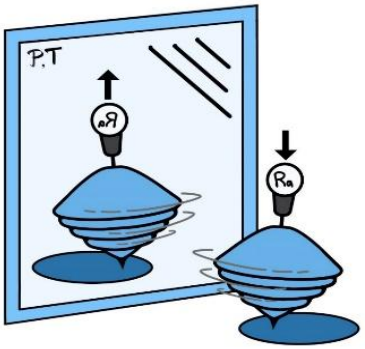


St Petersburg University

P, T violating effects in molecules

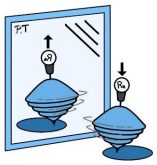
Zakharova Anna

Saint Petersburg State University

Petersburg Nuclear Physics Institute named by B.P.Konstantinov (ОТФ)

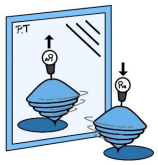
zakharova.annet@gmail.com

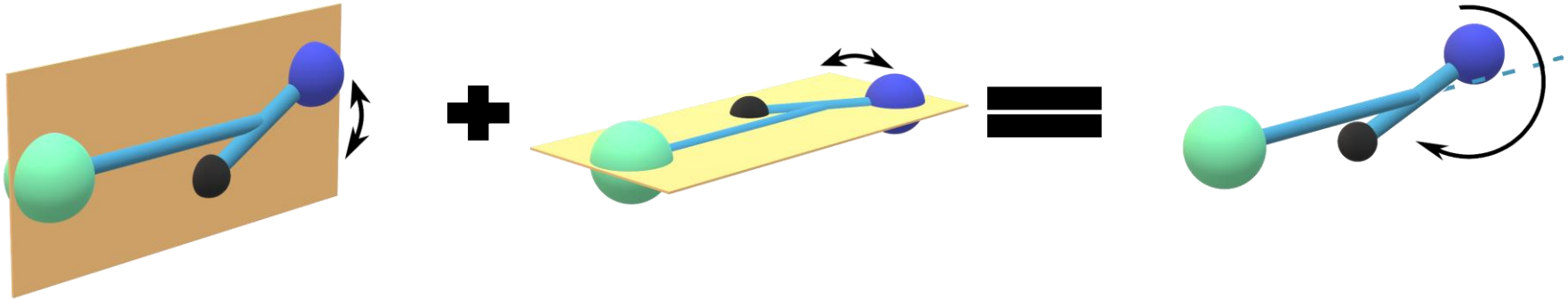
Search for the P, T violation with molecules



- Spectrum of the heavy-atomic molecules is sensitive to the P, T violation effects while having rather small Standard Model background
- Opposite parity doublets - T-violation can be easily distinguished compensating systematic effects from non-T violating noise
- Polyatomic molecules (triatomic, symmetric tops) - combine parity doublets with laser-cooling - next generation of the experiments
- Experiments with molecules - leaders in searches of the eEDM
- Can we use them to search other effects, like caused by presence of the axions?

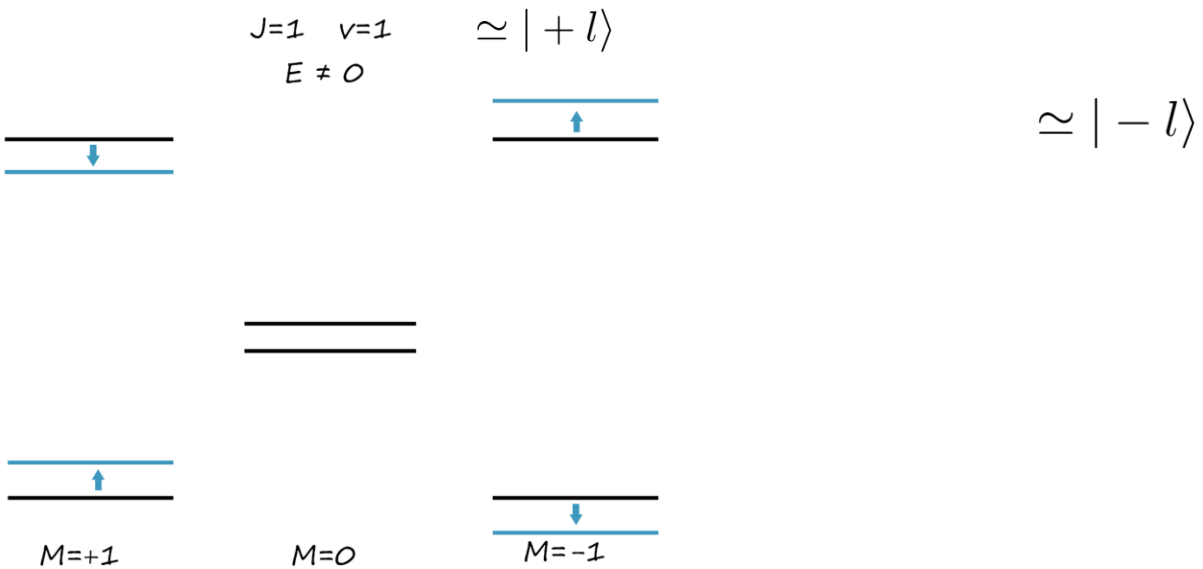
l-doublet



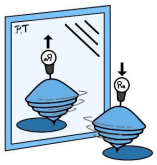


For free molecule eigenstates are $|\pm\rangle = \frac{1}{\sqrt{2}}\left(|+l\rangle \pm |-l\rangle\right)$

in External electric field the molecule polarizes and is sensitive to T violation



Example of P, T violating effects



Consider a P, T even Hamiltonian $\hat{H}_0$ perturbed by a P, T violating terms

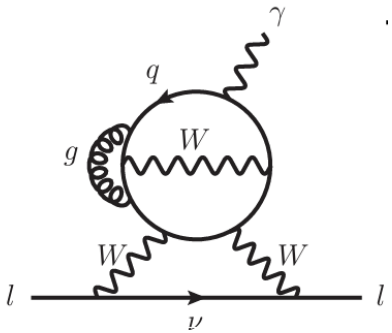
$$\hat{H} = \hat{H}_0 + \hat{H}_{\not P \not T}$$

$$\hat{H}_{\not P \not T} = \hat{H}_d + \hat{H}_s,$$

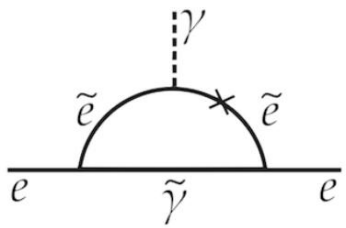
- Electron electric dipole moment

(suppressed in SM, larger in BSM)

$$\hat{H}_d = 2d_e \sum_i \begin{pmatrix} 0 & 0 \\ 0 & \sigma_i \mathbf{E_i} \end{pmatrix},$$



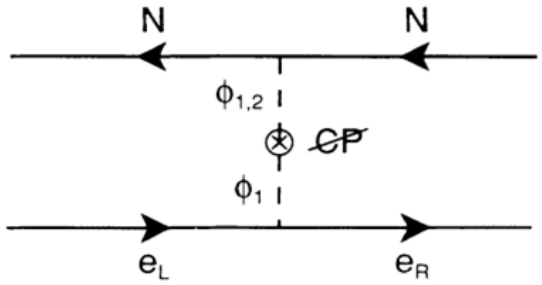
SM



SUSY

- Scalar-pseudoscalar electron-nucleon interaction

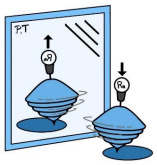
$$\hat{H}_s = ik_s \frac{G_F}{\sqrt{2}} \sum_{j=1}^{N_{elec}} \sum_{I=1}^{N_{nuc}} \rho_I(\vec{r_j}) Z_I \gamma^0 \gamma^5$$



Local effective interactions - main contribution from core region near heavy nucleus, weakly dependent on the molecule configutation

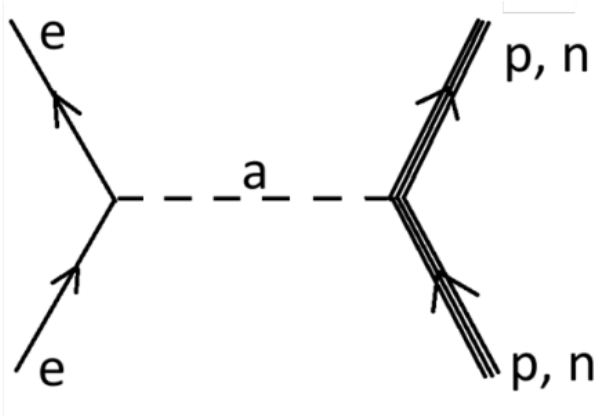
$$\delta E = P(d_e E_{eff} + k_s E_s) \qquad E_{\text{eff}} = \frac{\langle \Psi | \hat{H}_d | \Psi \rangle}{d_e}, \qquad E_{\text{s}} = \frac{\langle \Psi | \hat{H}_s | \Psi \rangle}{k_s}$$

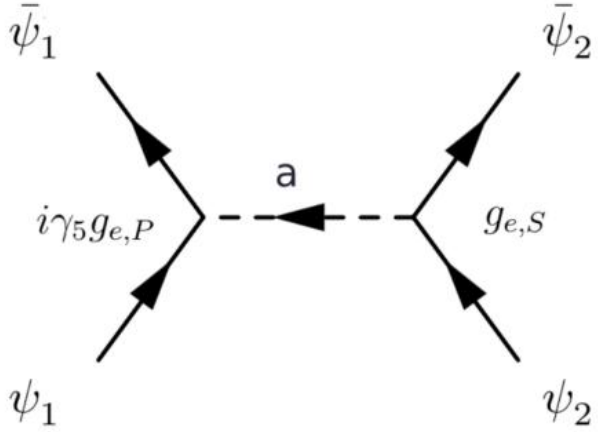
Axion mediated interaction



Axion interactions with fermions of SM - scalar and pseudoscalar

$$\mathcal{S}_{\rm int} = a \sum_{f \in {\rm SM}} \bar{\Psi}_f \left(g_{f,S} + i g_{f,P} \gamma_5 \right) \Psi_f$$

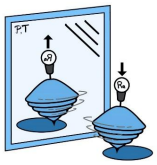




$$\hat{H}_{eN} = i \frac{g_{e,P}}{4\pi} \sum_{i=1}^{N_e} \sum_{k=1}^{A} \int d^3\mathbf{R}_k \, g_{N_k,S} \rho_k(\mathbf{R}_k) \frac{e^{-m_a c|\mathbf{r}_i - \mathbf{R}_k|}}{|\mathbf{r}_i - \mathbf{R}_k|} \gamma_0^{(i)} \gamma_5^{(i)}$$

$$\hat{H}_{ee} = \frac{g_S^{(e)} g_P^{(e)}}{4\pi} \sum_{i,j=1}^{N_e} \left(i\gamma_0\gamma_5 \right)_i \left(\gamma_0 \right)_j \frac{e^{-m_a c|\vec{r}_i - \vec{r}_j|}}{|\vec{r}_i - \vec{r}_j|}$$

Computations with GRECP

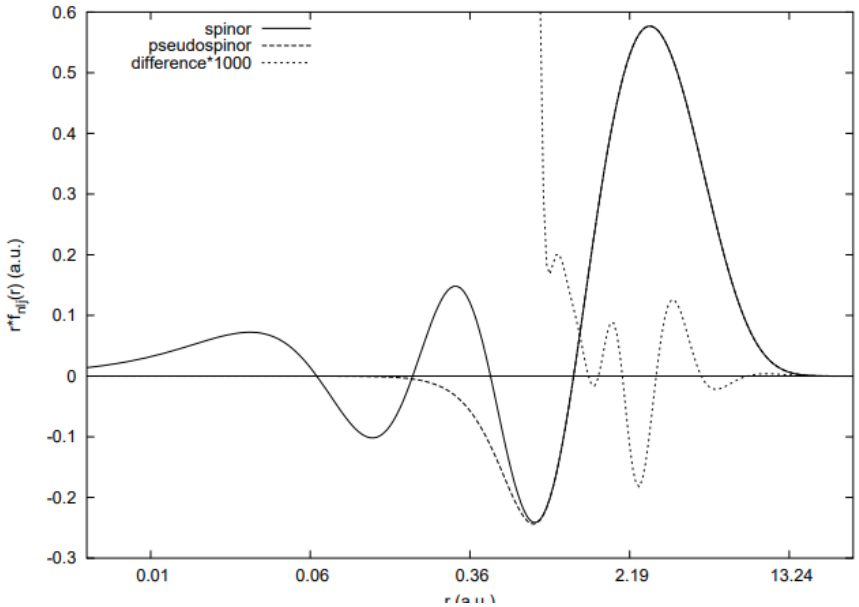


Full-electron computation - large computational complexity due to the large size of the basis required. GRECP - freeze core electrons and replace interaction with them by the effective potential operator

Molecular computation is much faster - good for study of the polyatomic molecules taking into account their vibrations

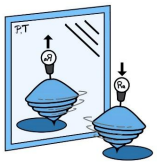
But the behavior of the wavefunction becomes incorrect in the core region

- 2-component formalism
- In the core region the solutions do not have the correct oscillatory behavior

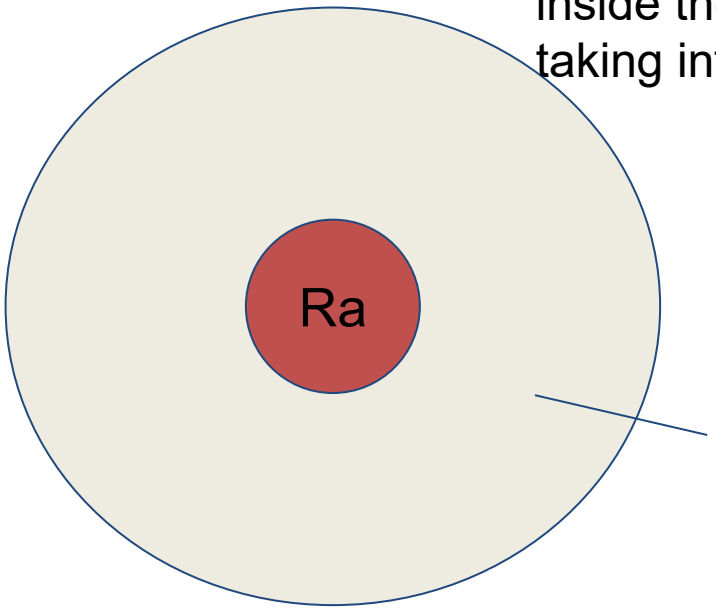


from A.V.Titov et al //
Prog.Theor.Chem.Phys., v.15, chapt.II (2006)

Restoration idea

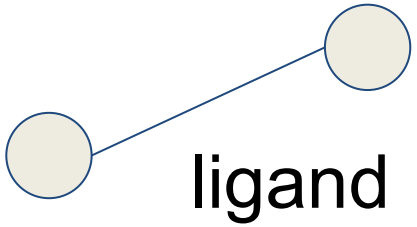


Near region - heavy atom dominates
inside the wavefunction can be described
taking into account only heavy atom field

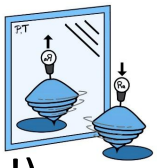


Matching the behavior in the transition region
we can reconstruct the correct behavior in the near region

far region - core electrons are not important
GRECP obtained wavefunction is correct



One center restoration method



Construct two sets of solutions of the atomic problem (once for the element!)

1). Two-component basis of solutions of atomic problem with GRECP

$$\tilde{\Phi}_{nm} = \frac{\tilde{f}_n(r)}{r}\Omega_{\kappa_n,m}(\theta,\phi) \qquad \Omega_{\kappa,m} = \begin{pmatrix} \omega_{\uparrow\kappa} Y_{l,m-\frac{1}{2}} \\ \omega_{\downarrow\kappa} Y_{l,m+\frac{1}{2}} \end{pmatrix}, \quad \kappa = \begin{cases} j+\frac{1}{2} = l, & \kappa > 0 \\ -j-\frac{1}{2} = -(l+1), & \kappa < 0 \end{cases}$$

2). Four-component basis of full-electron problem solutions

$$\Phi_{nm} = \frac{1}{r}\begin{pmatrix} f_n(r)\Omega_{\kappa_n m}(\theta,\phi) \\ i g_n(r)\Omega_{-\kappa_n,m}(\theta\phi) \end{pmatrix} \qquad \Phi_{nm}\Big|_{\text{transitional } r} \simeq \begin{pmatrix} \tilde{\Phi}_{nm} \\ 0 \end{pmatrix}$$

In the molecular computation:
2-component orbitals =
superposition of multi-center gaussians

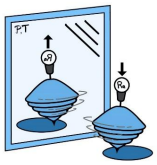
$$\psi_a = \sum_{K=1}^{N_{atoms}} \sum_{I=1}^{N_{bas,K}} \begin{pmatrix} A_{a,KI} \\ B_{a,KI} \end{pmatrix} \phi_{KI}\left(\vec{r} - \vec{r}_K\right)$$

$$\psi_a \simeq \sum_{nm} C_{a,nm}\tilde{\Phi}_{nm} \longrightarrow \Psi_a = \sum_{nm} C_{a,nm}\Phi_{nm}$$

4-component spinor with good oscillatory behavior

$$\langle \Psi_a | \hat{O}_{1-el} | \Psi_b \rangle \equiv \sum_{n_a m_a} \sum_{n_b m_b} C^*_{a,n_a m_a} C_{b,n_b m_b} \langle \Phi_{n_a m_a} | \hat{O}_{1-el} | \Phi_{n_b m_b} \rangle$$

Electron–Nucleon interaction



$$\hat{O}_{1-el} = \begin{pmatrix} \hat{O}_{LL} & \hat{O}_{LS} \\ \hat{O}_{SL} & \hat{O}_{SS} \end{pmatrix}, \quad \hat{O}_{AB} = \hat{O}_{AB,0}\hat{1} + \hat{O}_{AB,k}\hat{\sigma}_k$$

If only 0-term are present:

$$\langle \Phi_{nm} | \hat{O}_{1-el} | \Phi_{\tilde{n}\tilde{m}} \rangle = \int_0^\infty dr \Big\{ \Big(f_n \hat{O}_{0,LL} f_{\tilde{n}} + g_n \hat{O}_{0,SS} g_{\tilde{n}} \Big) \delta_{\kappa\tilde{\kappa}} \delta_{m\tilde{m}}$$

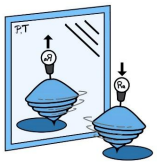
$$+ i \Big(f_n \hat{O}_{0,LS} g_{\tilde{n}} + g_n \hat{O}_{0,SL} f_{\tilde{n}} \Big) \delta_{\kappa,-\tilde{\kappa}} \delta_{m\tilde{m}} \Big\}$$

$$H_{eN} = A \frac{g_P^{(e)} g_S^N}{4\pi} i\gamma_0\gamma_5 \frac{e^{-m_a c r}}{r} = A \frac{g_P^{(e)} g_S^N}{4\pi} \begin{pmatrix} 0 & i\hat{1}e^{-m_a c r}/r \\ -i\hat{1}e^{-m_a c r}/r & 0 \end{pmatrix}$$

$$\frac{1}{m_a c} \sim 1\,\text{a.u.} \quad \mapsto \quad m_a \sim \frac{m_e}{137} \sim 5\,\text{KeV}$$

For most astrophysically interesting axion mass ranges this interaction is long-range compared to the molecular scales

Electron–Electron interaction



Neglecting exponent we can use usual Coulomb decomposition

$$\frac{1}{r_{12}} = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} \left(\frac{4\pi}{2L+1} \right) \left(\frac{r_<^L}{r_>^{L+1}} \right) Y_{LM}^*(\hat{r}_1) Y_{LM}(\hat{r}_2)$$

Then we can represent the two-electron matrix element as

$$\langle \Phi_{n_a m_a} \Phi_{n_b m_b} | \frac{(i\gamma_0\gamma_5)_1 (\gamma_0)_2}{|\vec{r}_1 - \vec{r}_2|} | \Phi_{n_c m_c} \Phi_{n_d m_d} \rangle =$$

$$\sum_{LM} (-1)^{j_a - m_a + L - M + j_b - m_b} \begin{pmatrix} j_a & L & j_c \\ -m_a & M & m_c \end{pmatrix} \begin{pmatrix} j_b & L & j_d \\ -m_b & -M & m_d \end{pmatrix} \mathcal{R}^{(L)}_{ab,cd}$$

$$\mathcal{R}^{(L)}_{ab,cd} = - \int_0^\infty dr_1 dr_2 (-1)^L \mathcal{G}_L(\kappa_a, -\kappa_c) \mathcal{G}_L(\kappa_b, \kappa_d) \frac{r_<^L}{r_>^{L+1}} \mathcal{P}_{ac}(r_1) \mathcal{S}_{bd}(r_2)$$

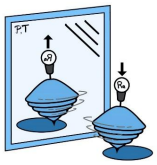
Angular factor $\mathcal{G}_L(\kappa_a, \kappa_b) = (-1)^{j_a + \frac{1}{2}} \sqrt{[j_a][j_b][l_a][l_b]} \begin{pmatrix} l_a & L & l_b \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} j_a & L & j_b \\ l_b & \frac{1}{2} & l_a \end{Bmatrix}$

$[j] \equiv 2j + 1$

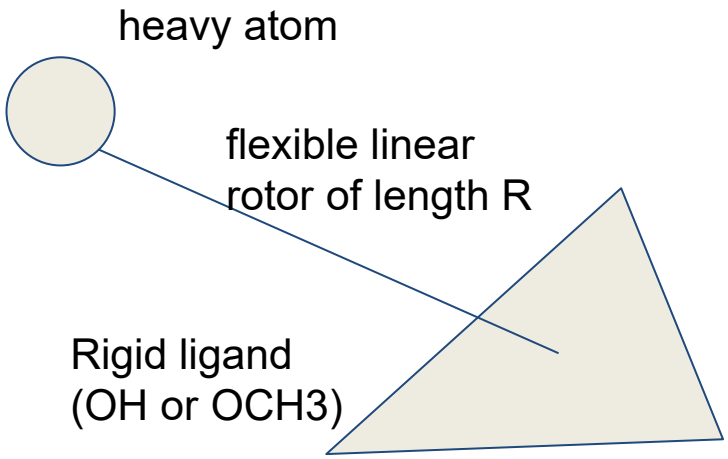
Pseudo-scalar factor $\mathcal{P}_{ac}(r) = f_a(r) g_c(r) + g_a(r) f_c(r)$

Scalar factor $\mathcal{S}_{bd}(r) = f_b(r) f_d(r) - g_b(r) g_d(r)$

Nuclear motion wavefunction



Coupled channel method



Decompose the nuclear motion wavefunction into the product of eigenvalues of:

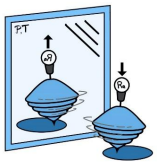
1. Total angular momentum l of the linear rotor heavy-atom – ligand c.o.m. and its space-fixed z projection m_l
2. Total angular momentum j of the rigid ligand, its space-fixed z projection m, for OCH3 - its ligand-fixed projection k

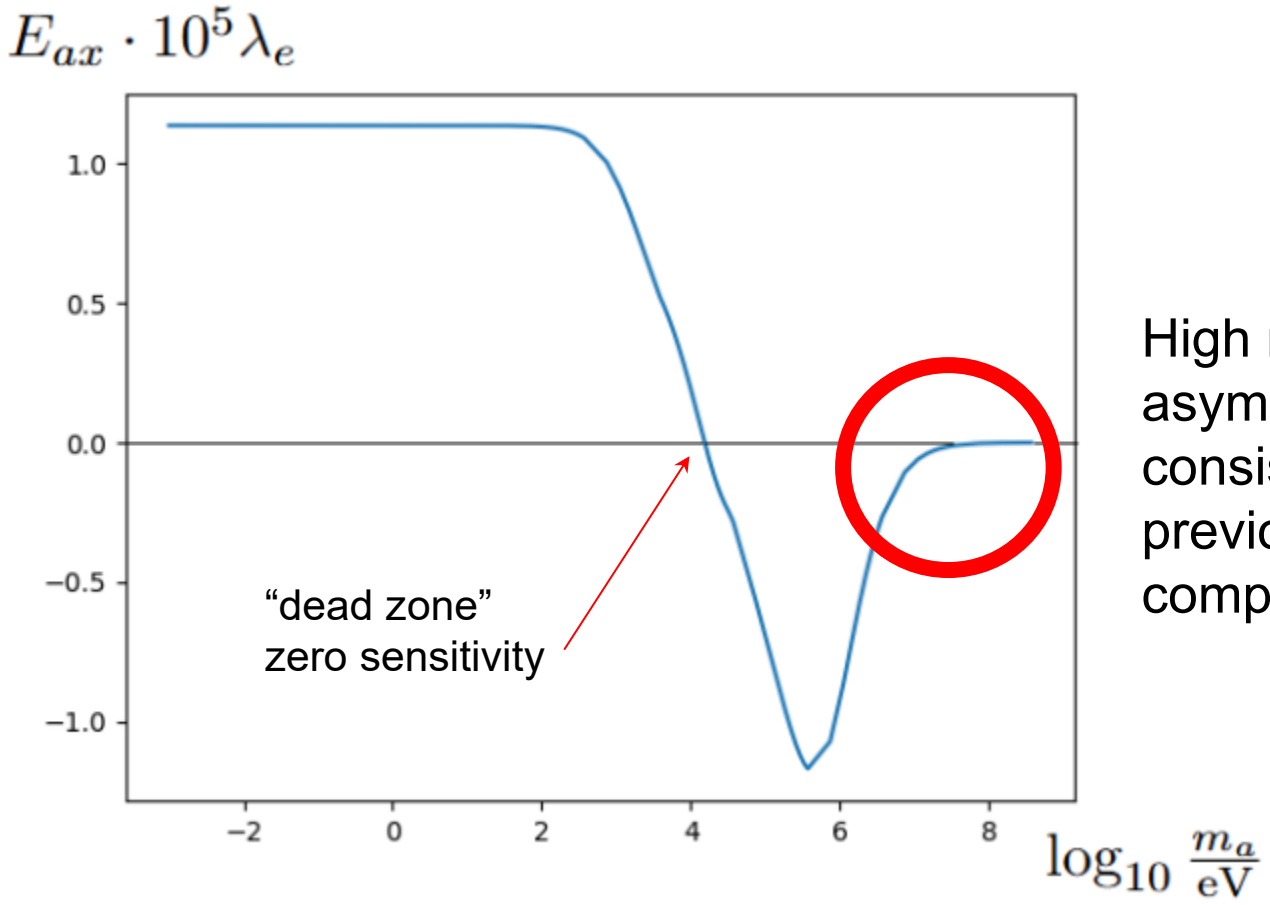
As result - 1D Schrodinger equation for the multi-component wavefunction with adiabatic potential becoming a matrix potential

Decompose all dependence on R in terms of the longitudinal harmonic oscillator wavefunctions - Hamiltonian becomes just a discrete matrix

This matrix can be written to include all anharmonic and rotational effects, thus all can be taken into account

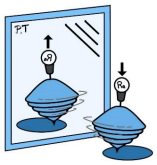
eN interaction dependence on m_a





High mass asymptotics is consistent with previous Es computations

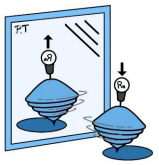
Results



State	EeN 10^-5 lambda_e^-1
RaOH equilibrium	1.141
RaOH l-doublet	1.127
YbOH equilibrium	3.36
BaF equilibrium	1.77

State	Eee 10^-5 lambda_e^-1
RaOH equilibrium	1.383
RaOH l-doublet	1.367
RaOCH3 equilibrium	17.37
RaOCH3 l-doublet	17.3
YbOH equilibrium	1.46
BaF equilibrium	0.8

Are molecules useful for axion searches?



Coupled channel method

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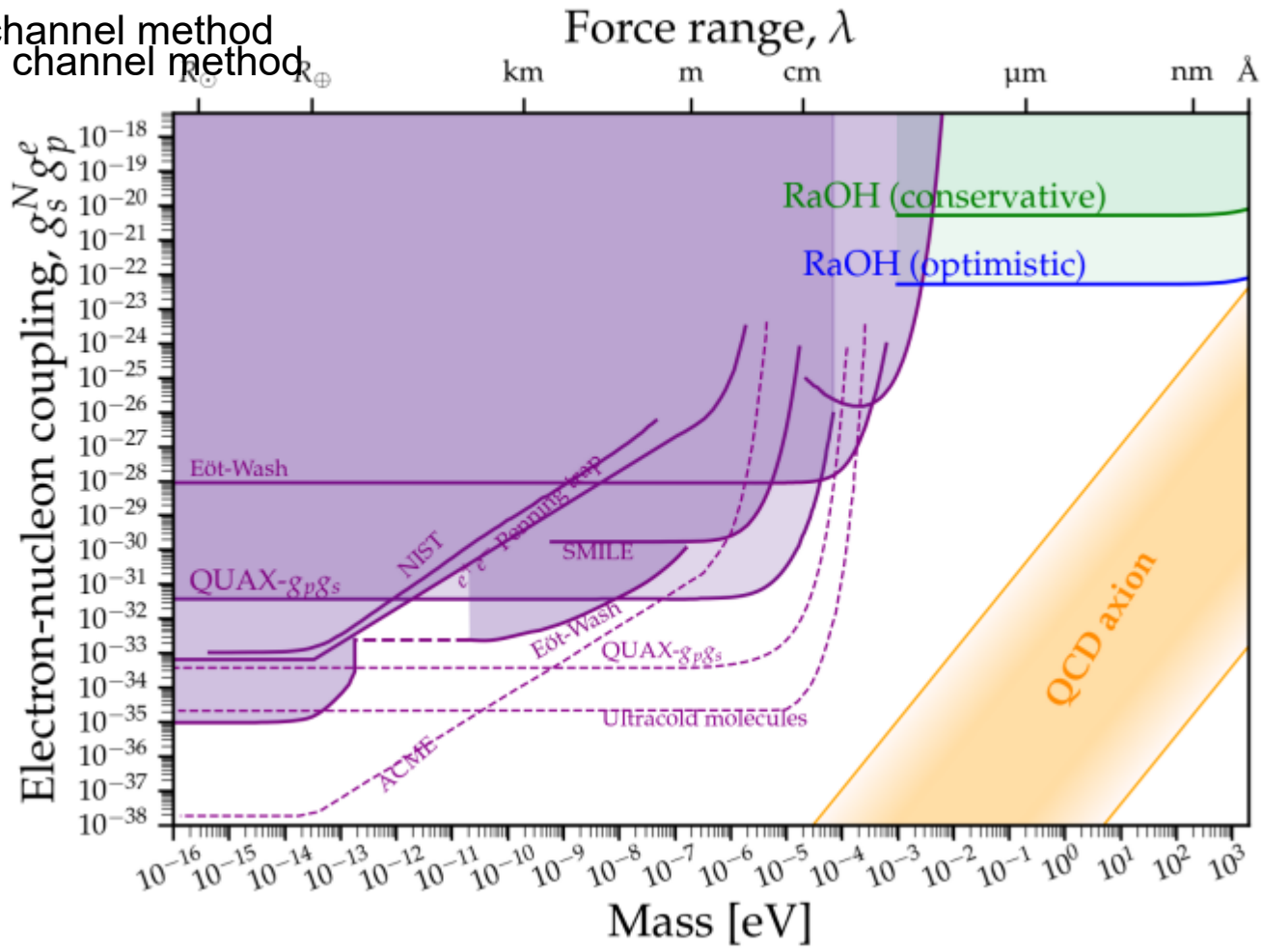
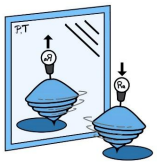


Conclusion



- We have developed tools for computing the properties induced by axion exchange using the one-center restoration technique. **First time this method was used to compute two-electron property (ee exchange)**

- The sensitivity to the axions obtained is comparable to the full-electron computations, but its dependence on the vibrations could be studied. Surprisingly, despite long-range nature, this dependence is small

- While the molecular experiments can't compete with astrophysical red-giant limits, they can become best laboratory experiments for a certain axion mass range

- **The developed techniques can now be applied to study other long range one- and two-electron interactions such as induced by the loop processes** (axion interaction with photon loop, loops induced by exchange of light fermions, such as neutrinos and gravitinos) - stay tuned for the new results