oldsymbol{j}(oldsymbol{r})$$

$$\hat{\boldsymbol{a}}_{s} = \frac{\pi e}{m} \sum_{i=1}^{A} \mu_{i} (\boldsymbol{r}_{i} \times \boldsymbol{\sigma}_{i})$$
$$\mu_{i} = \mu_{p} (1/2 + t_{z,i}) + \mu_{n} (1/2 - t_{z,i})$$

$$a_s = \langle \psi_{\rm gs} \ I \ I_z = I | \hat{a}_{s,0}^{(1)} | \psi_{\rm gs} \ I \ I_z = I \rangle$$

Here is what we want to calculate:

$$\kappa_{A} = \frac{\sqrt{2}e}{G_{F}}a_{s} \qquad \qquad \kappa_{A} = -i4\pi \frac{e^{2}}{G_{F}}\frac{\hbar}{mc}\frac{(II10|II)}{\sqrt{2I+1}} \sum_{j} \langle \psi_{\rm gs} \ I^{\pi} ||\sqrt{4\pi/3}\sum_{i=1}^{A}\mu_{i}r_{i}[Y_{1}(\hat{r}_{i})\sigma_{i}]^{(1)}||\psi_{j} \ I^{-\pi} \rangle \frac{1}{E_{\rm gs} - E_{j}} \langle \psi_{j} \ I^{-\pi} |V_{\rm NN}^{\rm PNC}|\psi_{\rm gs} \ I^{\pi} \rangle$$

NCSM applications to parity-violating moments: How to calculate the sum of intermediate unnatural parity states?

$$a_s = \langle \psi_{\rm gs} \ I \ I_z = I | \hat{a}_{s,0}^{(1)} | \psi_{\rm gs} \ I \ I_z = I \rangle$$

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- Solving Schroedinger equation with inhomogeneous term $(E_{\rm gs} H)|\psi_{\rm gs} \ I\rangle = V_{\rm NN}^{\rm PNC}|\psi_{\rm gs} \ I^{\pi}\rangle$
- To invert this equation, we apply the Lanczos algorithm



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Solving Schroedinger equation with inhomogeneous term

 $(E_{\rm gs} - H)|\psi_{\rm gs} I\rangle = V_{\rm NN}^{\rm PNC}|\psi_{\rm gs} I^{\pi}\rangle$

- To invert this equation, we apply the Lanczos algorithm
 - Bring matrix to tri-diagonal form (v_1 , v_2 ... orthonormal, H Hermitian)

 $H\mathbf{v}_{1} = \partial_{1}\mathbf{v}_{1} + b_{1}\mathbf{v}_{2}$ $H\mathbf{v}_{2} = b_{1}\mathbf{v}_{1} + \partial_{2}\mathbf{v}_{2} + b_{2}\mathbf{v}_{3}$ $H\mathbf{v}_{3} = b_{2}\mathbf{v}_{2} + \partial_{3}\mathbf{v}_{3} + b_{3}\mathbf{v}_{4}$ $H\mathbf{v}_{4} = b_{3}\mathbf{v}_{3} + \partial_{4}\mathbf{v}_{4} + b_{4}\mathbf{v}_{5}$

- nth iteration computes 2nth moment
- Eigenvalues converge to extreme (largest in magnitude) values
- ~ 150-200 iterations needed for 10 eigenvalues (even for 10⁹ states)



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$$|\psi_{\rm gs} I\rangle = |\psi_{\rm gs} I^{\pi}\rangle + \sum_{j} |\psi_{j} I^{-\pi}\rangle \frac{1}{E_{\rm gs} - E_{j}} \langle \psi_{j} I^{-\pi} | V_{\rm NN}^{\rm PNC} | \psi_{\rm gs} I^{\pi}\rangle$$

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- To invert this equation, we apply the Lanczos algorithm

$$|\mathbf{v}_1\rangle = V_{\rm NN}^{\rm PNC} |\psi_{\rm gs} \ I^{\pi}\rangle$$

$$\psi_{\rm gs} I \rangle \approx \sum_k g_k(E_0) |\mathbf{v}_k\rangle$$

$$\hat{g}_1(\omega) = \frac{1}{\omega - \alpha_1 - \frac{\beta_1^2}{\omega - \alpha_2 - \frac{\beta_2^2}{\omega - \alpha_3 - \beta_3^2}}}$$

Lanczos continued fraction method



Few-Body Systems 33, 259-276 (2003) DOI 10.1007/s00601-003-0017-z



Prin

Efficient Method for Lorentz Integral Transforms of Reaction Cross Sections

 $a_s = \langle \psi_{gs} I I_z = I | \hat{a}_{s,0}^{(1)} | \psi_{gs} I I_z = I \rangle$

M. A. Marchisio¹, N. Barnea², W. Leidemann¹, and G. Orlandini¹

Parity and time-reversal violating nucleon-nucleon interaction

Introduced through Hamiltonian H_{PVTV} :

PHYSICAL REVIEW C 70, 055501 (2004)

P- and *T*-odd two-nucleon interaction and the deuteron electric dipole moment

$$H_{PVTV}(\mathbf{r}) = \frac{1}{2m_n} \boldsymbol{\sigma}_- \cdot \nabla \left(-\bar{G}^0_\omega y_\omega(r) \right)$$

$$+ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \, \boldsymbol{\sigma}_- \cdot \nabla \left(\bar{G}^0_\pi y_\pi(r) - \bar{G}^0_\rho y_\rho(r) \right)$$

$$+ \frac{\boldsymbol{\tau}_+^z}{2} \boldsymbol{\sigma}_- \cdot \nabla \left(\bar{G}^1_\pi y_\pi(r) - \bar{G}^1_\rho y_\rho(r) - \bar{G}^1_\omega y_\omega(r) \right)$$

$$+ \frac{\boldsymbol{\tau}_-^z}{2} \boldsymbol{\sigma}_+ \cdot \nabla \left(\bar{G}^1_\pi y_\pi(r) + \bar{G}^1_\rho y_\rho(r) - \bar{G}^1_\omega y_\omega(r) \right)$$

$$+ (3\tau_1^z \tau_2^z - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \boldsymbol{\sigma}_- \cdot \nabla \left(\bar{G}^2_\pi y_\pi(r) - \bar{G}^2_\rho y_\rho(r) \right)$$

- Based on one meson exchange model
- $y_x(r) = e^{-m_x r}/(4\pi r)$

$$\sigma_{\pm} = \sigma_1 \pm \sigma_2$$
$$\tau_{\pm}^z = \tau_1^z \pm \tau_2^z$$

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- Based on one meson exchange model
- $y_{\chi}(r) = e^{-m_{\chi}r}/(4\pi r)$
- Coupling constants

Parity and time-reversal violating nucleon-nucleon interaction and nuclear EDM or Schiff moment ²¹ H_{PVTV} introduces parity admixture in the ground state (perturbation theory):

$$|0\rangle \longrightarrow |0\rangle + |\tilde{0}\rangle$$
$$|\tilde{0}\rangle = \sum_{n \neq 0} \frac{1}{E_0 - E_n} |n\rangle \langle n|H_{PVTV}|0\rangle$$

Nuclear EDM is dominated by polarization contribution:

$$D^{(pol)} = \langle 0 | \widehat{D}_z | \widetilde{0} \rangle + c.c.$$

$$S = \frac{e}{10} \sum_{i=1}^{Z} \left(r_i^2 \boldsymbol{r}_i - \frac{5}{3} \langle r^2 \rangle_{ch} \boldsymbol{r}_i \right)$$
$$\widehat{D}_Z = \frac{e}{2} \sum_{i=1}^{A} \left(1 + \tau_i^Z \right) z_i$$

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 $|0\rangle \longrightarrow |0\rangle + |\tilde{0}\rangle$

Low lying states of opposite parity can lead to enhancement!

Ab initio calculations of electric dipole moments of light nuclei

Paul Froese^{*} TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada and Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

> Petr Navrátil ©[†] TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

N_{max} convergence for ³He N³LO NN



³He EDM Benchmark Calculation

Discrepancy between calculations?

	PLB 665:165-172 (2008) (NN EFT)	PRC 87:015501 (2013)	PRC 91:054005 (2015)	Our calculation (NN EFT)
\overline{G}_{π}^{0}	0.015	(x 1/2)	(x 1/2)	0.0073 (x 1/2)
\overline{G}_{π}^{1}	0.023	(x 1/2)	(x 1/2)	0.011 (x 1/2)
\overline{G}_{π}^{2}	0.037	(x 1/5)	(x 1/2)	0.019 (x 1/2)
$\overline{G}^0_ ho$	-0.0012	(x 1/2)	(x 1/2)	-0.00062 (x 1/2)
$\overline{G}^1_ ho$	0.0013	(x 1/2)	(x 1/2)	0.00063 (x 1/2)
$\overline{G}_{ ho}^2$	-0.0028	(x 1/5)	(x 1/2)	-0.0014 (x 1/2)
\overline{G}^0_ω	0.0009	(x 1/2)	(x 1/2)	0.00042 (x 1/2)
\overline{G}^1_ω	-0.0017	(x 1/2)	(x 1/2)	-0.00086 (x 1/2)

Our results confirm those of Yamanaka and Hiyama, PRC 91:054005 (2015)

NCSM applications to parity-violating moments: EDMs of light stable nuclei







Editors' Suggestion

Nuclear spin-dependent parity-violating effects in light polyatomic molecules

Yongliang Hao[®],¹ Petr Navrátil[®],² Eric B. Norrgard[®],³ Miroslav Iliaš[®],⁴ Ephraim Eliav,⁵ Rob G. E. Timmermans[®],¹ Victor V. Flambaum[®],⁶ and Anastasia Borschevsky[®],^{*} 25

Nuclear spin-dependent parity-violating effects from NCSM

Contributions from nucleon axial-vector and the anapole moment

	⁹ Be	¹³ C	14 N	15 N	²⁵ Mg
I^{π}	3/2-	1/2-	1+	1/2-	$5/2^{+}$
$\mu^{ ext{exp.}}$	-1.177^{a}	0.702 ^b	0.404 ^c	-0.283^{d}	-0.855 ^e
		NCSM	calculations		
μ	-1.05	0.44	0.37	-0.25	-0.50
κ _A	0.016	-0.028	0.036	0.088	0.035
$\langle s_{p,z} \rangle$	0.009	-0.049	-0.183	-0.148	0.06
$\langle s_{n,z} \rangle$	0.360	-0.141	-0.1815	0.004	0.30
$\kappa_{\rm ax}$	0.035	-0.009	0.0002	0.015	0.024
ĸ	0.050	-0.037	0.037	0.103	0.057

$$\kappa_{ax} \simeq -2C_{2p} \langle s_{p,z} \rangle - 2C_{2n} \langle s_{n,z} \rangle \simeq -0.1 \langle s_{p,z} \rangle + 0.1 \langle s_{n,z} \rangle$$
$$\langle s_{\nu,z} \rangle \equiv \langle \psi_{gs} I^{\pi} I_z = I | \hat{s}_{\nu,z} | \psi_{gs} I^{\pi} I_z = I \rangle$$
$$C_{2p} = -C_{2n} = g_A (1 - 4 \sin^2 \theta_W) / 2 \simeq 0.05$$



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⁶He β-decay



Discovery, accelerated

- Precision measurements of β-decay observables offer the possibility to search for deviations from the Standard Model
 - β-decay observables are sensitive to interference of currents of SM particles and hypothetical BSM physics
 - Discovering such small deviations from the SM predictions demands also high-precision theoretical calculations
 - ⇒ Nuclear structure calculations with quantified uncertainties

⁶He β-decay

Decay rate proportional to

$$d\omega \propto 1 + a_{\beta\nu}\vec{\beta}\cdot\hat{\nu} + b_{\mathrm{F}}\frac{m_e}{E} \qquad \qquad \vec{\beta} = \frac{\vec{k}}{E} \quad \vec{\nu} = \nu\hat{\nu}$$

- $a_{\beta\nu}$ angular correlation coefficient between the emitted electron and the antineutrino
- *b*_F Fierz interference term that can be extracted from electron energy spectrum measurements
- The V-A structure of the weak interaction in the Standard Model implies for a Gamow-Teller transition
 - $a_{\beta\nu} = -\frac{1}{3}$

 $b_{\rm F}=0$





In the presence of Beyond the Standard Model interactions

$$a_{\beta\nu}^{\text{BSM}} = -\frac{1}{3} \left(1 - \frac{|C_T|^2 + |C_T'|^2}{2|C_A|^2} \right)$$

 $b_{\text{Fierz}}^{\text{BSM}} = \frac{C_T + C_T'}{C_A}$

- with tensor and pseudo-tensor contributions
- However, deviations also within the Standard Model caused by the finite momentum transfer, higher-order transition operators, and nuclear structure effects
 - Detailed, accurate, and precise calculations required





Higher-order Standard Model recoil and shape corrections

 $a_{\beta\nu}^{1^{+}\beta^{-}} = -\frac{1}{2} \left(1 + \tilde{\delta}_{a}^{1^{+}\beta^{-}} \right)$ $b_{\rm F}^{1^+\beta^-} = \delta_{\rm h}^{1^+\beta^-}$ $\delta_1^{1+\beta^-} \equiv \frac{2}{3} \Re \epsilon \left[-E_0 \frac{\langle \| \hat{C}_1^A / q \| \rangle}{\langle \| \hat{L}_1^A \| \rangle} + \sqrt{2} \left(E_0 - 2E \right) \frac{\langle \| \hat{M}_1^V / q \| \rangle}{\langle \| \hat{L}_1^A \| \rangle} \right]$ $-\frac{4}{7}ER\alpha Z_f-\frac{233}{630}\left(\alpha Z_f\right)^2,$ $\tilde{\delta}_{a}^{1+\beta^{-}} \equiv \frac{4}{3} \Re e \left[2E_{0} \frac{\langle \|\hat{C}_{1}^{A}/q\| \rangle}{\langle \|\hat{L}_{1}^{A}\| \rangle} + \sqrt{2} \left(E_{0} - 2E \right) \frac{\langle \|\hat{M}_{1}^{V}/q\| \rangle}{\langle \|\hat{L}_{1}^{A}\| \rangle} \right]$ $+\frac{4}{7}ER\alpha Z_f-\frac{2}{5}E_0R\alpha Z_f,$ $\delta_b^{1^+\beta^-} \equiv \frac{2}{3} m_e \Re e \left[\frac{\langle \| \hat{C}_1^A / q \| \rangle}{\langle \| \hat{L}_1^A \| \rangle} + \sqrt{2} \frac{\langle \| \hat{M}_1^V / q \| \rangle}{\langle \| \hat{L}_1^A \| \rangle} \right],$

$$\vec{q} = \vec{k} + \vec{v}$$
 momentum transfer

 \hat{C}_1^A axial charge

 \hat{M}_1^V vector magnetic or weak magnetism

 $\hat{L}_1^A \propto 1$ Gamow-Teller leading order

 \hat{C}_1^A \hat{M}_1^V NLO recoil corrections, order q/m_N

/doi.org/10.1088/1361-6471/ac7ed
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Higher-order Standard Model recoil and shape corrections

$$\frac{\hat{C}_{JM_{J}}^{A}}{q} = \sum_{j=1}^{A} \frac{i}{m_{N}} \left[g_{A} \hat{\Omega}_{JM_{J}}^{\prime}(q\vec{r}_{j}) - \frac{1}{2} \frac{\tilde{g}_{P}}{2m_{N}} \left(E_{0} + \Delta E_{c} \right) \hat{\Sigma}_{JM_{J}}^{\prime\prime}(q\vec{r}_{j}) \right] \tau_{j}^{+},$$

$$\hat{L}_{JM_{J}}^{A} = \sum_{j=1}^{A} i \left(g_{A} + \frac{\tilde{g}_{P}}{(2m_{N})^{2}} q^{2} \right) \hat{\Sigma}_{JM_{J}}^{\prime\prime}(q\vec{r}_{j}) \tau_{j}^{+},$$

$$\frac{\hat{M}_{JM_{J}}^{V}}{q} = \sum_{j=1}^{A} \frac{-i}{m_{N}} \left[g_{V} \hat{\Delta}_{JM_{J}}(q\vec{r}_{j}) - \frac{1}{2} \mu \hat{\Sigma}_{JM_{J}}^{\prime}(q\vec{r}_{j}) \right] \tau_{j}^{+}$$

Hadronic vector, axial vector and pseudo-scalar charges

$$g_V = 1$$
 $g_A = -1.2756(13)$ $\tilde{g}_P = -\frac{(2m_N)^2}{m_\pi^2 - q^2} g_A$

 $\mu \approx 4.706$ is the nucleon isovector magnetic moment $\Delta E_c \equiv \langle {}^{6}\text{Li} \ 1^{+}_{gs} | V_c | {}^{6}\text{Li} \ 1^{+}_{gs} \rangle - \langle {}^{6}\text{He} \ 0^{+}_{gs} | V_c | {}^{6}\text{He} \ 0^{+}_{gs} \rangle$

$$\hat{\Sigma}_{JM_{J}}^{\prime\prime}(q\vec{r}_{j}) = \left[\frac{1}{q}\vec{\nabla}_{\vec{r}_{j}}M_{JM_{J}}(q\vec{r}_{j})\right] \cdot \vec{\sigma}(j),$$

$$\hat{\Omega}_{JM_{J}}^{\prime}(q\vec{r}_{j}) = M_{JM_{J}}(q\vec{r}_{j}) \vec{\sigma}(j) \cdot \vec{\nabla}_{\vec{r}_{j}} + \frac{1}{2}\hat{\Sigma}_{JM_{J}}^{\prime\prime}(q\vec{r}_{j}),$$

$$\hat{\Delta}_{JM_{J}}(q\vec{r}_{j}) = \vec{M}_{JJM_{J}}(q\vec{r}_{j}) \cdot \frac{1}{q}\vec{\nabla}_{\vec{r}_{j}},$$

$$\hat{\Sigma}_{JM_{J}}^{\prime}(q\vec{r}_{j}) = -i\left[\frac{1}{q}\vec{\nabla}_{\vec{r}_{j}} \times \vec{M}_{JJM_{J}}(q\vec{r}_{j})\right] \cdot \vec{\sigma}(j),$$

$$M_{JM_{J}}(q\vec{r}_{j}) = j_{J}(qr_{j})Y_{JM_{J}}(\hat{r}_{j}),$$

$$\vec{M}_{JLM_{J}}(q\vec{r}_{j}) = j_{L}(qr_{j})\vec{Y}_{JLM_{J}}(\hat{r}_{j})$$

Ultimately, we need to calculate ${}^{6}\text{He}(0^{+} 1) \rightarrow {}^{6}\text{Li}(1^{+} 0)$ matrix elements of these "one-body" operators





Apply *ab initio* No-Core Shell Model to calculate the ⁶Li and ⁶He wave functions and the operator matrix elements

Matrix elements of the relevant operators

$$\begin{split} \hat{\Sigma}_{JM_J}^{\prime\prime}(q\vec{r}_j) &= \left[\frac{1}{q}\vec{\nabla}_{\vec{r}_j}M_{JM_J}(q\vec{r}_j)\right]\cdot\vec{\sigma}(j),\\ \hat{\Omega}_{JM_J}^{\prime}(q\vec{r}_j) &= M_{JM_J}(q\vec{r}_j)\,\vec{\sigma}(j)\cdot\vec{\nabla}_{\vec{r}_j} + \frac{1}{2}\hat{\Sigma}_{JM_J}^{\prime\prime}(q\vec{r}_j),\\ \hat{\Delta}_{JM_J}(q\vec{r}_j) &= \vec{M}_{JJM_J}(q\vec{r}_j)\cdot\frac{1}{q}\vec{\nabla}_{\vec{r}_j},\\ \hat{\Sigma}_{JM_J}^{\prime}(q\vec{r}_j) &= -i\left[\frac{1}{q}\vec{\nabla}_{\vec{r}_j}\times\vec{M}_{JJM_J}(q\vec{r}_j)\right]\cdot\vec{\sigma}(j), \end{split}$$

- Convergence investigation
 - Variation of HO frequency
 - hΩ = 16 24 MeV
 - Variation of basis size
 - $N_{\text{max}} = 0 14 \text{ for NNLO}_{\text{opt}}$
 - $N_{\text{max}} = 0 12 \text{ for NNLO}_{\text{sat}}$



Petr Navráti

Overall results for ⁶He(0⁺ 1) \rightarrow ⁶Li(1⁺ 0) + e⁻ + $\overline{\nu}$

- We find up to 1% correction for the β spectrum and up to 2% correction for the angular correlation
- Propagating nuclear structure and χ EFT uncertainties results in an overall uncertainty of 10⁻⁴
 - Comparable to the precision of current experiments

$$b_{\rm F}^{1^+\beta^-} = \delta_b^{1^+\beta^-} = -1.52\,(18)\cdot 10^{-3}$$

$$\left\langle \tilde{\delta}_{a}^{1^{+}\beta^{-}} \right\rangle = -2.54\,(68)\cdot 10^{-3}$$

Non-zero Fierz interference term due to nuclear structure corrections



Nuclear *ab initio* calculations of ⁶He β -decay for beyond the Standard Model studies Ayala Glick-Magid^a, Christian Forssén^{b,*}, Daniel Gazda^c, Doron Gazit^{a,*}, Peter Gysbers^{d,e}, Petr Navrátil^d



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Super-allowed Fermi transitions - electroweak radiative correction δ_{NS}



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Synergy of precision experiments and *ab initio* nuclear theory to test CKM unitarity Structure corrections for the extraction of the V_{ud} matrix element from the ¹⁰C \rightarrow ¹⁰B Fermi transition



- δ_{NS} parametrizes correction to free γW box
- Ab initio no-core shell model (NCSM)
 - A very good convergence consistent with what used in latest evaluation with a substantially reduced theoretical uncertainties

$$\delta_{NS} = 2\left[\Box_{\gamma W}^{VA, \text{nuc.}} - \Box_{\gamma W}^{VA, \text{free n}}\right]$$

An *ab initio* strategy for taming the nuclear-structure dependence of V_{ud} extractions: the ${}^{10}C \rightarrow {}^{10}B$ superallowed transition arXiv: 2405.19281

Michael Gennari^{1,2}, Mehdi Drissi¹, Mikhail Gorchtein^{3,4}, Petr Navrátil^{1,2}, and Chien-Yeah Seng^{5,6}

NCSM applicable also to ${}^{14}O \rightarrow {}^{14}N$ and possibly ${}^{18}Ne \rightarrow {}^{18}F$, ${}^{22}Mg \rightarrow {}^{22}Na$



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Isospin-symmetry breaking correction δ_{C}



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The pathway to δ_{C}

δ_C in *ab initio* NCSM over 20 years ago

PHYSICAL REVIEW C 66, 024314 (2002)

Ab initio shell model for A = 10 nuclei

E. Caurier,¹ P. Navrátil,² W. E. Ormand,² and J. P. Vary³ ¹Institut de Recherches Subatomiques (IN2P3-CNRS-Université Louis Pasteur), Batiment 27/1, 67037 Strasbourg Cedex 2, France ²Lawrence Livermore National Laboratory, L-414, P.O. Box 808, Livermore, California 94551 ³Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011 (Received 10 May 2002; published 13 August 2002)



The pathway to δ_C

• δ_{C} in *ab initio* NCSM now



The pathway to δ_{C}



Isospin-symmetry breaking interaction admixes continuum intruder states in the ground state

- Poorly described in the HO expansion
- Need to include continuum effects explicitly
- → No-Core Shell Model with Continuum

Combine NCSM with resonating group method (RGM)



Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

$$Y^{(A)} = \mathop{a}_{l} c_{l} \left| \stackrel{(A)}{\Longrightarrow}, l \right\rangle + \mathop{a}_{n} \grave{0} d\vec{r} g_{v}(\vec{r}) \hat{A}_{n} \left| \stackrel{\bullet}{\underbrace{\bullet}}_{(A-a)}^{\vec{r}} \stackrel{\bullet}{\bullet}, n \right\rangle$$

IOP Publishing | Royal Swedish Academy of Sciences
Phys. Scr. 91 (2016) 053002 (38pp)

Physica Scripta doi:10.1088/0031-8949/91/5/053002

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Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil¹, Sofia Quaglioni², Guillaume Hupin^{3,4}, Carolina Romero-Redondo² and Angelo Calci¹

S. Baroni, P. Navratil, and S. Quaglioni, PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

$$Y^{(A)} = \bigotimes_{I}^{a} c_{I} | \stackrel{(A)}{\Longrightarrow}, I \rangle + \bigotimes_{n}^{a} \bigotimes_{n}^{b} d\vec{r} g_{v}(\vec{r}) \hat{A}_{n} | \underset{(A-a)}{\overset{\vec{r}}{\Longrightarrow}}, n \rangle$$

$$N = N_{\max} + 1 \xrightarrow{\overset{(A)}{\longrightarrow}} \hbar\Omega$$

$$N = 1 \xrightarrow{\Delta E} = N_{\max} \hbar\Omega$$

$$N = 0$$

Static solutions for aggregate system, describe all nucleons close together

Phys. Scr. 91 (2016) 053002 (38pp)

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Unified *ab initio* approaches to nuclear structure and reactions

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Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)



Static solutions for aggregate system, describe all nucleons close together

S. Baroni, P. Navratil, and S. Quaglioni, PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

structure and reactions

Petr Navrátil¹, Sofia Quaglioni², Guillaume Hupin^{3,4}, Carolina Romero-Redondo² and Angelo Calci¹

Unified *ab initio* approaches to nuclear

Invited Comment

doi:10.1088/0031-8949/91/5/05

Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)



Static solutions for aggregate system, describe all nucleons close together

Continuous microscopic cluster states, describe long-range projectile-target

> OP Publishing | Boyal Swedish Academy of Sci Phys. Scr. 91 (2016) 053002 (38pp doi:10.1088/0031

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil¹, Sofia Quaglioni², Guillaume Hupin^{3,4}, Carolina Romero-Redondo² and Angelo Calci

S. Baroni, P. Navratil, and S. Quaglioni, PRL 110, 022505 (2013); PRC 87, 034326 (2013).

Ab initio calculation of the β decay from ¹¹Be to a ¹⁰Be + p resonance

Compute Fermi matrix element in NCSMC

 $\delta_{\rm C}$ in NCSMC

$$M_F = \left\langle \Psi^{J^{\pi}T_f M_{T_f}} \Big| T_+ \Big| \Psi^{J^{\pi}T_i M_{T_i}} \right\rangle \longrightarrow |M_F|^2 = |M_{F0}|^2 (1 - \delta_C)$$

• Total isospin operator $T_+ = T_+^{(1)} + T_+^{(2)}$ for partitioned system

$$M_{F} \sim \left\langle A\lambda_{f}J_{f}T_{f}M_{T_{f}}|T_{+}|A\lambda_{J_{i}}T_{i}M_{T_{i}}\rangle + \left\langle A\lambda J_{f}T_{f}M_{T_{f}}|T_{+}\mathcal{A}_{\nu i}|\Phi_{\nu r}^{J_{i}T_{i}M_{T_{i}}}\rangle \right\rangle + \left\langle \Phi_{\nu r}^{J_{f}T_{f}M_{T_{f}}}|\mathcal{A}_{\nu f}T_{+}\mathcal{A}_{\nu i}|\Phi_{\nu r}^{J_{i}T_{i}M_{T_{i}}}\rangle \right\rangle$$

$$NCSM matrix element$$

$$NCSM Cluster metrix element$$

$$Continuum (cluster) matrix element$$

NCSM-Cluster matrix elements

¹⁰C structure from chiral EFT NN(N⁴LO)+3N(N²LO,InI) interaction ($N_{max} = 9$)

$$|^{10}\mathrm{C}\rangle = \sum_{\alpha} c_{\alpha} |^{10}\mathrm{C}, \alpha\rangle_{\mathrm{NCSM}} + \sum_{\nu} \int dr \,\gamma_{\nu}^{J^{\pi}T}(r)\mathcal{A}_{\nu} |^{9}\mathrm{B} + \mathrm{p}, \nu\rangle$$

- Treat as mass partition of proton plus ⁹B
- Use 3/2⁻ and 5/2⁻ states of ⁹B
- Known bound states captured by NCSMC

State	E _{NCSM} (MeV)	E (MeV)	E _{exp} (MeV)
0+	-3.09	-3.46	-4.006
2+	+0.40	-0.03	-0.652



¹⁰C structure from chiral EFT NN(N⁴LO)+3N(N²LO,InI) interaction ($N_{max} = 9$)



¹⁰B structure from chiral EFT NN(N⁴LO)+3N(N²LO,InI) interaction ($N_{max} = 9$)

$$|^{10}\mathrm{B}\rangle = \sum_{\alpha} c_{\alpha} |^{10}\mathrm{B}, \alpha\rangle_{\mathrm{NCSM}} + \sum_{\nu} \int dr \,\gamma_{\nu}(r)\mathcal{A}_{\nu} |^{9}\mathrm{Be} + p, \nu\rangle + \sum_{\mu} \int dr \,\gamma_{\mu}(r)\mathcal{A}_{\mu} |^{9}\mathrm{B} + n, \mu\rangle$$



Use 3/2⁻ and 5/2⁻ states of ⁹B and ⁹Be
Eight of twelve bound states predicted

State	E (MeV)	E _{exp} (MeV)
3+	-5.75	-6.5859
1+	-5.33	-5.8676
0+	-4.30	-4.8458
1+	-4.26	-4.4316
2+	-2.69	-2.9988
2+	-0.93	-1.4220
2+	-0.70	-0.6664
4+	-0.19	-0.5609

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⁷Li(p,e⁺e⁻)⁸Be internal pair creation and the X17 anomaly



Discovery, accelerate



Fig. from PLB 813, 136061 (2021)

NCSMC calculations of ⁸Be structure and ⁷Li+p scattering and capture

Wave function ansatz

$$\Psi_{\mathsf{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} \left| {}^{8}\mathrm{Be}, \lambda \right\rangle + \sum_{\nu} \int \mathrm{d}r \gamma_{\nu}(r) \hat{A}_{\nu} \left| {}^{7}\mathrm{Li} + p, \nu \right\rangle + \sum_{\mu} \int \mathrm{d}r \gamma_{\mu}(r) \hat{A}_{\mu} \left| {}^{7}\mathrm{Be} + n, \mu \right\rangle$$

- 3/2⁻, 1/2⁻, 7/2⁻, 5/2⁻, 5/2⁻ ⁷Li and ⁷Be states in cluster basis
- 15 positive and 15 negative parity states in ⁸Be composite state basis



TUNL Nuclear Data Evaluation Project

NCSMC calculations of ⁸Be structure and ⁷Li+p scattering and capture

Wave function ansatz

$$\Psi_{\mathsf{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} \left| {}^{8}\mathrm{Be}, \lambda \right\rangle + \sum_{\nu} \int \mathrm{d}r \gamma_{\nu}(r) \hat{A}_{\nu} \left| {}^{7}\mathrm{Li} + p, \nu \right\rangle + \sum_{\mu} \int \mathrm{d}r \gamma_{\mu}(r) \hat{A}_{\mu} \left| {}^{7}\mathrm{Be} + n, \mu \right\rangle$$

- 3/2⁻, 1/2⁻, 7/2⁻, 5/2⁻, 5/2⁻ ⁷Li and ⁷Be states in cluster basis
- 15 positive and 15 negative parity states in ⁸Be composite state basis





⁸Be structure – calculated positive-parity eigenphase shifts





Additional resonances are seen compared to TUNL data

PHYSICAL REVIEW C 110, 015503 (2024)

Editors' Suggestion

Ab initio investigation of the ${}^{7}\text{Li}(p, e^+e^-){}^{8}\text{Be}$ process and the X17 boson

- Motivated by ATOMKI experiments (Firak, Krasznahorkay et al., EPJ Web of Conferences 232, 04005 (2020))
- No-core shell model with continuum (NCSMC) with wave function ansatz

$$\Psi_{\mathsf{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} \left| {}^{8}\mathrm{Be}, \lambda \right\rangle + \sum_{\nu} \int \mathrm{d}r \gamma_{\nu}(r) \hat{A}_{\nu} \left| {}^{7}\mathrm{Li} + p, \nu \right\rangle + \sum_{\mu} \int \mathrm{d}r \gamma_{\mu}(r) \hat{A}_{\mu} \left| {}^{7}\mathrm{Be} + n, \mu \right\rangle$$



Internal electron-positron pair conversion correlation



Calculating properly the pair production cross section with the interference of different multipoles improves description.

Still not a perfect agreement with ATOMKI data

PHYSICAL REVIEW C 110, 015503 (2024)

Editors' Suggestion

Ab initio investigation of the ${}^{7}\text{Li}(p, e^+e^-){}^{8}\text{Be}$ process and the X17 boson

P. Gysbers ^{1,2,3} P. Navrátil^{1,4} K. Kravvaris^{1,5} G. Hupin^{1,6} and S. Quaglioni⁵



New ATOMKI measurements in-between & at resonance energies

N. J. Sas et al., "Observation of the X17 anomaly in the ⁷Li(p,e^+e^-)⁸Be direct proton-capture reaction," arXiv:2205.07744



NCSMC calculations match well resonance data. Disagree in-between resonances – flat E1 distribution. Proton slow-down in the thick target?

Modeling hypothetical X17 boson

Integrated cross sections ⁷Li $(p, X)^8$ Be 10^{-2} σ_{γ} $-- \sigma_{\gamma}(M1)$ $\sigma_{\gamma}(E1)$ 10^{-4} $\sigma_{\gamma \to ee}$ σ_{E} σ_V 10^{-6} σ_A Data: γ_0 [q] 10^{-8} 10^{-10} Using g_x estimates from Backens et al. arXiv:2110.06055 10^{-12} -0.20.40.6 0.81.01.21.4 0.0E [MeV]

Gamma capture data: Zahnow *et al.* Z.Phys.A **351** 229-236 (1995)



PHYSICAL REVIEW C 110, 015503 (2024)

Editors' Suggestion

Ab initio investigation of the ${}^{7}\text{Li}(p, e^+e^-){}^{8}\text{Be}$ process and the X17 boson

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Conclusions & topics for discussion



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Conclusions & topics for discussion

- Ab initio nuclear theory
 - Makes connections between the low-energy QCD and many-nucleon systems
- No-core shell model is an *ab initio* extension of the original nuclear shell model
 - Applicable to nuclear structure, reactions including those relevant for astrophysics, electroweak processes, tests of fundamental symmetries

Open questions

- How to accurately and precisely evaluate the isospin-symmetry breaking correction $\delta_{\rm C}$?
- How to evaluate the radiative nuclear structure correction δ_{NS} beyond light nuclei?
- What is the importance of sub-leading chiral 3N contributions for electro-weak processes in nuclei?
- What is the particle physics interpretation of the X17 anomaly?

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Backup slides



Discovery, accelerated

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2024-09-24

Unique first-forbidden beta decay $^{16}N(2^{-}) \rightarrow {}^{16}O(0^{+})$

- The unique first-forbidden transition, J^{Δπ} =2⁻, is of great interest for BSM searches
 - Energy spectrum of emitted electrons sensitive to the symmetries of the weak interaction, gives constraints both in the case of right and left couplings of the new beyond standard model currents
 - Ayala Glick-Magid *et al.*, PLB 767 (2017) 285
- Ongoing experiment at SARAF, Israel



¹⁶N(2⁻) Gamow-Teller transitions to the negative parity excited states of ¹⁶O ⁶³

- Tests of NCSM wave functions
 - B(GT)s overestimated operator SRG, 2BC need to be included, continuum
 - Correct hierarchy of transitions





Unique first-forbidden beta decay $^{16}N(2^{-}) \rightarrow ^{16}O(0^{+})$

Preliminary results for electron energy spectrum and angular correlations



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Ab initio calculations of muon capture on light nuclei



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Muon capture on ⁶Li, ¹²C, ¹⁶N from *ab initio* nuclear theory



Ab initio no-core shell-model calculations in good agreement with experiments

See talk by Lotta Jokiniemi on Saturday