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EUROPEAN CENTRE FOR THEORETICAL STUDIES
IN NUCLEAR PHYSICS AND RELATED AREAS

TIFPA
Trento Institute for
Fundamental Physics
and Applications

Path Integral MD/MC for many-body properties
&
Ab-initio Beta-decay calculations

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Outline

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- Path Integral Monte Carlo / Molecular Dynamics:
  a) Theory;
  b) Applications:
    1) vibrational properties of high-pressure hydrogen;
    2) proton distribution in water clusters;

- Ab-initio beta-decay simulations:
  a) Theory;
  b) Application: Nickel spectrum and rate;
  c) Improving the calculation of matrix elements (at least) in a few-body system;

- Perspectives

Path Integral MD/MC

$$\hat{H} = \sum_{I=1}^{3N_n} \frac{\hat{P}_I^{\,2}}{2M_I} + \sum_{i=1}^{3N_e} \frac{\hat{p}_i^{\,2}}{2m_i} + \hat{V}_{n-e}\left(R_1, \ldots, R_{3N}, x_1, \ldots, x_{3N}\right)$$

Non-relativistic Hamiltonian:
interacting system made by
N_n nuclei (treated as Coulomb-point particles)
and
N_e electrons

Goal → extract properties of the system such as vibrational properties, pair distribution functions, phase diagrams...

Path Integral MD/MC

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interacting system made by
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Goal → extract properties of the system such as vibrational properties, pair distribution functions, phase diagrams...

Born-Oppenheimer:
Integrating out the
Electronic degrees of freedom

$$\hat{H} = \sum_{I=1}^{3N_n} \frac{\hat{P}_I^{\,2}}{2M_I} + \hat{U}_n(R_1, \ldots, R_{3N})$$

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Born-Oppenheimer:
Integrating out the electronic degrees of freedom

How do we treat the ground state electronic many-body problem?

Density Functional Theory → Quantum Espresso (QE) engine.
Functionals benchmarked by QMC.
Features of QE: planewave expansion of the wf/density, pseudopotentials.
Wf is simple a Slater determinant (Kohn-Sham approach): $\Psi_{el} = \Phi_{SD}$

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QUANTUMESPRESSO

Variational QMC → TurboRVB code.
Features of TurboRVB: Slater/Pfaffian + Jastrow factor to represent the ground state wf.
Gaussian basis set.

$$\Psi_{el} = \Phi_{AS} \exp\left(J\right)$$

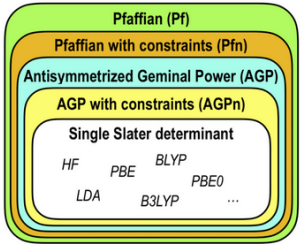


FIG. 3. *Ansatz* hierarchy. The output of Hartree–Fock (HF) or DFT simulations with different exchange-correlation functionals are special instances of the SD *Ansatz*.

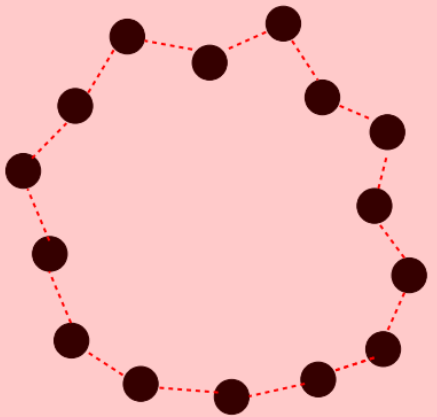
TurboRVB
Quantum Monte Carlo Package SISSA

Path Integral MD/MC

Quantum partition function

$$Z(T)=Tr[e^{-\beta\hat{H}}]$$

$$\hat{H}=\sum_{i=1}^{3N}\frac{\hat{P}_I^{\,2}}{2M_I}+\hat{U}(X_1,\ldots,X_{3N})$$



$$Z_M(T)=\frac{1}{(2\pi\hbar)^M}\int d^{3NM}\vec{X}\int d^{3NM}\vec{P}\,e^{-\frac{\beta}{M}H_M(\vec{X},\vec{P})}$$

Classical partition function of a chain of M beads (ring polymer)

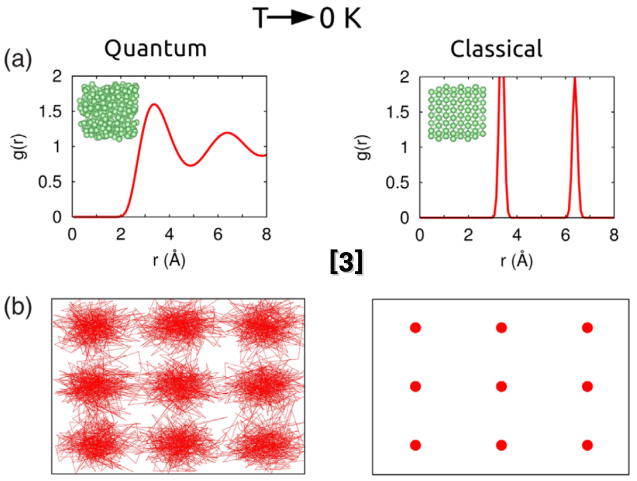
$$H_{PIMD}\equiv H_M=\sum_{i=1}^{3N}\sum_{j=1}^{M}\left(\frac{[P_i^{(j)}]^2}{2M_I}+\frac{1}{2}m_i\omega_M^2[X_i^{(j)}-X_i^{(j-1)}]^2\right)+\sum_{j=1}^{M}U(X_1^{(j)},\ldots,X_{3N}^{(j)})$$

D.M. Ceperley, *Path integrals in the theory of condensed helium,* Rev. Mod. Phys. 1995, 67, 279–355

Path Integral MD

Path Integral Molecular Dynamics (PIMD):

- **Molecular dynamics for quantum nuclei (full account of nuclear quantum effects);**
- **Sampling the exact thermal distribution of quantum nuclei → including anharmonicity at all orders.**
- **Thermal effects included by a Langevin thermostat [1,2]**

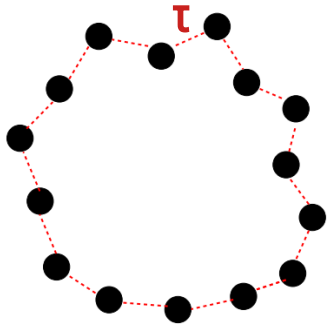


[1] - M. Ceriotti et al., *Efficient stochastic thermostatting of path integral molecular dynamics,* J. Chem. Phys. 133, 124104 (2010)

[2] - F. Mouhat et al., *Path Integral Langevin Dynamics driven by Quantum Monte Carlo forces*, J. Chem. Theory Comput. 13, 2400 (2017)

[3] - C. Cazorla and J. Boronat, *Simulation and understanding of atomic and molecular quantum crystals*, *Rev. Mod. Phys.* 89, (2017)

Matsubara Green's function



$$G_{ij}(\tau) = -\langle T\, \delta\hat{x}_i(\tau)\delta\hat{x}_j(0)\rangle$$

$$G(i\omega_n) = \frac{-1}{\omega_n^2 + D^{harm} + \Pi(i\omega_n)}$$

PIMD → G(ω) from G(τ):

Ill defined inversion problem
+
Stochastic noise

But within PIMD we can access G for $i\omega_n=0$ (Kubo-transform)

$$\widetilde{G} = \frac{1}{\beta}\int_0^\beta G(\tau)d\tau = \frac{1}{\beta}G(i\omega_0) = \frac{1}{\beta}\frac{-1}{D^{harm}+\Pi(0)}$$

$$\widetilde{G}_{ij} = \frac{1}{\beta Z}\sum_{l,m}\langle m|\delta\hat{x}_i|l\rangle\langle l|\delta\hat{x}_j|m\rangle\frac{e^{-\beta E_l}-e^{\beta E_m}}{E_m-E_l}$$

- **Poles of the phononic Green's function (excitation energies weighted by displacement matrix elements)**
- **Static Self-Energy (no linewidths)**

→ **The displacement-displacement correlator from PIMD gives exactly $\widetilde{G}$**

$$\widetilde{G}_{il} = \frac{1}{M^2}\left\langle \sum_{j_1}^{M}\delta x_i^{(j_1)} \sum_{j_2}^{M}\delta x_l^{(j_2)}\right\rangle$$

TM et al., *Probing anharmonic phonons by quantum correlators: A path integral approach*, J. Chem. Phys. **154**, 224108 (2021)

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High pressure (@500 GPa) hydrogen

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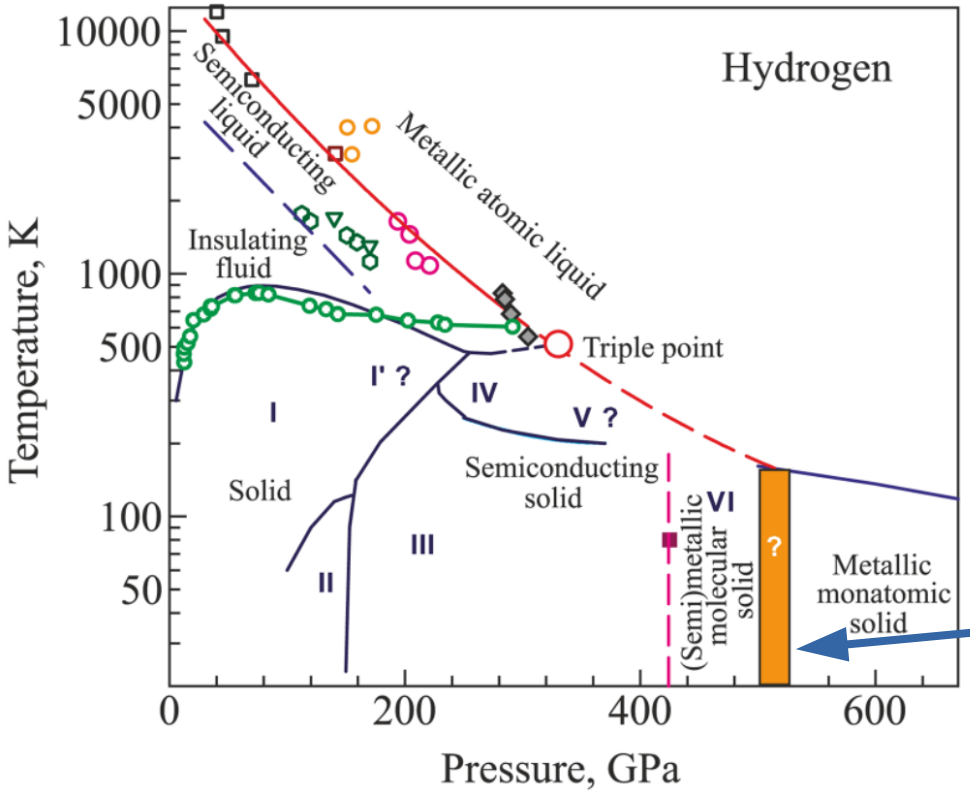
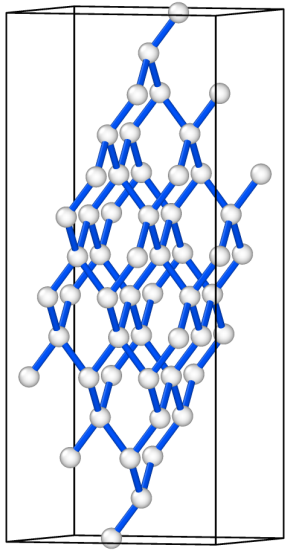
PIMD + DFT application

I application: solid hydrogen vibrational properties





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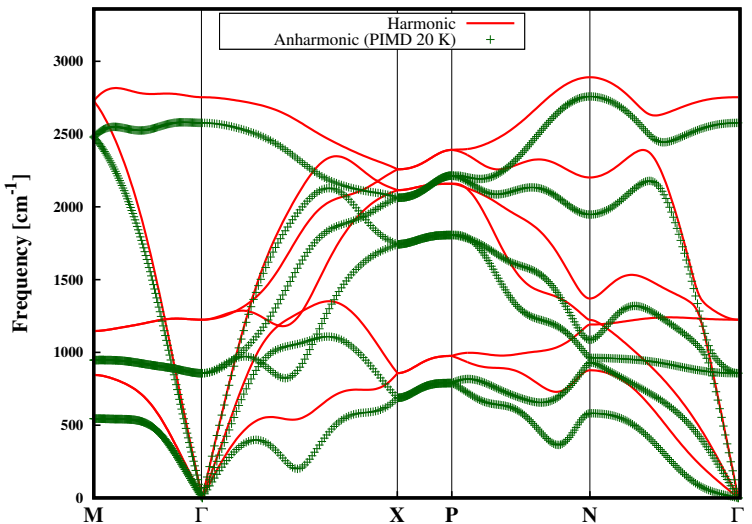
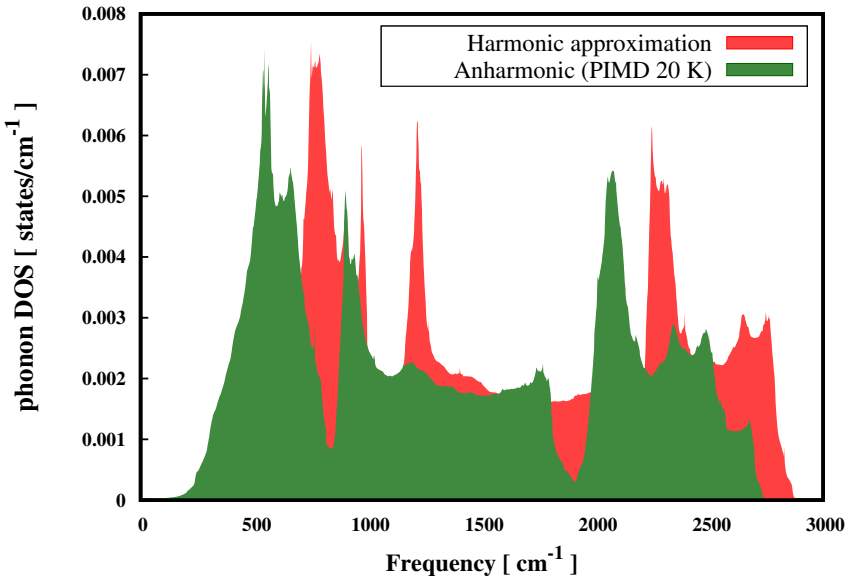
PIMD + DFT application

phonon dispersion



phonon DOS

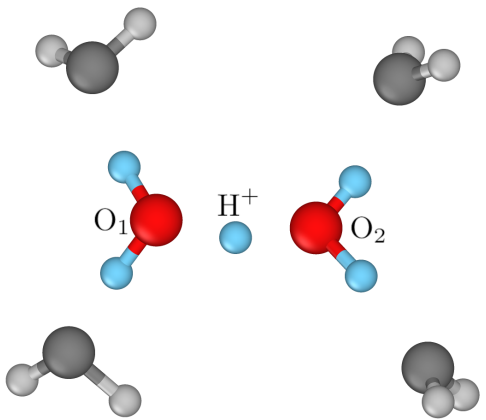


TM et al., *Probing anharmonic phonons by quantum correlators: A path integral approach*, J. Chem. Phys. **154**, 224108 (2021)

Water clusters

II application: pair correlation function in water

PIMD + QMC application



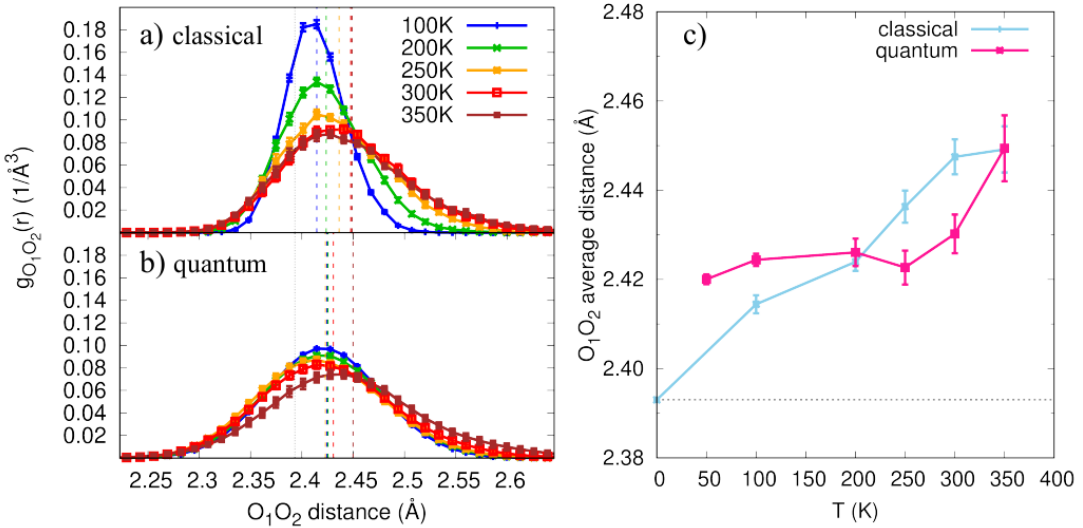


Figure 2: Classical (panel a)) and quantum (panel b)) oxygen-oxygen $g_{O_1O_2}$ pair correlation functions of the $H_{13}O_6^+$ ion as a function of temperature. The dashed vertical lines indicate the average $\langle d_{O_1O_2} \rangle$ distance for each simulation, at the corresponding temperature. The dotted vertical line is located at the classical equilibrium geometry. Panel c) shows the T-dependence of the $\langle d_{O_1O_2} \rangle$ average distance. The classical equilibrium geometry is represented by a short-dashed horizontal black line. At 250 K and 300 K the oxygen-oxygen distance is *shortened* by NQEs with respect to the classical counterpart.

F. Mohuat, M. Peria, TM et al., *Thermal dependence of the hydrated proton and optimal proton transfer,* arXiv:2301.01825, (2023)

Beta-decay

Aim:
compute electronic spectra (‘easy’ task)
and
decay-rates (‘hard’ task)

Fermi’s golden rule:

$$P = 2\pi \int |\langle f|\hat{H}_\beta|i\rangle|^2 \rho(W_f)\delta(W_f - W_i)dW_f \qquad \hat{H}_\beta = \int \mathcal{H}_\beta \, d^3x$$

$J^{\mu,H}$: *hadronic current* J^{L}_{μ}: *leptonic current*

$$\mathcal{H}_\beta = \frac{G_\beta}{\sqrt{2}}(\bar{\psi}_p(\mathbf{r})\gamma^\mu(1 - x\gamma^5)\hat{\psi}_n(\mathbf{r})) \cdot (\bar{\psi}_e(\mathbf{r})\gamma_\mu(1 - \gamma^5)\hat{\psi}_\nu(\mathbf{r})) + h.c.$$

Weak interaction Hamiltonian

$$x = \frac{C_A}{C_V}$$

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Weak interaction Hamiltonian

$$x = \frac{C_A}{C_V}$$

$$|i\rangle = |h_i\rangle \otimes |e_i\rangle$$
$$|f\rangle = |h_f\rangle \otimes |e_f\rangle \otimes |\bar{\nu}_f\rangle,$$

Initial state: tensorial product of nuclear and electronic wfs

Non-orthogonal (different nuclei = different Hamiltonians !!!)

Final state: tensorial product of nuclear and electronic wfs + (anti)neutrino

Beta-decay

To deal with the relativistic weak-interaction Hamiltonian, we set up a relativistic mean-field framework to compute leptonic and hadronic matrix elements.

Generalized Dirac equation for N interacting fermions

$$\left\{ \sum_{i}^{N} \left(c\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + \beta_i mc^2 + V_i \right) + \sum_{i<j}^{N} \left[\beta_i \beta_j g_{S,ij} + \left(1 - \boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j \right) g_{V,ij} \right] \right\} \psi \left(\mathbf{r}_1, \cdots \mathbf{r}_N \right) = E \psi \left(\mathbf{r}_1, \cdots \mathbf{r}_N \right)$$

external potential — **Scalar interaction** — **Vectorial interaction**

TM et al., *Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Medium-Heavy Nuclei and of Atomic and Molecular Electronic Structure*, Advanced Theory and Simulations, 1, 1870030 (2018)

Beta-decay: leptonic current

To deal with the relativistic weak-interaction Hamiltonian, we set up a relativistic mean-field framework to compute leptonic and hadronic matrix elements.

$$\begin{pmatrix} mc^2 + W_V + \cancel{W_S} - E & -c\boldsymbol{\sigma}\cdot i\boldsymbol{\nabla} \\ -c\boldsymbol{\sigma}\cdot i\boldsymbol{\nabla} & -mc^2 + W_V - \cancel{W_S} - E \end{pmatrix} \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} = 0 \longrightarrow$$

single particle equations

For electrons → $W_s = 0$ and W_v is the (self-consistent Dirac-Hartree-Fock) Coulomb field

Simplified version: To find the electronic wavefunctions, we assume that the non-local exchange Fock term is substituted by an exchange potential V_{ex} derived by the non-relativistic approximation to the free-electron gas theory [Salvat]

$$V_{ex}[\rho] = \frac{9}{4}\left[\frac{3}{\pi}\rho(r)\right]^{\frac{1}{3}}$$

[Salvat] – F. Salvat et al., *Analytical Dirac-Hartree-Fock-Slater screening function for atoms (Z=1 - 92)*, Phys. Rev. A 36, 467 (1987)

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→ **single particle equations**

For electrons → $W_s = 0$ and W_v is the (self-consistent Dirac-Hartree-Fock) Coulomb field

Initial electronic state

$$|e_i\rangle = |\bigwedge_B n_B^i, \kappa_B^i, \mu_B^i\rangle_e \equiv \prod_{B=1}^{N} \hat{a}_{B,e}^{i\dagger}|0\rangle_e \qquad (17)$$

where $\bigwedge_B$ implies the complete antisymetrization of the total spatial wavefunction and where quantum numbers $n_B^i, \kappa_B^i, \mu_B^i$ completely identify an initial electron. Indeed, the latter is assumed to be eigenfunction of a single particle Dirac Hamiltonian in which the potential energy operator is spherically symmetric. The eigenfunction of the total Dirac Hamiltonian will thus be a Slater determinant constructed with single particle wavefunctions.

Final electronic state

$$|e_f\rangle = |\bigwedge_{B,C} n_B^f, \kappa_B^f, \mu_B^f, W_C^f, \kappa_C^f, \mu_C^f\rangle_e \equiv \prod_{B=1}^{N} \hat{a}_{B,e}^{f\dagger}\hat{a}_{C,e}^{f\dagger}|0\rangle_e$$

Final (anti)neutrino state

$$|\bar{\nu}_f\rangle = |W_\nu, \kappa_\nu, \mu_\nu\rangle_\nu \equiv \hat{b}_\nu^\dagger|0\rangle_\nu$$

Beta-decay: leptonic current

To deal with the relativistic weak-interaction Hamiltonian, we set up a relativistic mean-field framework to compute leptonic and hadronic matrix elements.

$$\begin{pmatrix} mc^2 + W_V + \cancel{W_S} - E & -c\boldsymbol{\sigma}\cdot i\boldsymbol{\nabla} \\ -c\boldsymbol{\sigma}\cdot i\boldsymbol{\nabla} & -mc^2 + W_V - \cancel{W_S} - E \end{pmatrix} \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} = 0$$

→ **single particle equations**

For electrons → $W_s = 0$ and W_v is the (self-consistent Dirac-Hartree-Fock) Coulomb field

Leptonic current: determinant of the overlap between initial and final electronic states

$$J^L_\mu(r_h) = \sum_{j=1}^{N} \prod_{B\neq j} (-)^j \langle 0;0|\hat{a}'_{B,e}\hat{a}'_{C,e}\hat{a}^+_{1,e}\cdots\hat{a}^+_{N,e}|0;0\rangle$$

$$\int dr_l \int d\Omega_l\, Y_{L',-q}(\theta_l,\phi_l)\langle n'_B,\kappa'_B,\mu'_B|\mathbf{r}_l\rangle\gamma^0\gamma_\mu$$

$$(1-\gamma^5)\langle \mathbf{r}_l|W_v,\kappa_v,\mu_v\rangle\delta(r_h-r_l)$$

→ The β-electron excites a bound electron

$$+\langle 0;0|\hat{a}'_{1,e}\ldots\hat{a}'_{N,e}\hat{a}^+_{1,e}\cdots\hat{a}^+_{N,e}|0;0\rangle$$

$$\int dr_l \int d\Omega_l\, Y_{L',-q}(\theta_l,\phi_l)\langle W'_C,\kappa'_C,\mu'_C|\mathbf{r}_l\rangle\gamma^0\gamma_\mu$$

$$(1-\gamma^5)\langle \mathbf{r}_l|W_v,\kappa_v,\mu_v\rangle\delta(r_h-r_l)$$

→ The β-electron is directly emitted

Beta-decay: hadronic current

To deal with the relativistic weak-interaction Hamiltonian, we set up a relativistic mean-field framework to compute leptonic and hadronic matrix elements.

$$\begin{pmatrix} mc^2 + W_V + W_S - E & -c\boldsymbol{\sigma}\cdot i\boldsymbol{\nabla} \\ -c\boldsymbol{\sigma}\cdot i\boldsymbol{\nabla} & -mc^2 + W_V - W_S - E \end{pmatrix} \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} = 0$$

For nuclei → $W_s + W_v$ and $W_v - W_s$ are parametrized by Wood-Saxon shapes

$$(W_S + W_V)_{p/n} = \frac{V^0_{p/n}}{1 + e^{(r - R_{p/n})/a_{p/n}}}$$

$$(W_S - W_V)_{p/n} = -\lambda_{p/n} \frac{V^0_{p/n}}{1 + e^{(r - R^{ls}_{p/n})/a^{ls}_{p/n}}}$$

→ *Spin – orbit potential*

$$V^0_{p/n} = V\left(1 \pm \kappa \frac{N - Z}{N + Z}\right) \qquad R_{p/n} = r_o^{p/n} A^{1/3} \qquad R^{ls}_{p/n} = r_o^{ls,\,p/n} A^{1/3}$$

Table 3. Parameters of the equivalent Saxon-Woods potentials

Particles	V (MeV)	κ	λ	r_0 (fm)	a (fm)	r_0^{ls} (fm)	a^{ls} (fm)
Neutrons	−71.28	0.462	11.12	1.233	0.615	1.144	0.648
Protons	−71.28	0.462	8.97	1.250	0.612	1.140	0.647

W. Koepf and P. Ring, *The spin-orbit field in superdeformed nuclei: a relativistic investigation*, Z. Phys. A 339, 81 (1991)

Beta-decay: hadronic current

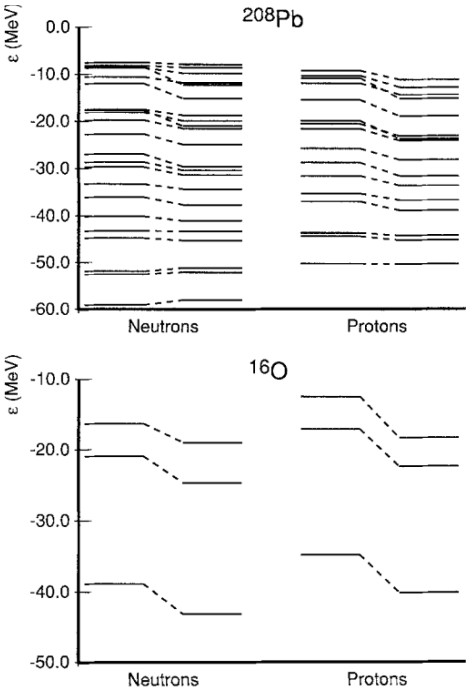
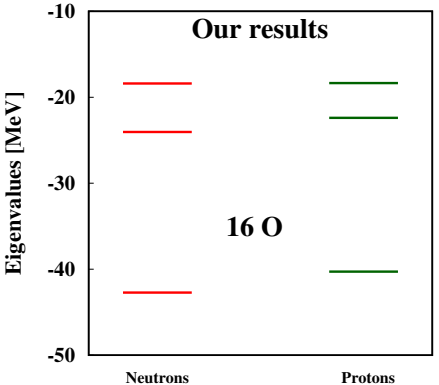


Fig. 1. Single particle levels below the Fermi surface for protons and neutrons in the nuclei ^{208}Pb and ^{16}O. The exact eigenvalues of a fully self-consistent solution of the relativistic mean field equations (left hand side) are compared with eigenvalues of a Dirac equation containing the fitted Saxon-Woods fields, $U = V + S$ and $W = V - S$ from (23) (right hand side). For the self-consistent calculations in ^{208}Pb the parameter set $NL1$ was used and for ^{16}O we used $NL2$



W. Koepf and P. Ring, *The spin-orbit field in superdeformed nuclei: a relativistic investigation*, Z. Phys. A 339, 81 (1991)

Beta-decay: a computational perspective

$$\frac{d\Gamma_t}{dW_e^t} = \frac{\pi G_\beta^2}{(2j_n+1)(2J_B^i+1)} \sum_{n_B^f,\kappa_B^f} \sum_{\mu_n,\mu_p} \sum_{\mu_B^f,\mu_B^i} \sum_{\kappa_C^f,\mu_C^f} \sum_{\kappa_\nu,\mu_\nu} \int |I|^2 \rho(W_f)\delta(Q - W_e^t - W_\nu) dW_\nu \qquad (43)$$

In this expression, more than the sum over the magnetic quantum numbers, the sum runs over all the possible final state in which the final atom can be left (the initial atom naturally is supposed to be in its ground state).
If now one put together the expressions for $I_\mu^n(r_a)$ and $I_\mu^l(r_a)$, I can be written as

$$I = \sum_{L,q} (-)^q \begin{vmatrix} \langle\psi_1^f|\phi_1^i\rangle & \langle\psi_1^f|\phi_2^i\rangle & \cdots & \langle\psi_1^f|\phi_N^i\rangle & M_{L,q,1} \\ \langle\psi_2^f|\phi_1^i\rangle & \langle\psi_2^f|\phi_2^i\rangle & \cdots & \langle\psi_2^f|\phi_N^i\rangle & M_{L,q,2} \\ \vdots & & \ddots & & \vdots \\ \langle\psi_N^f|\phi_1^i\rangle & \langle\psi_N^f|\phi_2^i\rangle & \cdots & \langle\psi_N^f|\phi_N^i\rangle & M_{L,q,N} \\ \langle\psi_C^f|\phi_1^i\rangle & \langle\psi_C^f|\phi_2^i\rangle & \cdots & \langle\psi_C^f|\phi_N^i\rangle & M_{L,q,C} \end{vmatrix}$$

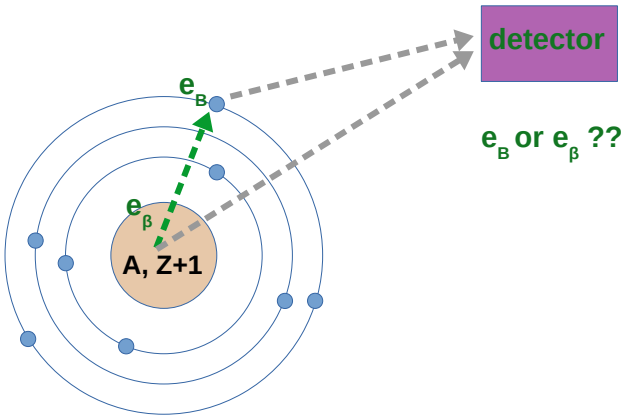
Within this approach we take into account:

- Shake-up, shake-off;
- Non-orthogonality;
- Exchange effects;

$$M_{L,q,B} = \int \left[\int d\Omega_a Y_{L,q}(\theta_h,\phi_h) \langle \xi_p, j_p, \mu_p | \mathbf{r_h} \rangle \, \gamma^0\gamma^\mu(1-x\gamma^5) \langle \mathbf{r_h} | \xi_n, j_n, \mu_n \rangle \cdot r_h^2 \cdot \right.$$
$$\left. \cdot \int d\Omega_l Y_{L,-q}(\theta_l,\phi_l) \langle n_B^f, \kappa_B^f, \mu_B^f | \mathbf{r_l} \rangle \gamma^0\gamma_\mu(1-\gamma^5) \langle \mathbf{r_l} | W_\nu, \kappa_\nu, \mu_\nu \rangle \delta(r_h - r_l) \right] dr_h;$$

$$M_{L,q,C} = \int \left[\int d\Omega_h Y_{L,q}(\theta_h,\phi_a) \langle \xi_p, j_p, \mu_p | \mathbf{r_h} \rangle \, \gamma^0\gamma^\mu(1-x\gamma^5) \langle \mathbf{r_h} | \xi_n, j_n, \mu_n \rangle \cdot r_h^2 \cdot \right.$$
$$\left. \cdot \int d\Omega_l Y_{L,-q}(\theta_l,\phi_l) \langle W_C^f, \kappa_C^f, \mu_C^f | \mathbf{r_l} \rangle \gamma^0\gamma_\mu(1-\gamma^5) \langle \mathbf{r_l} | W_\nu, \kappa_\nu, \mu_\nu \rangle \delta(r_h - r_l) \right] dr_h;$$

Determinant of the matrix of overlaps between initial and final electronic states



Beta-decay: a computational perspective

$$\frac{d\Gamma_t}{dW_e^t} = \frac{\pi G_\beta^2}{(2j_n+1)(2J_B^i+1)} \sum_{n_B^f,\kappa_B^f} \sum_{\mu_n,\mu_p} \sum_{\mu_B^f,\mu_B^i} \sum_{\kappa_C^f,\mu_C^f} \sum_{\kappa_\nu,\mu_\nu} \int |I|^2 \rho(W_f)\delta(Q - W_e^t - W_\nu) dW_\nu \qquad (43)$$

In this expression, more than the sum over the magnetic quantum numbers, the sum runs over all the possible final state in which the final atom can be left (the initial atom naturally is supposed to be in its ground state).
If now one put together the expressions for $I_\mu^n(r_a)$ and $I_\mu^l(r_a)$, I can be written as

$$I = \sum_{L,q} (-)^q \begin{vmatrix} \langle\psi_1^f|\phi_1^i\rangle & \langle\psi_1^f|\phi_2^i\rangle & \cdots & \langle\psi_1^f|\phi_N^i\rangle & \\ \langle\psi_2^f|\phi_1^i\rangle & \langle\psi_2^f|\phi_2^i\rangle & \cdots & \langle\psi_2^f|\phi_N^i\rangle & \\ \vdots & & \ddots & & \\ \langle\psi_N^f|\phi_1^i\rangle & \langle\psi_N^f|\phi_2^i\rangle & \cdots & \langle\psi_N^f|\phi_N^i\rangle & \\ & & & & M_{L,q,C} \end{vmatrix}$$

Determinant of the matrix of overlaps between initial And final electronic states

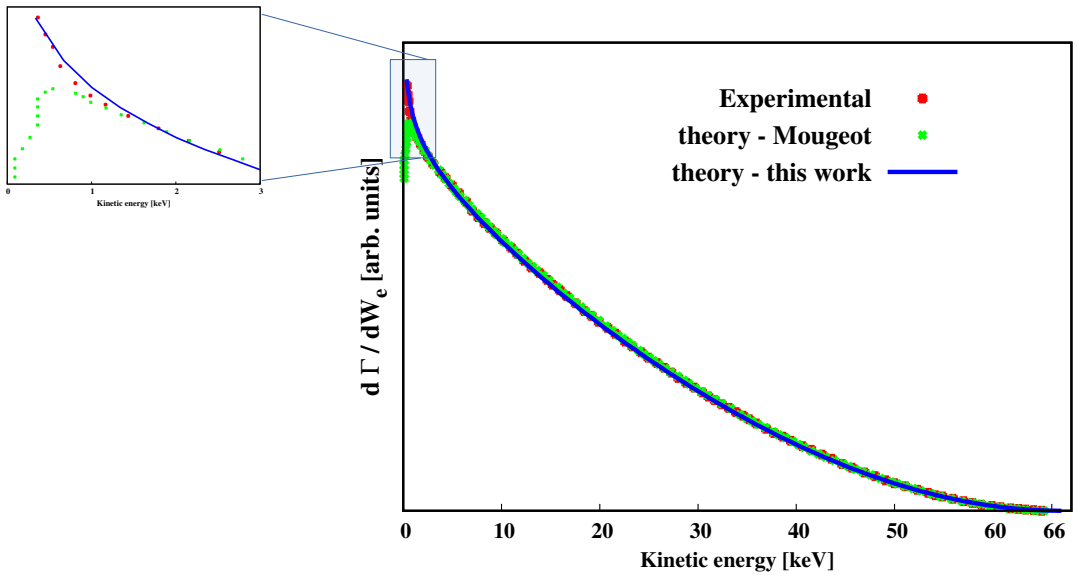
$$M_{L,q,B} = \int \left[\int d\Omega_a Y_{L,q}(\theta_h,\phi_h) \langle \xi_p, j_p, \mu_p | \mathbf{r_h} \rangle \, \gamma^0\gamma^\mu(1-x\gamma^5) \langle \mathbf{r_h} | \xi_n, j_n, \mu_n \rangle \cdot r_h^2 \cdot \right.$$
$$\left. \cdot \int d\Omega_l Y_{L,-q}(\theta_l,\phi_l) \langle n_B^f, \kappa_B^f, \mu_B^f | \mathbf{r_l} \rangle \gamma^0\gamma_\mu(1-\gamma^5) \langle \mathbf{r_l} | W_\nu, \kappa_\nu, \mu_\nu \rangle \delta(r_h - r_l) \right] dr_h;$$
$$M_{L,q,C} = \int \left[\int d\Omega_h Y_{L,q}(\theta_h,\phi_a) \langle \xi_p, j_p, \mu_p | \mathbf{r_h} \rangle \, \gamma^0\gamma^\mu(1-x\gamma^5) \langle \mathbf{r_h} | \xi_n, j_n, \mu_n \rangle \cdot r_h^2 \cdot \right.$$
$$\left. \cdot \int d\Omega_l Y_{L,-q}(\theta_l,\phi_l) \langle W_C^f, \kappa_C^f, \mu_C^f | \mathbf{r_l} \rangle \gamma^0\gamma_\mu(1-\gamma^5) \langle \mathbf{r_l} | W_\nu, \kappa_\nu, \mu_\nu \rangle \delta(r_h - r_l) \right] dr_h;$$

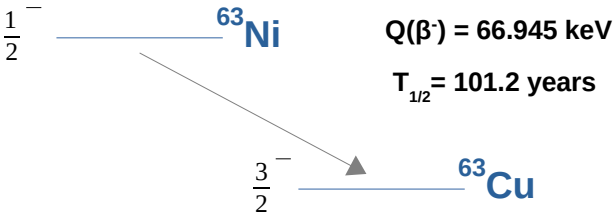
By considering the submatrix in which the emitted electron is the one escaping from the atom, one can recover the traditional spectrum

Beta-decay

$$^{63}_{28}Ni_{35} \rightarrow {}^{63}_{29}Cu_{34} + e^{-} + \bar{\nu}_e$$

The 63Ni nucleus (even–odd) decays 100% via β− to 63Cu (odd–even)





This spectrum is computed computing the nuclear matrix element using a neutron in the $2p_{1/2}$ level and a proton in the $2p_{3/2}$ level

This gives an half-life $T_{1/2}$ ~ 0.1 years !!!!

Need to go beyond the simple shell model to compute rates !!!

[Mougeot] - X. Mougeot et al., *Consistent calculation of the screening and exchange effects in allowed β− transitions*, Phys. Rev. A 90, 012501 (2014)

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Beta-decay

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Generalizing to different temperatures and densities

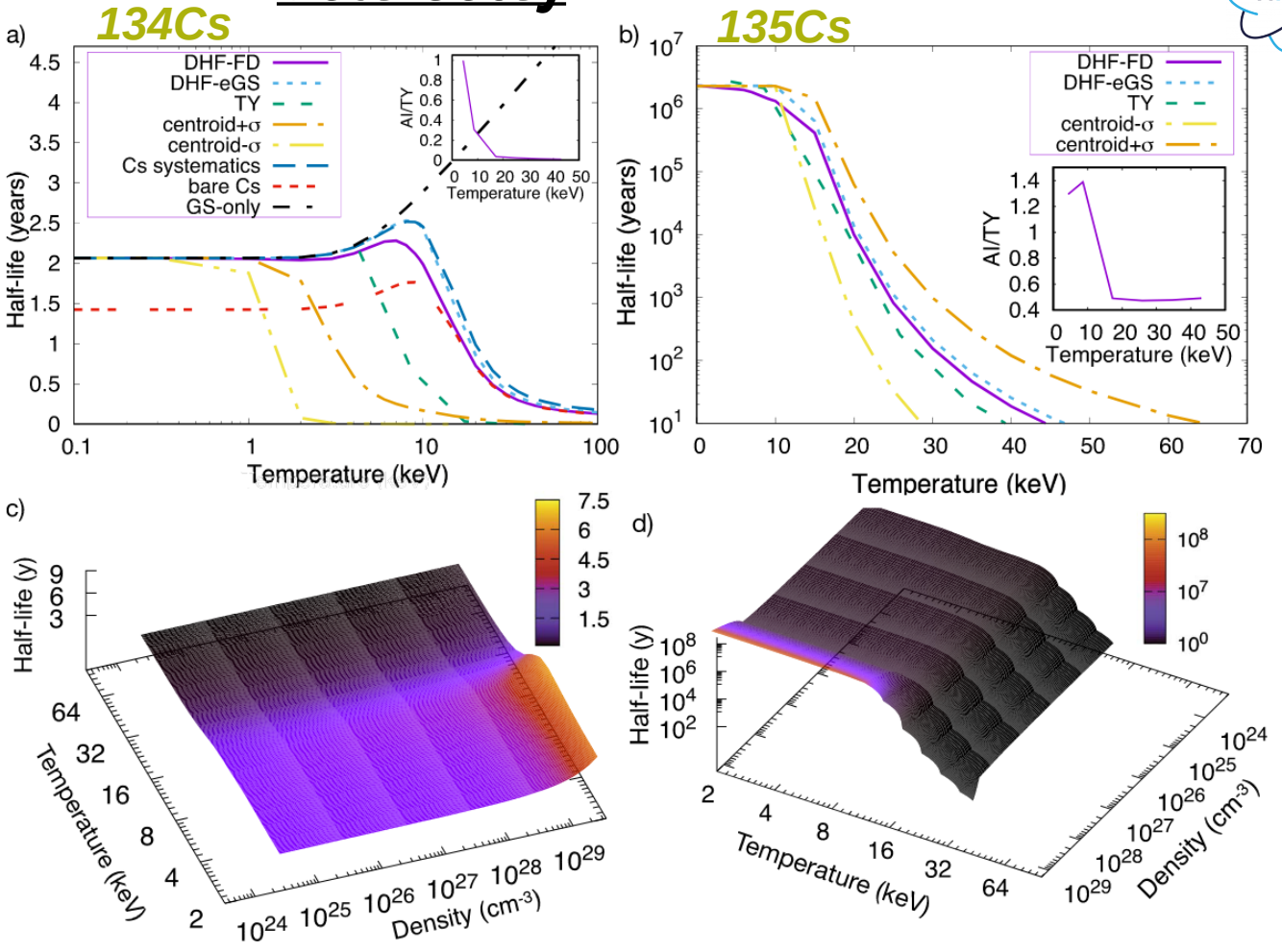
$$P_{i\to f} = 2\pi Tr\left[\hat{\rho}_i H_\beta S_f H_\beta\right]\delta(W_i - W_f)$$

where

$$\hat{\rho}_i = p_i |i\rangle\langle i|$$

and

$$S_f = \sum_f |f\rangle\langle f|$$



S. Taioli et al., *Theoretical Estimate of the Half-life for the Radioactive 134Cs and 135Cs in Astrophysical Scenarios*, The Astrophysical Journal, 933:158, (2022)

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Beta-decay: improving the framework (at least for small systems)

TIFPA Trento Institute for Fundamental Physics and Applications

We consider the beta-decay of the T_2 molecule

$$\Psi = \psi^{(1)}_{nnp} \otimes \psi^{(2)}_{nnp} \otimes \Phi$$

$\psi^{(i)}_{nnp}$ → **Nuclear wavefunction computed using hyperspherical harmonics and realistic potential (chiral EFT)**

$$\Phi = \sum_k C_k P(T_1, T_2) P(e_1, e_2) [g_k(\boldsymbol{r}_{T_1}, \boldsymbol{r}_{T_2}, \boldsymbol{r}_{e_1}, \boldsymbol{r}_{e_2}) \Theta(T_1, T_2) \Theta(e_1, e_2)]$$

$$g_k(\boldsymbol{r}_{T_1}, \boldsymbol{r}_{T_2}, \boldsymbol{r}_{e_1}, \boldsymbol{r}_{e_2}) = e^{-(\boldsymbol{r}-\boldsymbol{b})^T A_k (\boldsymbol{r}-\boldsymbol{b})}$$

Explicitly correlated Gaussian as basis set to solve the fully non-adiabatic non-relativistic many-body problem

A_k is a positive definite NxN matrix, where N is the number of particles (N=4 for Tritium)

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Perspectives

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- **Path Integral Monte Carlo / Molecular Dynamics:**
  1) study of the structural phase transition of H3S in the superconducting phase;
  2) machinery to develop Machine Learning potential energy surfaces;
  3) benchmarking 3-body potentials for Helium-4 in the superfluid phase;

- **Ab-initio beta-decay simulations:**
  1) building a framework to include both hadronic and leptonic matrix elements at the highest level of accuracy;
  2) Tritium beta-decay: bechmark system.

Thanks for your attention!

Main collaborators:

Michele Casula (Sorbonne University)

Stefano Simonucci (UNICAM)

Simone Taioli (ECT*)

Giovanni Garberoglio (ECT*)

The work on hydrogen and water clusters was performed using HPC resources from GENCI-IDRIS (Grant 2021-0906493)

European Centre of Excellence in Exascale Computing TREX (Targeting Real Chemical Accuracy at the Exascale)

Tracking H_3S structural phase transition

asymmetric

symmetric

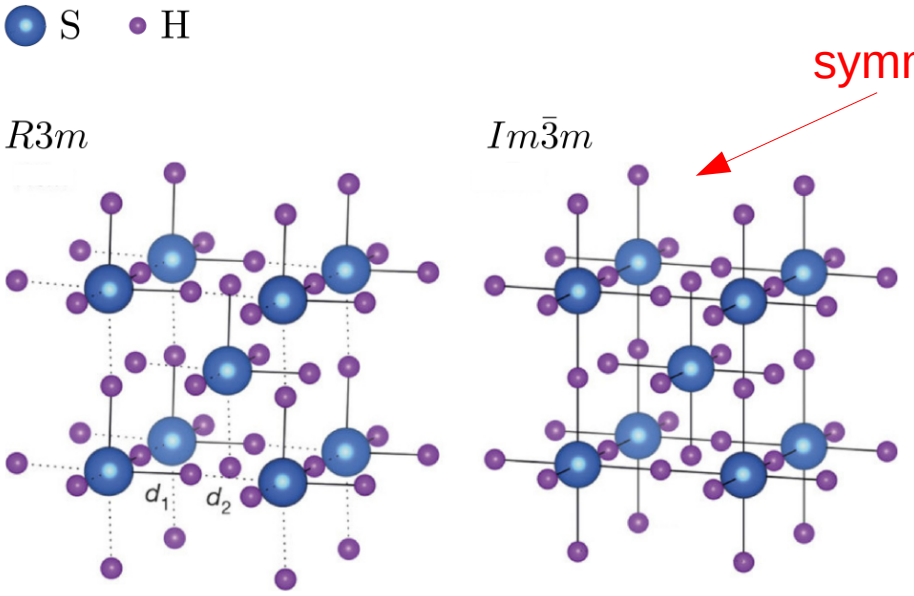


FIG. 1. Crystal structure in the conventional bcc cell of the $Im\bar{3}m$ phase (right) and of a $R3m$ phase (left) of H_3S. In the $R3m$ structure, the H-S covalent bond of length d_1 is marked with a solid line and the longer $H\cdots S$ hydrogen bond of length d_2 with a dotted line. In the $Im\bar{3}m$ phase $d_1 = d_2$. Blue and pink spheres represent S and H atoms, respectively.

Published: 17 August 2015

Conventional superconductivity at 203 kelvin at high pressures in the sulfur hydride system

A. P. Drozdov, M. I. Eremets ✉, I. A. Troyan, V. Ksenofontov & S. I. Shylin

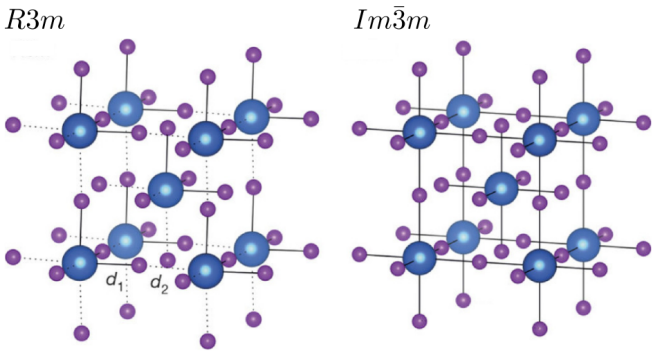
Nature **525**, 73–76(2015) | Cite this article

15k Accesses | **934** Citations | **678** Altmetric | Metrics

Picture from:
High-pressure phase diagram of hydrogen and deuterium sulfides from first principles: Structural and vibrational properties including quantum and anharmonic effects,
R. Bianco, I. Errea, M. Calandra and F. Mauri, PRB 97, 214101 (2018)

Tracking H_3S structural phase transition

S H



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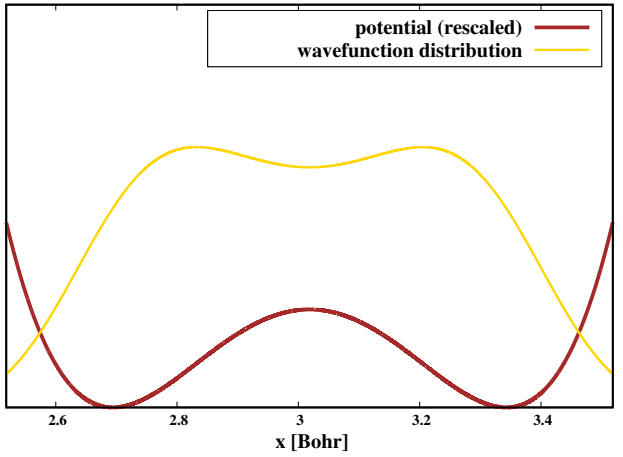
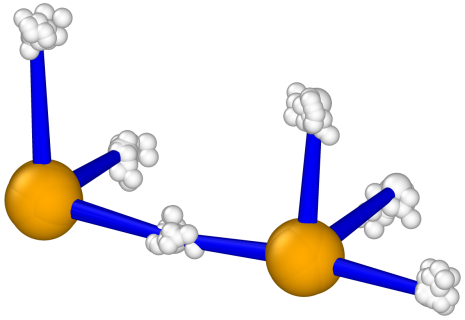
From PIMD simulations, the average position of H atoms is *always* symmetric!!





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Tracking H_3S structural phase transition

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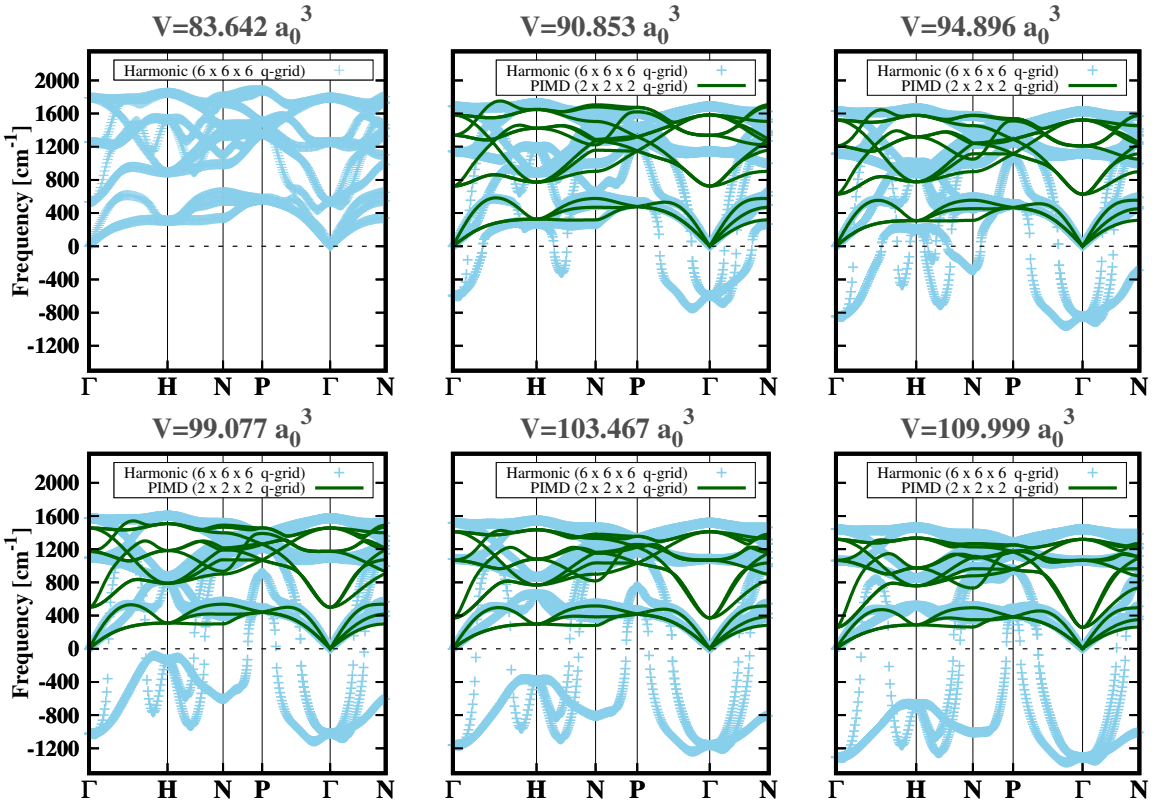
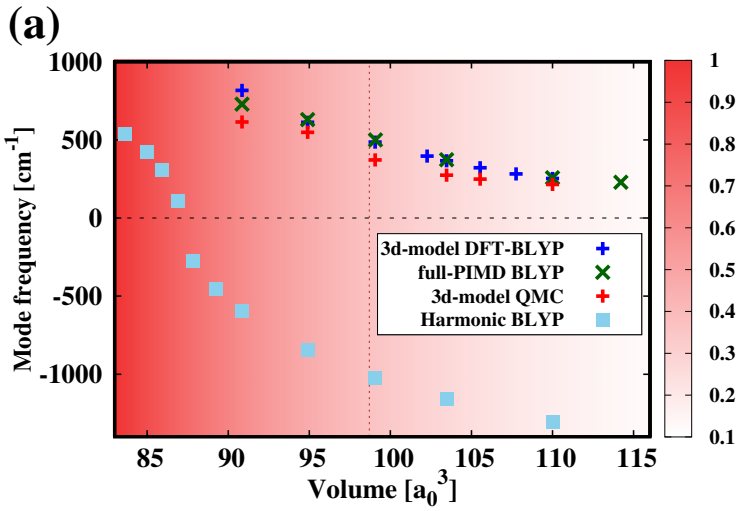




Beta-decay

Tritium beta decay

$$^{3}_{1}H_{2} \rightarrow {}^{3}_{2}He_{1} + e^{-} + \bar{\nu}_{e}$$

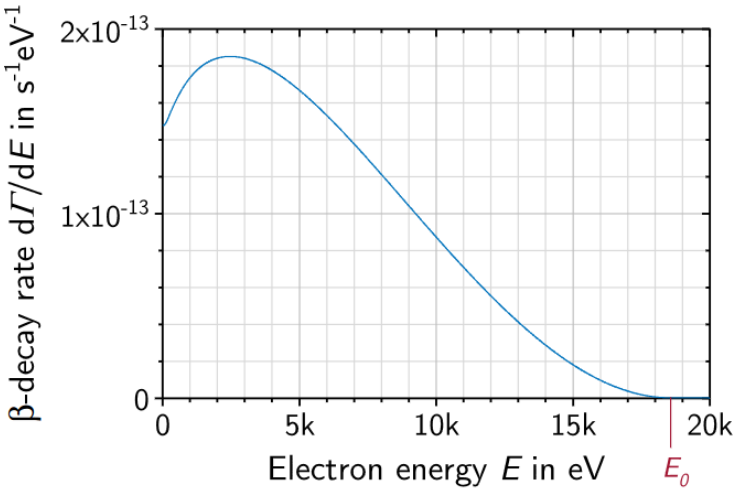
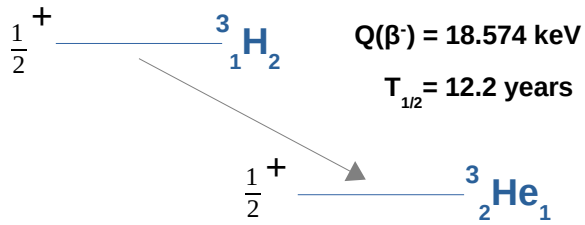
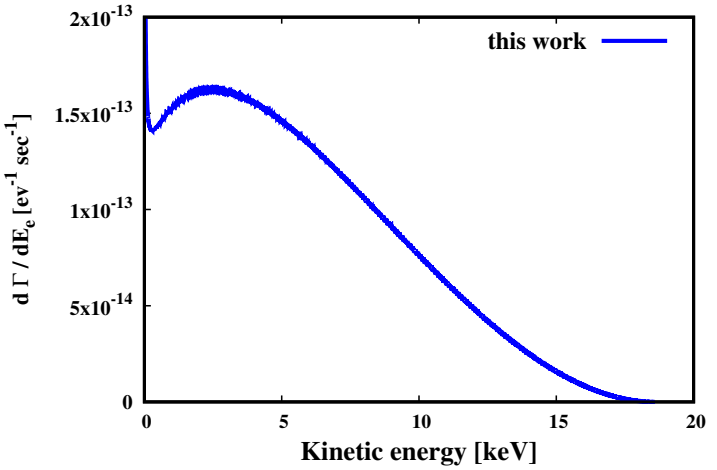


Fig. 1 The differential β-electron energy spectrum for the β-decay of molecular tritium with the endpoint energy E_0 of 18.574 keV. The given units correspond to the decay rate of a single tritium nucleus

Eur. Phys. J. C (2019) 79:204, https://doi.org/10.1140/epjc/s10052-019-6686-7

The 3H nucleus (even–odd) decays 100% via β− to 3He (odd–even)





This spectrum is computed computing the nuclear matrix element using a neutron in the $1p_{1/2}$ level and a proton in the $1p_{1/2}$ level

This gives an half-life $T_{1/2}$ ~ 25 years !!!!

Beta-decay

To deal with the relativistic weak-interaction Hamiltonian, we set up a relativistic mean-field framework to compute leptonic and hadronic matrix elements.

$$\begin{pmatrix} mc^2 + W_V + W_S + \mathbf{A}_P \cdot \boldsymbol{\sigma} - E & -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} - \boldsymbol{\sigma} \cdot \mathbf{A} + W_{PS} \\ -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} - \boldsymbol{\sigma} \cdot \mathbf{A} + W_{PS} & -mc^2 + W_V + \mathbf{A}_P \cdot \boldsymbol{\sigma} - W_S - E \end{pmatrix} \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} = 0$$

where

- W_S - scalar potential
- W_V - vectorial potential
- ~~W_{PS} - pseudoscalar potential~~
- ~~$\mathbf{A}_P$ - pseudo-vectorial potential~~

$$\rightarrow \quad \begin{pmatrix} mc^2 + W_V + W_S - E & -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} \\ -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} & -mc^2 + W_V - W_S - E \end{pmatrix} \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} = 0$$

TM et al., *Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Medium-Heavy Nuclei and of Atomic and Molecular Electronic Structure*, Advanced Theory and Simulations, 1, 1870030 (2018)

Beta-decay

To deal with the relativistic weak-interaction Hamiltonian, we set up a relativistic mean-field framework to compute leptonic and hadronic matrix elements.

$$H = \sum_{s_1 s_2} \int d\mathbf{r}\ \hat{\psi}^+_{s_1}(\mathbf{r}) \left[-ic\boldsymbol{\alpha}_{s_1 s_2} \cdot \boldsymbol{\nabla} + \beta_{s_1 s_2} mc^2 + \delta_{s_1 s_2} V(\mathbf{r})\right] \hat{\psi}_{s_2}(\mathbf{r}) +$$
$$+ \frac{1}{2} \sum_{s_1 s_2 s'_1 s'_2} \int d\mathbf{r} d\mathbf{r}'\ \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}^+_{s'_1}(\mathbf{r}') \left[\beta_{s_1 s_2} \beta_{s'_1 s'_2} g_S(\mathbf{r}, \mathbf{r}') + \left(\delta_{s_1 s_2} \delta_{s'_1 s'_2} - \boldsymbol{\alpha}_{s_1 s_2} \cdot \boldsymbol{\alpha}'_{s'_1 s'_2}\right) g_V(\mathbf{r}, \mathbf{r}')\right] \hat{\psi}_{s'_2}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r})$$

Hartree-Fock approximation

$$\left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}^+_{s'_1}(\mathbf{r}') \hat{\psi}_{s'_2}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle = \left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle \left\langle \hat{\psi}^+_{s'_1}(\mathbf{r}') \hat{\psi}_{s'_2}(\mathbf{r}') \right\rangle - \left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}_{s'_2}(\mathbf{r}') \right\rangle \left\langle \hat{\psi}^+_{s'_1}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle$$

TM et al., *Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Medium-Heavy Nuclei and of Atomic and Molecular Electronic Structure*, Advanced Theory and Simulations, 1, 1870030 (2018)

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$$+ \frac{1}{2} \sum_{s_1 s_2 s'_1 s'_2} \int d\mathbf{r} d\mathbf{r}'\ \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}^+_{s'_1}(\mathbf{r}') \left[\beta_{s_1 s_2} \beta_{s'_1 s'_2} g_S(\mathbf{r}, \mathbf{r}') + \left(\delta_{s_1 s_2} \delta_{s'_1 s'_2} - \boldsymbol{\alpha}_{s_1 s_2} \cdot \boldsymbol{\alpha}'_{s'_1 s'_2}\right) g_V(\mathbf{r}, \mathbf{r}')\right] \hat{\psi}_{s'_2}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r})$$

Hartree-Fock approximation

$$\left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}^+_{s'_1}(\mathbf{r}') \hat{\psi}_{s'_2}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle = \left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle \left\langle \hat{\psi}^+_{s'_1}(\mathbf{r}') \hat{\psi}_{s'_2}(\mathbf{r}') \right\rangle - \left\langle \hat{\psi}^+_{s_1}(\mathbf{r}) \hat{\psi}_{s'_2}(\mathbf{r}') \right\rangle \left\langle \hat{\psi}^+_{s'_1}(\mathbf{r}') \hat{\psi}_{s_2}(\mathbf{r}) \right\rangle$$

$$\begin{pmatrix} mc^2 + W_V + W_S + \mathbf{A}_P \cdot \boldsymbol{\sigma} - E & -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} - \boldsymbol{\sigma} \cdot \mathbf{A} + W_{PS} \\ -c\boldsymbol{\sigma} \cdot i\boldsymbol{\nabla} - \boldsymbol{\sigma} \cdot \mathbf{A} + W_{PS} & -mc^2 + W_V + \mathbf{A}_P \cdot \boldsymbol{\sigma} - W_S - E \end{pmatrix} \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} = 0$$

where

- W_S - scalar term
- W_V - vectorial term
- W_{PS} - pseudoscalar term
- $\mathbf{A}_P$ - pseudo-vectorial term

Single particle equations