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The influence of electronic correlation on weak decays

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I am deep in debt to

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Outline

- Introduction to our (relativistic) approach to weak decays in astrophysical scenarios
- β-decay and EC are not only nuclear but also atomic processes (electron correlation)
- Application of our approach to a number of βdecay processes of light (⁷Be) and heavy (¹³⁴Cs and ¹³⁵Cs) atoms
- Perspectives, future developments

β-decay: a multiscale scenario

 10^{-2} (t= 10^{-15} s, 10^{-10} m)

L (W t= 10^{-24} s, 10^{-15} m)



Coupl. const.=10⁻⁷ (t>10⁻⁸ s, 10⁻¹⁸ m)

 Standard model of particles: weak interaction is mediated by the emission or absorption of massive bosons



The enrichment of Li in the Universe is still unexplained

Li is one of the primordial elements produced in Big Bang nucleosynthesis: very fragile Galactic Cosmic Rays do not produce much ⁷Li



In interstellar medium Li content is higher than that expected by BBN For low mass star (below 2
- 3 M_☉) Li is predicted to be destroyed in the early phases of evolution, preceding the MS

⁷Li is produced in Novae and a small amount of ⁷Li in H-burning intermediate mass stars at the base of their envelope, but is thought to be burned during MS as fast as produced when convective processes carry it to temperatures of a few millions K, where it undergoes p-captures.

The cosmic Li problem before BSM....

Thus, stellar burning may form and deplete Li and its abundance is strongly influenced by several nuclear burning mechanisms as well as by the extension of the convective envelope.

- Production of $^7\mathrm{Li}$ via EC (hereinafter "EC") of $^7\mathrm{Be}$

 $^{7}\mathrm{Be} + e^{-} \longrightarrow ^{7}\mathrm{Li} + \nu_{e}$

- production of 7 Li via antineutrino capture of 7 Be

 $^{7}\mathrm{Be} + \overline{\nu}_{e} \longrightarrow ^{7}\mathrm{Li} + e^{+}$

- production of ⁷Be via positron capture of ⁷Li

 $^{7}\mathrm{Li} + e^{+} \longrightarrow ^{7}\mathrm{Be} + \overline{\nu}_{e}$

├ production of ⁷Be via neutrino capture of ⁷Li

$$^{7}\mathrm{Li} + \nu_{e} \longrightarrow ^{7}\mathrm{Be} + e^{-}$$

These reactions are interesting since previous simulations, which didn't account for electroweak processes at $10 < K_BT < 100$ KeV, gave a too high (or low) ⁷Li abundance compared to observations

State-of-the-art of 7Be beta-decay in solar-like systems

- Bachall (1962): ~ 20% of 7Be in the center of the Sun might have a bound electron —-> 7Be lifetime in solar conditions for partially ionised atoms using DH screening for the e-e interaction: total-to-continuum capture ratio is 1.217

- Shaviv et al. (2001): ⁷Be lifetime larger by \sim 20%–30% as compared to Bahcall due to fully ionized ⁷Be is in the solar plasma

- Quarati et al. (2009): ⁷Be lifetime shorter by about 10%, using a modified DH screening potential.

Despite the main decay channel in the Sun's interior is the free EC, bound e- can significantly change the decay probability of ⁷Be

Out-of-solar conditions

Adelberger (2011): data extrapolation from Bahcall's calculations, a procedure rather insecure due to the very different conditions

The situation is unsatisfactory with a lot of scattered data and uncertainties, in particular related to the T and g dependence of the rate.

Motivation of this work: provide the missing weakinteraction input data for Li nucleosynthesis calculations

Contrary to this simple view, there is evidence of changes in nuclear decay rates with these parameters

β-decay: standard approach A typical nuclear β-decay process reads: ${}^{A}_{Z}X_{N} \rightarrow {}^{A}_{Z+1}X'_{N-1} + e^{-} + \bar{\nu}_{e}$

<u>**Q-value</u></u>: total energy released by the reaction (m_{\nu} = 0)</u>**

ra-nuclear tacto

 $Z \pm 1$

$$Q_{eta^-} = m_N(^A X) - m_N(^A X') \qquad m_N(^A X) = m(^A X) - Zm_e + \sum_i B_i$$

$$Q_{\beta^{-}} = \{ [m(^{A}X) - Z \cdot m_{e}] - [m(^{A}X') - (Z+1) \cdot m_{e}] - m_{e} \} \cdot c^{2} + \{ \sum_{i=1}^{2} B_{i} - \sum_{i=1}^{2} B_{$$

In the traditional theory of β -decay processes, spectra are typically calculated as product of three factors:

 $\frac{dN}{dW} \propto pWq^2 F(Z,W)C(W)$

- a phase-space factor to deal with the momentum sharing between the βelectron (p) and neutrino (q);
- a Fermi function F(Z,W) to take into account the static corrections due to the Coulomb field of the nucleus;
- a shape factor C(W) to include the coupling between nuclear and lepton dynamics.

β-decay: standard approach A typical nuclear β-decay process reads: ${}^{A}_{Z}X_{N} \rightarrow {}^{A}_{Z+1}X'_{N-1} + e^{-} + \bar{\nu}_{e}$ <u>Q-value</u>: total energy released by the reaction ($m_{\nu} = 0$) $Q_{\beta^{-}} = m_N(^A X) - m_N(^A X') \qquad m_N(^A X) = m(^A X) - Zm_e + \sum B_i$ **Extra-nuclear factor** $Q_{\beta^{-}} = \{ [m(^{A}X) - Z \cdot m_{e}] - [m(^{A}X^{'}) - (Z+1) \cdot m_{e}] - m_{e} \} \cdot c^{2} + \{ \sum_{i=1}^{n} B_{i} - \sum_{i=1}^{n-1} B_{i} \}$ In the traditional theory of β -decay processes, spectra are typically calculated as product of three factors: $\frac{dN}{dW} \propto pWq^2 F(Z,W)C(W) \quad F(Z,W) = \frac{2\pi\nu}{1 - \exp^{-2\pi\nu}} = \frac{2\pi \nu}{1 - \exp^{-2\pi\nu}}$ • a phase-space factor to deal with the momentum sharing between the β -

- a phase-space factor to deal with the momentum sharing between the βelectron (p) and neutrino (q);
- a Fermi function F(Z,W) to take into account the static corrections due to the Coulomb field of the nucleus;
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β-decay: standard approach

$$\frac{dN}{dW} \propto pWq^2 F(Z,W)C(W)$$

It works well to predict the lineshape of allowed transitions (Δ L=0,1 π conserved), at odds forbidden non-unique transitions (Δ L>1 and π can or cannot be conserved) are out of reach of this relation

Still a rigours treatment of these transitions including electronic and nuclear DOF is missing!!!

Our approach to beta-decay aims to solve these issues using first-principles simulations as in condensed matter

Open issues in Li depletion

Li could be produced by coupled mixing and nucleosynthesis episodes, in which the depletion of Li by downward diffusion is overcompensated by an upward transport of 7Be from burning regions, at a pace fast enough to survive destruction by p- and e-captures, reaches the stellar envelope and eventually decays there

Poor knowledge of the Be decay rate dependence on the conditions below the envelopes of Red Giants (T=1:80 MK, $\rho = 1:5$ o.o.m. lower than the Sun), very different from our Sun (T_{core} = 10⁷ K a nd $\rho \sim 10^5$ kg/m³)

In calculating rates in these conditions you need to take into account conditions in which:

1. ⁷Be can be partially or totally ionized, decay may occur by capturing an e⁻ from both bound (excited) and continuum states;



3. the DH approx to model the e-e interaction may not hold and introduce large deviations in the capture rate

(degenerate Fermi gas ???)





Condition of the stellar material at high T DEGENERACY CONDITIONS: CLASSICAL vs. QUANTUM

The electronic density must be >> N_Q N_Q is the number of available quantum states

To have degeneracy $\rho_e >> n_{NQ} = (2\pi m_e kT/h^2)^{3/2}$

 $T << h^2 \rho_e^{2/3}/(2\pi m_e k) = 9.12 \times 10^6 \ {\rm K}$

Solar core: T=15.6 X 10⁶ K -----> ⁷Be atoms are all ionized (12000 K = 1 eV)!!!

In the solar core the temperature is marginally too high for degeneracy of electrons, classical gas, but decreasing R can set in...

 $T \propto 1/R$ and thus $n_{QNR} \propto T^{(3/2)} \propto R^{-3/2}$, which cannot keep the pace with $\rho_e \propto R^{-3}$ Cold? Fermi gas can be degenerate even at millions of K. THE DH model of e-e interaction is questionable Inside a star I have a plasma of Be nuclei, protons, electrons in mutual interaction this means to solve the coupled el-nuc many-body



 $V_e(\mathbf{r}), V_n(\mathbf{R})$: external scalar potentials acting on the electrons/nuclei. This is a very tricky computational problem

Electronic Structure and BO approximation: panettone/plasma

Sponge keeps together panettone. Only sponge no taste...

The source of the interesting properties in stellar plasma is the rearrangement of electrons due to the arrangement of the nuclei

Sultana change the taste, but we assume that the taste does not depend much on their distribution (basically we still have a panettone).

 $M_N/m_e \ge 10^4$

Electronic transitions ~10¹⁷ Hz

lonic vibration ~ 10^{12} Hz .

$$\chi = \tau_p / \tau_e = 10^5$$



Timescales are not comparable: electronic and nuclear motion can be decoupled.

Nonrelativistic Schrödinger equation



 $V_e(\mathbf{r}), V_n(\mathbf{R})$: external scalar potentials acting on the electrons/nuclei.

Born-Oppenheimer approximation

- Decouple the electronic and nuclear dynamics. This is a good approximation since nuclei are much heavier than electrons.
 Treat the nuclei as classical particles at fixed positions.
- Write down electronic Hamiltonian for a given nuclear configuration (here we ignore any external fields):

$$\begin{split} \hat{H}_{BO}(\{\mathbf{r}\},\{\mathbf{R}\}) &= -\sum_{j=1}^{N_e} \frac{\nabla_j^2}{2} + \frac{1}{2} \sum_{j \neq k}^{N_e} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} + \frac{1}{2} \sum_{j \neq k}^{N_e} \frac{Z_j Z_k}{|\mathbf{R}_j - \mathbf{R}_k|} \\ &- \sum_{j=1}^{N_e} \sum_{k=1}^{N_n} \frac{Z_k}{|\mathbf{r}_j - \mathbf{R}_k|} \end{split}$$
This is just a constant

The problem of doing realistic simulations of stellar plasma breaks into two questions: first, how do you find the electronic states of the system of electrons when the Be nuclei are sitting in certain positions and second, how should the nuclei move?

The electronic many-body problem

$$\Psi(x_1, x_2, ..., x_N)$$
 $x_j = (\mathbf{r}_j, \sigma_j)$ space and spin

antisymmetric N-electron wave function

$$\begin{split} \hat{H}\Psi_{j}(x_{1},...,x_{N}) &= E_{j}\Psi_{j}(x_{1},...,x_{N}) \\ \hat{H} &= -\sum_{j=1}^{N} \frac{\nabla_{j}^{2}}{2} + \sum_{j=1}^{N} V(\mathbf{r}_{j}) + \frac{1}{2} \sum_{j \neq k}^{N} \frac{1}{|\mathbf{r}_{j} - \mathbf{r}_{k}|} &\equiv \hat{T} + \hat{V} + \hat{W} \end{split}$$

Even a two-electron problem (Helium) is very difficult:

$$\begin{cases}
-\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \Psi_j(\mathbf{r}_1, \mathbf{r}_2) = E_j \Psi_j(\mathbf{r}_1, \mathbf{r}_2) \\
\text{This is a 6-dimensional partial differential equation!}
\end{cases}$$

Correlation within BO approximation

A first simple case: one electron hydrogen atom

The allowed energies are given by:

$$H_T |\Psi_n(r)\rangle = E_n |\Psi_n(r)\rangle$$

where

$$H_T = \frac{\hbar^2}{2m} \nabla^2 + V(r), \ V(r) = -e^2/(4\pi\epsilon r)$$

More than one electron (like bound and continuum electrons in a plasma with Be): attraction with the nuclei and repulsion with other e-



Two one-body problem

$$|\Psi(r_1, r_2)\rangle = \psi_a(r_1)\psi_b(r_2)$$
$$E_{tot} = E_1 + E_2$$

One two-body problem

$$|\Psi(r_1, r_2)\rangle \neq \psi_a(r_1)\psi_b(r_2)$$
$$E_{tot} \neq E_1 + E_2$$

Repulsion destroys the independent particles model

Hartree-Fock within BO approximation

Hartree theory: include static repulsion, but ignore correlation

Electrons are independent and feel an average potential $V_m(r)$



Many-body problem has been replaced by many one-body problems with electrons moving in $V_m(r)$

Hartree-Fock: electrons are unsociable $\Psi(r) = \psi_{a\uparrow}(r_1)\psi_{b\uparrow}(r_2) - \psi_{b\uparrow}(r_2)\psi_{a\uparrow}(r_1)$

There are two mechanisms to avoid each other: exchange and correlation and both lower the total energy and dress the electron-electron bare interaction.

> Correlation is the remaining repulsion energy: keeps electrons apart!!!

How do we actually calculate e-capture rates?

We can define the T-matrix of the weak interaction as:

$$\left\langle \psi_{f,\boldsymbol{k}}^{-}|W|\phi_{i,\boldsymbol{p}}^{+}\right\rangle = \left\langle \phi_{f,\boldsymbol{k}}^{-}|\mathbf{T}_{W}|\phi_{i,\boldsymbol{p}}^{+}\right\rangle$$

By multiplying the c.s. by the e⁻ current one obtains the e-capture rate:

- 1. 1st Be e.s. is found at 429.4 keV=5X10⁹ K above the ground state 2. $T_W \propto \delta(r)$ = very short range contact interaction
- 3. $t_{f,i}$ are chosen equal to those measured on the Earth, neglect dependence on T and $p^2/2m_e$

IMPORTANT OUTCOME!

⁷Be-e⁻ can be modelled as a two-body scattering process at a given relative electron momentum p. The rate is proportional to $\rho_e(0)$.

Which Hamiltonian? Climbing the electronic **correlation ladder** be n mean iel LowerAccuracy Hartree-Fock **Thomas-Fermi** model model Loner acch **Debye-Hückel** model

Energy of the Isolated Beryllium Atom in Atomic Units and Spin-up Density at the Nucleus Obtained Through the HF and CI Calculations

Some data...

	Energy			$ ho_{e\uparrow}(0)$	UUII		
Hartree-Fock		-14.573 -14.660		17.68521 17.68060 Degenerate condition			
Full-CI							
ρ (g cm ⁻³)	<i>T</i> (10 ⁶ K)	$\lambda_{\text{Debye}} a.u.$	$\lambda_{\text{De Broglie}}$ (e - p)	$\rho_{\rm HF}(0) a.u.$	$\rho_{\rm TF}(0)$	$\rho_B(0)$	$\rho_{\rm DH}(0)$
1000.	1.	0.038	1.409-0.0329	71.87÷71.97	68.99 ÷ 69.11	$42.61 \div 42.74$	47.46 ÷ 47.55
100.		0.119		33.52 ÷ 33.53	$29.53 \div 29.55$	$4.027 \div 4.031$	19.13 ÷ 19.14
10.		0.377		17.37 ÷ 17.37	13.83 ÷ 13.83	$0.945 \div 0.945$	13.33 ÷ 13.33
1. Sol	ar	1.193		7.839 ÷ 7.837	$5.708 \div 5.707$	$0.184 \div 0.184$	8.151 ÷ 8.149
0.1 cor	ndition	3.771		$1.940 \div 1.940$	$1.415 \div 1.415$	$0.044 \div 0.044$	$2.059 \div 2.058$
0.01		11.93		$0.278 \div 0.278$	$0.220 \div 0.220$	$0.0075 \div 0.0075$	$0.279 \div 0.279$
0.001		37.71		$0.0308 \div 0.0308$	$0.0264 \div 0.0264$	$0.0012 \div 0.0012$	0.0303 ÷ 0.0303
1009.	10.	0.119	0.445-0.0103	122.43 ÷ 122.89	116.21 ÷ 116.68	51.77 ÷ 52.05	$108.56 \div 109.01$
100.		0.377		$20.23 \div 20.27$	19.53 ÷ 19.57	$10.36 \div 10.39$	19.54 ÷ 19.58
10.		1.193		$2.578 \div 2.581$	$2.554 \div 2.558$	$2.515 \div 2.519$	$2.570 \div 2.573$
1.		3.771		$0.274 \div 0.275$	$0.274 \div 0.275$	$0.274 \div 0.274$	$0.274 \div 0.275$
0.1		11.93		$0.0281 \div 0.0282$	$0.0281 \div 0.0282$	$0.0281 \div 0.0282$	$0.0281 \div 0.0281$
0.01		37.71		$(2.84 \div 2.84) \times 10^{-3}$	$(2.84 \div 2.84) \times 10^{-3}$	$(2.84 \div 2.84) \times 10^{-3}$	$(2.83 \div 2.83) \times 10^{-3}$
0.001		119.3		$(2.84 \div 2.84) \times 10^{-4}$	$(2.84 \div 2.84) \times 10^{-4}$	$(2.84 \div 2.84) \times 10^{-4}$	$(2.84 \div 2.84) \times 10^{-4}$
1000.	100.	0.377	0.141-0.0033	78.31 ÷ 80.39	$78.24 \div 80.32$	76.57 ÷ 78.64	$78.22 \div 80.30$
100.		1.193		9.051 ÷ 9.289	$9.051 \div 9.288$	9.031 ÷ 9.268	$9.051 \div 9.288$
10.		3.771		$0.773 \div 0.787$	$0.773 \div 0.787$	$0.773 \div 0.787$	0.773 ÷ 0.787
1.		11.93		$0.0775 \div 0.0789$	$0.0775 \div 0.0789$	$0.0775 \div 0.0789$	$0.0775 \div 0.0789$
0.1		37.71		$(7.75 \div 7.90) \times 10^{-3}$	$(7.75 \div 7.90) \times 10^{-3}$	$(7.75 \div 7.90) \times 10^{-3}$	$(7.75 \div 7.90) \times 10^{-3}$
0.01		119.3		$(7.75 \div 7.90) \times 10^{-4}$	$(7.75 \div 7.90) \times 10^{-4}$	$(7.75 \div 7.90) \times 10^{-4}$	$(7.75 \div 7.90) \times 10^{-4}$
0.001		377.1		$(7.75 \div 7.90) \times 10^{-5}$	$(7.75 \div 7.90) \times 10^{-5}$	$(7.75 \div 7.90) \times 10^{-5}$	$(7.75 \div 7.90) \times 10^{-5}$

⁷Be half-life

half-life (days)= 941.86881/g(0)



Astrophysical consequences of the new rate



typical RGB conditions

AGB stages

Equilibrium abundances of ⁷Be and ⁷Li in the layers above the H-burning shell using our ⁷Be life-time (red line) and the solar extrapolated rate (black line), in a 2 M^o evolved star of solar metallicity. The matter density is also shown (blue line), and is referred to the scale on the right axis.

AGB: the HF values of $\rho_e(0)$ are > than those of the DH model; the half-life is smaller and the e-capture is therefore faster; a lower equilibrium abundance of ⁷Be is established



• A smaller lifetime of ⁷Be EC: less destruction via the ⁷Be(p, γ)⁸B changing the yield of the solar neutrino flux.



 $n_e = 10^{12} \text{ cm}^{-3}$

OK for light nuclei! What about heavy ones?

- The s-process represents the mechanisms by which heavy nuclei are produced
 - The presence of several branching points along the s-process path require accurate rates of the competing β -decays and n-capture reactions



A new estimate of the 134Cs and 135Cs half-lives to reproduce isotopic ratios of heavy elements measured in presolar SiC grains. The abundance of Ba in AGB stars depends only on slow n-captures.

Climbing the correlation ladder be mean LowerAccuracy **Dirac-Hartree-Fock Thomas-Fermi** model model Lowerach **Debye-Hückel** model

Standard Model β-decay theory

β-decay rate is calculated by using Fermi's Golden Rule: $P_{i\to f} = 2\pi \int |\langle f | \hat{H}_{\beta} | i \rangle|^2 \rho(W_f) \delta(W_f - W_i) dW_f$

Probability *P* per unit time that a system undergoes a transition from an initial state, *i*, to a number of final states, *f*, under the influence of a perturbation described by the Hamiltonian H_β

Weak Interaction Hamiltonian



All the wavefunctions will be written as Dirac spinors

While nuclear excited state dynamics is the most relevant, with rate increasing by a factor of 15 at 100 KeV due to populating fast-decaying nuclear excited states, e⁻ temperature has the most pronounced impact at [0:15] keV, decreasing the half-life by 20% with respect to e-GS (cyan)



Astrophysical implications

Left panel: isotopic ratios of ¹³⁴Ba and ¹³⁵Ba with respect to ¹³⁶Ba, displayed as part-per-mil deviations (indicated by the symbol δ), with decay rates from TY.

Right panel: the results of the same models, where only the decay rates for ¹³⁴Cs and ¹³⁵Cs are changed, using those of the present work. Computations are for 2 M stars, where magneto-hydrodynamic processes induce the penetration of protons into He-rich layers, producing ¹³C then releasing neutrons through ¹³C(α ,n)¹⁶O. Abundances are computed in stellar winds, where magnetic blobs further add 5% of C-rich material in flare-like episodes.The symbol [Fe/H] indicates Log(X_{Fe}/X_H)_{star} - Log(¹³C)_{sun}



Percentage of s-process contributions (blue dots) to the isotope production (134,136Ba) as computed by M. Busso et al. ApJ 908, 55 (2021) for s-only nuclei near the magic neutron number N= 82.



Conclusions

- A new method for calculating β- and e-capture decay spectra in both light to heavy nuclei, which extends the standard approach in several ways
- This method can be applied to any nuclear beta decay and includes relativistic, many-body screening and post-collisional effects
- It works also in astrophysical environment by including temperature, density and charge state distribution
- Our approach can also take into account plasma induced variations of beta decay!

Outlook

- Inclusion of electro-nuclear dynamic correlation beyond meanfield approximation; DONE for electron! ECGBF; quantum neural network to estimate nuclear matrix elements
- Estimate of beta-decay rates of different elements (¹⁷⁶Lu, ⁹⁴Nb, any other suggestion from the Pandora collaboration AND you!)



