# **Cornering the Electron EDM with Ultracold AgRa**

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# Outline

in collaboration with



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• Molecular EDMs : AgRa

• Atomic EDMs : <sup>129</sup>Xe

# eEDM Constraint on Beyond-Standard-Model Theories<sup>1</sup> Single-source interpretation



Model	$ d_e [e \cdot cm]$
Standard model	$< 10^{-38}$
Left-right symmetric Lepton-flavor changing Multi-Higgs	$ \begin{array}{c} 10^{-28} \dots 10^{-26} \\ 10^{-29} \dots 10^{-26} \\ 10^{-28} \dots 10^{-27} \\ < 10^{-25} \end{array} $
Experimental limit (TI) <sup>2</sup> Experimental limit (YbF) <sup>3</sup> Experimental limit (ThO) <sup>4</sup>	$ \leq 10 $ $ < 1.6 \cdot 10^{-27} $ $ < 10.5 \cdot 10^{-28} $ $ < 9.6 \cdot 10^{-29} $

<sup>1</sup>Courtesy: DeMille (2005), Huliyar (2009)

<sup>2</sup>B.C. Regan, E.D. Commins, C.J. Schmidt, D.P. DeMille, *Phys Rev Lett* **88** (2002) *071805/1* 

<sup>3</sup>J.J. Hudson, D.M. Kara, I.J. Smallman, B.E. Sauer, M.R. Tarbutt, E.A. Hinds, *Nature* 473 (2011) 493

<sup>4</sup>D. DeMille, ICAP 2014, Washington D.C., ACME Collaboration, *Science* **6168** (2014) *269*, TF and M. K. Nayak, *J. Mol. Spectrosc.* **300** (2014) *16*, L. V. Skripnikov, A. N. Petrov, A. V. Titov, *J. Chem. Phys.* **139** (2013) *221103*, L. V. Skripnikov, A. V. Titov, *J. Chem. Phys.* **142** (2015) *024301*, M. Denis, TF, *J Chem Phys* **145** (2016) *214307* 

# More Stringent Bounds on (Semi-)Leptonic CP-odd Parameters<sup>5</sup>



<sup>b</sup>TF, M. Jung, J. High Energy Phys. 7 (2018) 012

J. Baron et al., Science 343 (2014) 269

M. Denis, T. F., J. Chem. Phys. 145 (2016) 214307

L. Skripnikov, J. Chem. Phys. 145 (2016) 214301

W.B. Cairncross, D.N. Gresh, M. Grau, K.C. Cossel, T.S. Roussy, Y. Ni, Y. Zhou, J. Ye, E.A. Cornell, *Phys. Rev. Lett.* **119** (2017) *153001* 

T. F., Phys. Rev. A (Rap. Comm.), 96 (2017) 040502(R)

L.V. Skripnikov, J. Chem. Phys., 147 (2017) 021101

 $\begin{aligned} & \mathsf{Multiple-source picture:} \\ & \Delta E_{\mathcal{P},\mathcal{T}} = - \left\langle \mathbf{d}_{\mathsf{sys}} \cdot \mathbf{E}_{\mathsf{ext}} \right\rangle \\ & = \left( \alpha_{d_e} \, d_e + \alpha_{C_S} \, C_S \right) \, \left\langle \mathbf{n} \cdot \mathbf{z} \right\rangle (E_{\mathsf{ext}}) \end{aligned}$ 

Previous resulting bound: From HfF<sup>+</sup>, ThO, YbF, TI  $|d_e|_{2017} < 6.4 \times 10^{-28}e$  cm

 $\label{eq:second} \begin{array}{l} \hline \mbox{New resulting bounds:} \\ \hline \mbox{From Hg, HfF^+, ThO, YbF, TI} \\ |d_e|_{2018} < 3.8 \times 10^{-28} e \ \mbox{cm} \\ |C_S|_{2018} < 2.7 \times 10^{-8} \end{array}$ 

# eEDM Constraint on Beyond-Standard-Model Theories Single-source interpretation (2018)



#### ACME 2018 result<sup>6</sup> combined with 2016 theory

<sup>6</sup>ACME collaboration, *Nature*, **562** (2018) *355* 

## **Going Ultracold: From beams to traps**

PHYSICAL REVIEW A, VOLUME 63, 023405

#### Loading and compressing Cs atoms in a very far-off-resonant light trap

D. J. Han, Marshall T. DePue, and David S. Weiss

Department of Physics, University of California at Berkeley, Berkeley, California 94720-7300 (Received 25 May 2000; published 12 January 2001)

We describe an experiment in which  $3 \times 10^7$  Cs atoms are loaded into a 400  $\mu$ m crossed beam far-offresonant trap (FORT) that is only 2  $\mu$ K deep. A high-density sample is prepared in a magneto-optic trap, cooled in a three-dimensional far-off-resonant lattice (FORL), optically pumped into the lowest-energy state, adiabatically released from the FORL, magnetically levitated, and transferred to the final trap with a phasespace density of  $10^{-3}$ . Spontaneous emission in the FORT is negligible, and we have compressed the atoms in the FORT to a spatial density of  $2 \times 10^{13}$  atoms/cm<sup>3</sup>. Evaporative cooling under these conditions proceeds rapidly.

• Estimated sensitivity of Cs EDM measurement in DLT<sup>7</sup> is  $|d_e| \approx 10^{-29} ecm$ 

Cs atom:  $\Delta E = R E_{\text{ext}} d_e$  $E_{\text{int}} \approx 20 \left[\frac{\text{MV}}{\text{cm}}\right]$  Ultracold XY Molecule:  $\Delta E = E_{\text{eff}} d_e$  $E_{\text{eff}} \approx 50 \left[\frac{\text{GV}}{\text{cm}}\right]$ 

• A factor of  $\approx 2500$  gain in sensitivity!

<sup>&</sup>lt;sup>7</sup>DLT: Dipole light trap; D. Weiss (Penn State), 2014: "Measuring the eEDM using laser-cooled Cs atoms in optical lattices"

S. Chu, J.E. Bjorkholm, A. Ashkin, A. Cable, Phys. Rev. Lett. 57 (1986) 314

C. Chin, V. Leiber, V. Vuletić, A.J. Kerman, S. Chu, Phys. Rev. A 63 (2001) 033401

### **Atomic Electric Dipole Moment**

• Definition:<sup>8</sup>

 $d_a = -\lim_{E_{\text{ext}} \to 0} \left[ \frac{\partial (\Delta \varepsilon_{\mathbb{F}T})}{\partial E_{\text{ext}}} \right]$ 

 $\Delta \varepsilon_{\mathbb{P}T}$  is some P, T-odd energy shift.

• Example: Lorentz covariant electron EDM interaction

$$\hat{H}_{\text{EDM}} = \imath \frac{d_e}{2} \gamma^0 \gamma^5 \frac{\imath}{2} \left( \gamma^\mu \gamma^\nu - \gamma^\nu \gamma^\mu \right) F_{\mu\nu}$$
$$\{F_{\mu\nu}\} = \{\partial_\mu A_\nu - \partial_\nu A_\mu\} = \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & -B_z & B_y \\ -E_y & B_z & 0 & -B_x \\ -E_z & -B_y & B_x & 0 \end{pmatrix}$$
$$\hat{H}_{\text{EDM}} = -d_e \gamma^0 \left[ \mathbf{\Sigma} \cdot \mathbf{E} + \imath \mathbf{\alpha} \cdot \mathbf{B} \right]$$

$$d_a = \lim_{E_{\text{ext}} \to 0} \frac{\partial}{\partial E_{\text{ext}}} d_e \left\langle \gamma^0 \left[ \mathbf{\Sigma} \cdot \mathbf{E} + \imath \boldsymbol{\alpha} \cdot \mathbf{B} \right] \right\rangle_{\psi(E_{\text{ext}})}$$

<sup>8</sup>E.D. Commins, Adv. Mol. Opt. Phys. **40** (1999) 1

## **Atomic Electric Dipole Moment**

• With the definitions

$$(E+B)_{\rm eff} = -\left\langle \gamma^0 \left[ \mathbf{\Sigma} \cdot \mathbf{E} + \imath \boldsymbol{\alpha} \cdot \mathbf{B} \right] \right\rangle_{\psi(E_{\rm ext})}$$

$$R := \frac{d_a}{d_e} \qquad \qquad R_{\text{lin}} := -\frac{\Delta(E+B)_{\text{eff}}}{\Delta E_{\text{ext}}} = -\frac{(E+B)_{\text{eff}}(2) - (E+B)_{\text{eff}}(1)}{E_{\text{ext}}(2) - E_{\text{ext}}(1)}$$

• the linear-regime enhancement is:

$$R \approx R_{\rm lin} = -\frac{(E+B)_{\rm eff}}{E_{\rm ext}}$$

•  $E_{\text{ext}} \in \{10^{-5}, \dots, 10^{-4}\}$  a.u.

Corresponding expressions for other P, T-odd effects (Ne-SPS, Ne-TPT, Schiff, etc.) Magnetic EDM term will be of importance for constraints<sup>9</sup> on bounds from Xe (near future)

<sup>&</sup>lt;sup>9</sup>T. Chupp, M. Ramsey-Musolf, *Phys. Rev. C* **91** (2015) *035502* 

W. Dekens, J. de Vries, M. Jung, K.K. Vos, J. High En. Phys. 1 (2019) 069

## Atomic and Molecular Correlated Wavefunctions Hamiltonians

• Dirac-Coulomb Hamiltonian + external electric field (atoms)

$$\begin{split} \hat{H}^{\mathsf{Dirac-Coulomb}} + \hat{H}^{\mathsf{Int-Dipole}} \\ &= \sum_{i}^{n} \left[ c \, \boldsymbol{\alpha}_{i} \cdot \mathbf{p}_{i} + \beta_{i} c^{2} - \frac{Z}{r_{i}} \mathbb{1}_{4} \right] + \sum_{i,j>j}^{n} \frac{1}{r_{ij}} \mathbb{1}_{4} + \sum_{i}^{n} \, \mathbf{r}_{i} \cdot \mathbf{E}_{\mathsf{ext}} \, \mathbb{1}_{4} \end{split}$$

• Dirac-Coulomb Hamiltonian operator (molecules)

$$\hat{H}^{DC} = \sum_{i}^{n} \left[ c \, \boldsymbol{\alpha}_{i} \cdot \mathbf{p}_{i} + \beta_{i} c^{2} - \sum_{A}^{N} \frac{Z}{r_{iA}} \mathbb{1}_{4} \right] + \sum_{i,j>i}^{n} \frac{1}{r_{ij}} \mathbb{1}_{4} + \sum_{A,B>A}^{N} V_{AB}$$

• Dirac-Coulomb-Gaunt Hamiltonian operator (molecules)

$$\hat{H}^{DCG} = \sum_{i}^{n} \left[ c \, \boldsymbol{\alpha}_{i} \cdot \mathbf{p}_{i} + \beta_{i} c^{2} - \sum_{A}^{N} \frac{Z}{r_{iA}} \mathbb{1}_{4} \right] + \sum_{i,j>i}^{n} \left( \frac{1}{r_{ij}} \mathbb{1}_{4} - \frac{1}{2} \frac{\vec{\alpha}_{i} \vec{\alpha}_{j}}{r_{ij}} \right) + \sum_{A,B>A}^{N} V_{AB}$$

## **Atomic and Molecular Correlated Wavefunctions**

• All-electron Dirac-Coulomb Hartree-Fock (DC(G)HF) calculation set of time-reversal paired 4-spinors  $\hat{K}\varphi_i = \varphi_{\bar{i}}$  and  $\hat{K}\varphi_{\bar{i}} = -\varphi_i$ 

$$\hat{K}(n) := e^{-\frac{i}{2}\pi \left(\sum_{j=1}^{n} \boldsymbol{\sigma} \otimes \mathbb{1}_{2}(j)\right) \cdot \vec{e}_{y}} \prod_{j=1}^{n} \hat{K}_{0}(j)$$

• Expansion and variation<sup>10</sup> in *n*-electron sector of Fock space  $\begin{aligned} &|\psi_k\rangle = \sum_{I=1}^{\dim \mathcal{F}^t(\mathrm{M},\mathrm{n})} c_{kI} \left(\mathcal{S}\overline{\mathcal{T}}\right)_I | \rangle & \text{unbarred (Kramers up) string } \mathcal{S} = a_i^{\dagger} a_j^{\dagger} a_k^{\dagger} \dots \\ &\text{barred (Kramers down) string } \overline{\mathcal{S}} = a_i^{\dagger} a_m^{\dagger} a_n^{\dagger} \dots \end{aligned}$ 

#### Linear expansion: Configuration Interaction

Exponential expansion: Coupled Cluster

<sup>&</sup>lt;sup>10</sup>S. Knecht, H.J.Aa. Jensen, T.F., *J Chem Phys* **132** (2010) *014108* 

## $\mathcal{P}$ , $\mathcal{T}$ -odd Property Calculations

using correlated wavefunctions

Expectation values over relativistic Configuration Interaction wavefunctions<sup>11</sup>  $\left\langle \hat{O} \right\rangle_{\psi_{i}^{(0)}} = \sum_{I=1}^{\dim \mathcal{F}^{t}(M,n)} c_{kI}^{*} c_{kJ} \left\langle \left| \left( \mathcal{S}\overline{\mathcal{T}} \right)_{I}^{\dagger} \right| \hat{O} \right| \left( \mathcal{S}\overline{\mathcal{T}} \right)_{J} \right| \right\rangle$ 

Property operator  $\hat{O}$  in basis of Kramers-paired molecular spinors  $\hat{O} = \sum_{m,n=1}^{P_u} o_{mn} a_m^{\dagger} a_n + \sum_{m=1}^{P_u} \sum_{n=P_u+1}^{P} o_{m\overline{n}} a_m^{\dagger} a_{\overline{n}} + \sum_{m=P_u+1}^{P} \sum_{n=1}^{P_u} o_{\overline{m}n} a_{\overline{m}}^{\dagger} a_n + \sum_{m,n=P_u+1}^{P} o_{\overline{mn}} a_{\overline{m}}^{\dagger} a_{\overline{n}}$ 

First-term contribution to expectation value

$$W'(\Psi_k)_1 = \sum_{I,J=1}^{\dim \mathcal{F}^{t}(\mathbf{P},\mathbf{N})} c_{kI}^* c_{kJ} \sum_{m,n=1}^{P_u} o_{mn}^M$$
$$\begin{cases} N_p \in \mathcal{S}_I \ N_p \in \mathcal{S}_I + N_{\overline{p}} \in \overline{\mathcal{T}}_I \\ \langle \mid \prod_{p=1}^{N_p \in \mathcal{S}_I} \prod_{\overline{p}=N_p+1}^{N_p \in \overline{\mathcal{T}}_I} a_{\overline{p}} a_p \ a_m^{\dagger} a_n \prod_{q=1}^{N_p \in \mathcal{S}_J} \prod_{\overline{q}=N_p+1}^{N_p \in \overline{\mathcal{T}}_J} a_q^{\dagger} a_{\overline{q}}^{\dagger} \mid \rangle \end{cases}$$

<sup>11</sup> S. Knecht, Dissertation, HHU Düsseldorf 2009

### $\mathcal{P}$ , $\mathcal{T}$ -odd Properties as Expectation Values

Interaction constants / enhancement factors for n-electron system

• Electron eEDM interaction constant  $^{12}$  / enhancement  $^{13}$ 

$$\begin{split} W_d &:= \frac{1}{\Omega} \left\langle \sum_{j=1}^n \gamma_j^0 \, \mathbf{\Sigma}_j \cdot \mathbf{E}_j \right\rangle_{\psi^{(0)}} \approx -\frac{2ic}{\Omega \, e\hbar} \left\langle \sum_{j=1}^n \gamma_j^0 \gamma_j^5 \, \vec{p}_j^{-2} \right\rangle_{\psi_k^{(0)}} \\ E_{\text{eff}} &= -\Omega \, W_d \qquad \qquad R \approx R_{\text{lin}} = -\frac{E_{\text{eff}}}{E_{\text{ext}}} \end{split}$$

• S-PS nucleon-electron interaction constant  $^{14}$  / ratio  $^{15}$ 

$$W_{\mathcal{S}} := \frac{\imath}{\Omega} \frac{G_F}{\sqrt{2}} A \left\langle \sum_{j=1}^n \gamma_j^0 \gamma_j^5 \rho_N(\vec{r}_j) \right\rangle_{\psi_k^{(0)}} \qquad S = -\frac{\left\langle \imath \sum_j \gamma_j^0 \gamma_j^5 \rho_N(\mathbf{r}_j) \right\rangle_{\Psi(E_{\text{ext}})}}{E_{\text{ext}}}$$

- <sup>12</sup>E. Lindroth, E. Lynn, P.G.H. Sandars, J. Phys. B: At. Mol. Opt. Phys. 22 (1989) 559, stratagem II
- TF, M.K. Nayak, Phys. Rev. A 88 (2013) 032514
- <sup>13</sup>TF, L.V. Skripnikov, *arXiv:1910.11596* (2019)
- <sup>14</sup>M. Denis *et al.*, New J. Phys. **7** (2015) 043005
- <sup>15</sup>TF, M. Jung, J. High Energy Phys. (JHEP) **07** (2018) 012

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## **Towards Ultracold DLT EDM Measurement**

#### **Picking the cherry**

#### In the casting:

Alkali(-like) atoms: Li, Na, K, Rb, Cs; Ag, Au Earth-alkaline atoms: Sr, Ba, Ra; Yb

**Jury spreadsheet** for X partner of Ra and some contenders:

X	EA(X) [eV]	$E_{ m effmax}\left[rac{ m GV}{ m cm} ight]$	$B_v = \left\langle v   \frac{1}{\mu R^2}   v \right\rangle [\mathrm{cm}^{-1}]$	D [D]	$E_{\mathrm{pol}} = \frac{B_v}{D} \left[ \frac{\mathrm{kV}}{\mathrm{cm}} \right]$
Li	0.62	61	—	$\approx 1.5$	
Na	0.55	58	—	$\approx 1$	
K	0.50	50	—	$\approx 1$	
Rb	0.49	48	+	$\approx 1$	
Cs	0.47	44	+	$\approx 1$	
Ag	1.30	66	0.021	5.4	0.264
Au	2.31	60	+	$\approx 6$	
AgBa	1.30	6	+	$\approx 3$	
RbYb <sup>16</sup>		-0.7	0.001	0.21	5.5
$CsYb^{16}$		0.54	0.007	0.24	3.5

<sup>16</sup>E. R. Meyer, J. L. Bohn, *Phys. Rev. A* **80** (2009) 042508

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#### Au is forbidden fruit!

## $(\mathcal{P},\mathcal{T})\text{-}\text{odd}$ properties of AgRa

• Electron EDM effective electric field<sup>17</sup>

$$E_{\text{eff}} = \frac{2ic}{e\hbar} \left\langle \sum_{j=1}^{n} \gamma_j^0 \gamma_j^5 \vec{p}_j^2 \right\rangle_{\psi^{(0)}}$$

• S-PS nucleon-electron interaction constant<sup>18</sup>

$$W_{\mathcal{S}} := \frac{\imath}{\Omega} \frac{G_F}{\sqrt{2}} Z_{\text{heavy}} \left\langle \Psi_{\Omega} \right| \sum_{j=1}^n \gamma_j^0 \gamma_j^5 \rho_N(\vec{r}_j) \left| \Psi_{\Omega} \right\rangle$$

	$ $ $^{3}\Delta_{1}$			$^{2}\Sigma$		
	ThO	$HfF^+$	$ThF^+$	YbF	ÁgRa	
$ E_{\text{eff}} $	78	23	35	25	64	$\left[\frac{\text{GV}}{\text{cm}}\right]$
$ W_S $	106	20	51	40	175	[kHz]

- <sup>17</sup>E. Lindroth, E. Lynn, P.G.H. Sandars, *J. Phys. B: At. Mol. Opt. Phys.* **22** (1989) *559* T.F., M.K. Nayak, *Phys. Rev. A* **88** (2013) *032514*
- <sup>18</sup>V. G. Gorshkov, L. N. Labzovski, and A. N. Moskalev, Zh. Eksp. Teor. Fiz. 76 (1979) 414
  - M. Denis et al., New J. Phys. 7 (2015) 043005

# **Devising a AgRa DLT EDM Experiment**

• Photoassociating ultracold atoms into ultracold molecules<sup>19</sup>



- Does its electronic spectrum allow for efficient energy transfer (remove binding energy without heating) ?
- Which states are candidates for photoassociation ?

<sup>&</sup>lt;sup>19</sup>L. D. Carr, D. DeMille, R. V. Krems, J. Ye, New J. Phys. **11** (2009) 055049

## **AgRa - Electronic-structure model**

	# o	f Kramers pairs	accun # of el min.	nulated lectrons max.	
	(4 a.u.)				Determinant classes
		-1	01	- 1	$\mathrm{I}^{18}~\mathrm{II}^{3}~\mathrm{III}^{0}$ (Reference space)
III	Virtual Kramers pairs	71	21	21	$I^{18} II^2 III^1$ (Singles)
	Ag: 5p,6s				$\mathrm{I}^{18}~\mathrm{II}^{1}~\mathrm{III}^{2}$ (Valence correlating)
II	Ra: 7p,8p,6d	18	19	21	$I^{17} II^4 III^0$ (Singles)
	Ra: 7s σ				$I^{17} II^3 III^1$ (Singles)
Ι	Ra: 6s, 6p Ag: 4d	9	17	18	$\mathrm{I}^{17}~\mathrm{II}^2~\mathrm{III}^2$ (Core-val. correlating)
	Frozen core	(57)			$17.6 imes10^6$ expansion terms ( $\Omega=1/2$ )

cvTZ bases<sup>20</sup>

**KRCI** program<sup>21</sup>

<sup>20</sup>K.G. Dyall, *Theoret. Chim. Acta* **131** (2012) *1217* 

K.G. Dyall, A.S.P. Gomes, Theoret. Chim. Acta 125 (2010) 97

<sup>21</sup>S. Knecht, H.J.Aa. Jensen, T.F., *J. Chem. Phys.* **132** (2010) *014108* 

**DIRAC15** package (locally modified)

### AgRa - PECs



Frontiers in Quantum Matter Workshop: Electric Dipole Moments, Canberra, 25-27 November 2019

## **AgRa**

#### A Pathway To Assemble AgRa (X) from Trapped Ag-Ra Atom Pairs



Frontiers in Quantum Matter Workshop: Electric Dipole Moments, Canberra, 25-27 November 2019

## **Electronic Transition Dipole Moments :** $\Omega = 1/2$ states



Frontiers in Quantum Matter Workshop: Electric Dipole Moments, Canberra, 25-27 November 2019

## **Electronic Transition Dipole Moments :** $\Omega = 3/2$ states



# Long-Range Theory<sup>22</sup>

Van der Waals interaction potential for two neutral heteronuclear atoms:

$$V(R) = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} - \dots$$

Ground state:

$$C_6^{\Omega=1/2(1)} = \sum_{n_c(\ell_c=1), n_d(\ell_d=1)} \frac{3}{2} \frac{f_{ac}^{(1)} f_{bd}^{(1)}}{\Delta E_{ca} \Delta E_{db} \left(\Delta E_{ca} + \Delta E_{db}\right)}$$

 $a={}^2S_{1/2}(5s^1)$  for Ag and  $b={}^1S_0(7s^2)$  for Ra

Oscillator strengths:<sup>23</sup>

$$\begin{split} f_{IF}^{(1)} &= \frac{2}{3g_I} \left( E_F - E_I \right) \sum_{\substack{M_{LF}, M_{SF} \\ M_{LI}, M_{SI}}} \left| \left| \left\langle L_F, M_{LF}, S_F, M_{SF} \right| \sum_{k=1}^n \hat{\mathbf{r}}(k) \left| L_I, M_{LI}, S_I, M_{SI} \right\rangle \right| \right|^2 \\ g_I &= (2M_{LI} + 1)(2M_{SI} + 1) \\ \left| \psi_L \right\rangle &= \left| {}^2P \right\rangle = \left| 1, M_L; \frac{1}{2}, M_S \right\rangle \text{ are expanded as} \\ &= \left| 1, 0; \frac{1}{2}, \frac{1}{2} \right\rangle = \left\langle \frac{3}{2}, \frac{1}{2} \right| 1, 0; \frac{1}{2}, \frac{1}{2} \right\rangle + \left\langle \frac{1}{2}, \frac{1}{2} \right| 1, 0; \frac{1}{2}, \frac{1}{2} \right\rangle \\ \frac{22}{3}_{\text{T.N. Chang, Phys. Rev. A 36 (1987) 447} \end{split}$$

## **Atomic Transition Dipole Moments: Ag and Ra**<sup>24</sup>

Ag Transition	$D_{IF}^{rac{1}{2}-rac{1}{2}}$ [a.u.]	$D_{IF}^{rac{1}{2}-rac{3}{2}}$ [a.u.]	$D_{if}$ [a.u.]	$f_{if}$	$\Delta E \ [\mathrm{cm}^{-1}]$
${}^{2}S_{\frac{1}{2}}(5s) - {}^{2}P_{\frac{1}{2},\frac{3}{2}}(5p)$	-1.1007	1.5561	1.9061	0.9987	30165.796
${}^{2}S_{\frac{1}{2}}^{2}(5s) - {}^{2}P_{\frac{1}{2},\frac{3}{2}}^{2/2}(6p)$	-0.0515	0.1238	0.1308	0.0076	48433.009
${}^{2}S_{\frac{1}{2}}(5s) - {}^{2}P_{\frac{1}{2},\frac{3}{2}}(7p)$	-0.0820	0.0812	0.1142	0.0064	54094.418

Ra Transition	$D_{IF}^{0-1} \;$ [a.u.]	$f_{if}$	$f_{if}$ <sup>25</sup>	$\Delta \epsilon  [\mathrm{cm}^{-1}]$
$^{-1}S_0(7s^2) - {}^3P_1(7s7p)$	0.4995	0.0350		15391.
${}^{1}S_{0}(7s^{2}) - {}^{1}P_{1}(7s7p)$	3.3687	2.1422	1.91	20715.614
${}^{1}S_{0}(7s^{2}) - {}^{3}P_{1}(7s8p)$	0.3836	0.0402		30000.
${}^{1}S_{0}(7s^{2}) - {}^{1}P_{1}(7s8p)$	0.8252	0.2039		32857.537

Ra Transition	$f_{if}$	$\Delta E  [\mathrm{cm}^{-1}]$
${}^{1}P_{1}(7s7p) - {}^{3}S_{1}(7s8s)$	0.0053	3899.32
${}^{1}P_{1}(7s7p) - {}^{1}S_{0}(7s8s)$	0.2396	6414.14
${}^{1}P_{1}(7s7p) - {}^{1}S_{0}(7s9s)$	0.0046	23516.95
${}^{1}P_{1}(7s7p) - {}^{1}S_{0}(7s10s)$	0.0167	38210.06
${}^{1}P_{1}(7s7p) - {}^{3}D_{1}(7s7d)$	0.0258	23264.76
${}^{1}P_{1}(7s7p) - {}^{3}D_{2}(7s7d)$	0.2405	23405.31
${}^{1}P_{1}(7s7p) - {}^{1}D_{2}(7s7d)$	0.1968	24495.86

<sup>24</sup>TF, D. DeMille, "Using Ultracold Assembled AgRa Molecules to Search for Time-Reversal Violation", to be submitted.
 <sup>25</sup>V.A. Dzuba and V.V. Flambaum, J. Phys. B 40 (2007) 227

### Testing the approach: LiBe and RbSr

LiBe 
$$(^{2}\Sigma_{1/2})$$
 lin. CCSD<sup>26</sup>
 KRCI(FCI)

  $C_{6}$ [a.u.]
 478(3)
 462

5% residual deviation!

AgRa (
$$\Omega = 1/2(1)$$
)
 KRCI(MR-SD)

  $C_6$ [a.u.]
 1163

<sup>&</sup>lt;sup>26</sup>A. Derevianko, S.G. Porsev, J.F. Babb, At. Data Nucl. Data Tables **96** (2010) 323

M.S. Safronova, W.R. Johnson, A. Derevianko, Phys. Rev. A 60 (1999) 4476

### **Connecting LR- and SR-Potentials**

Ground potential  $\Omega = 1/2(1)$ 



20

R [AA]

25

30

15

-200890

10

- Pure short-range potentials produce artefacts! |
- $V(R) \approx -\frac{C_6}{R^6}$  and fit long-range to short-range curves
- Correct physics from careful fitting

<sup>&</sup>lt;sup>27</sup>R.J. LeRoy, Can. J. Phys. 52 (1974) 246
R.J. LeRoy, R. B. Bernstein, J. Chem. Phys. 52 (1970) 3869

## **Dispersion coefficients from oscillator strengths**

$$\begin{split} C_{6}^{\Omega=1/2(16)} &= C_{6}^{\Omega=3/2(11)} &= \sum_{nc(\ell_{c}=1),n_{d}(\ell_{d}=0)} \frac{3}{4} \frac{f_{ac}^{(1)} f_{bd}^{(1)}}{\Delta E_{ca} \Delta E_{db} (\Delta E_{ca} + \Delta E_{db})} \\ &+ \sum_{nc(\ell_{c}=1),n_{d}(\ell_{d}=1)} \frac{15}{8} \frac{f_{ac}^{(1)} f_{bd}^{(1)}}{\Delta E_{ca} \Delta E_{db} (\Delta E_{ca} + \Delta E_{db})} \\ &+ \sum_{nc(\ell_{c}=1),n_{d}(\ell_{d}=2)} \frac{57}{40} \frac{f_{ac}^{(1)} f_{bd}^{(1)}}{\Delta E_{ca} \Delta E_{db} (\Delta E_{ca} + \Delta E_{db})} \\ &\text{A test on LiBe:} \frac{2\Pi \ ^{1}P(\text{Be}\ 2s^{1}2p^{1})}{2\Sigma \ ^{1}P(\text{Be}\ 2s^{1}2p^{1})} \ 951.6 \ 714.0 \\ 1228 \ 1402 \end{split}$$

#### Ra(7p) excited states:

$\Omega = 1/2(m)$	$^M\Lambda_\Omega$ term	C <sub>6</sub> [a.u.]	$\Omega = 3/2(k)$	$^M\Lambda_\Omega$ term	C <sub>6</sub> [a.u.]
m = 1	$^{2}\Sigma_{1/2}$	1163	k = 1	$^{4}\Sigma_{3/2}$	1380
m = 4	${}^{4}\Pi_{1/2}$	478	k = 11	$^{2}\Pi_{3/2}$	478
m = 15	$^{2}\Sigma_{1/2}$	1380		,	
m = 16	$^{2}\Pi_{1/2}$	478			

<sup>28</sup>J.-Y. Zhang, Y. Cheng, J. Mitroy, J. Phys. B: At. Mol. Opt. Phys. 46 (2013) 125004

#### **Connecting LR- and SR-Potentials**

Excited potentials  $\Omega = 1/2(16), \Omega = 3/2(11)$ 

LeRoy radius:

$$R_{\rm LR} = 2 \left( \left\langle \hat{r}^2 \right\rangle_A^{1/2} + \left\langle \hat{r}^2 \right\rangle_B^{1/2} \right)$$

$$ig\langle \hat{r}^2 ig
angle_{\mathrm{Ag}_{5s}} = 13.90 \text{ a.u.} \qquad ig\langle \hat{r}^2 ig
angle_{\mathrm{Ra}_{7p_{3/2}}^+} = 60.63 \text{ a.u.}$$
$$\Rightarrow R_{\mathrm{LR}}^{\Omega = 1/2(1)} = 23.0 \text{ a.u.}$$



•  $V(R) \approx -\frac{C_6}{R^6}$  and fit long-range to short-range curves

## AgRa FCF for Proposed PA

FC overlap of  $\Omega = 1/2(1)$  and  $\Omega = 1/2(16)$  including trap potential  $\int \psi'_v \psi_v d\tau_v > 0.003$  for pair-bound state always exists.

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FCFs_XSHO_DEtimes0.99_OneHalf_16_10/Ag.d       -       -       ×         File       Edit       Format       View       Help       *         v_X\v_ex       104       105       106       107       108       *         127       0.28410       0.02376       0.01092       0.00432       0.00091       127         128       0.43894       0.44306       0.00016       0.00488       0.00091       127         128       0.43894       0.44306       0.00016       0.00432       0.00091       128         129       0.06740       0.08971       0.62117       0.17570       0.00592       130         131       0.00055       0.01362       0.01996       0.09643       0.74363       131         3131       0.00020       0.00042       0.00056       0.00296       0.00586       313         Image: Comparison of the state of the st	DissEng       -       ×         le       Edit       Format       View         27, -0.239036932508174       ^         28, -0.088042501821406       127       0.000         29, -0.0197678370221207       129       0.000         30, -0.000801889412685098       130       0.002         31, 0.000192059988259233       ×          DissEng       -       ×         Edit       Format       View       Help         V.2.V_ex       130       0.002         131       0.004       131       0.004         SissEng       -       ×       File       Edit       Format       View         0, -0.232844966667555       ^       -       128       0.138       129       0.580         0, -0.0855122982532279       -       -       128       0.138       129       0.580         0, -0.0855122982532279       -       -       129       0.580       129       0.580	0.99_OneHalf_16_107Ag.dat □ × w Help 104 105 106 107 108 053 0.00000 0.00011 0.00011 0.00003 262 0.00352 0.00156 0.00019 0.00002 016 0.77771 0.15456 0.01661 0.00038 131 0.06071 0.17071 0.51624 0.21875 003 0.00084 0.00303 0.00278 0.06738 ×  99_OneHalf_16_109Ag.dat - N □ × v Help 05 106 107 108 109 168 0.01045 0.00620 0.00246 0.00022 118 0.32866 0.00378 0.0015 0.00015	DissEng × File Edit Format View Help 127, -0.359021664074495 128, -0.151544304619359 129, -0.0458686700936669 130, -0.00609124005113412 131, 0.000110268275565008 × C DissEn × File Edit Format View Help 128, -0.201460899388427 ^ 129, -0.0699349748339458 120, 0.04136724019226620
FCFs_XSHO_DEtimes0.99_OneHalf_16_10/Ag.d       -       -       ×         File       Edit       Format       View       Help         v_X\v_ex       104       105       106       107       108         127       0.28410       0.02376       0.01092       0.00432       0.00091         128       0.43894       0.44306       0.00016       0.00488       0.00091         128       0.43894       0.44306       0.00016       0.00488       0.00091         129       0.06740       0.08971       0.62117       0.17570       0.00592         130       0.00655       0.01362       0.01996       0.09643       0.74363         131       0.00020       0.00042       0.00056       0.00296       0.00586       131         Statistic       Statistic       Statistic       Statistic       Statistic       131         131       0.00020       0.00042       0.00056       0.00296       0.00586       131         Statistic       Statistic       Statistic       Statistic       Statistic       Statistic         Statistic       Statistic       Statistic       Statistic       Statistic       Statist         Statistic	DissEng       —       ×         le       Edit       Format       View         PCFs_XSHO_C6times0       File       Edit       Format         PCFs_VSHO_C6times0       File       Edit       Format       View         PCFs_VSHO_C6times0       File       Edit       Format       View         PCFs_VSHO_C6times0       127       0.000       128       0.877         PCFs_VSHO_C6times0       128       0.877       129       0.000         PCFs_VSHO_00801889412685098       130       0.000       131       0.000         PCFs_VSHO_00192059988259233       ×         FCFs_VSHO_DEtimes0         PissEng       —       —       ×       File       Edit       Format       View         P, -0.232844966667555       ^        128       0.138       129       0.580         J, -0.040743368499376608       130       0.078       129       0.580       130       0.078	0.99_OneHalf_16_107Ag.dat	DissEng X File Edit Format View Help 127, -0.359021664074495 128, -0.151544304619359 129, -0.0458686700936669 130, -0.00609124005113412 131, 0.000110268275565008 C DissEn X File Edit Format View Help 128, -0.201460899388427 129, -0.0699349748339458 130, -0.0135749198226939 131, 0.00202727100606°22
FCFs_XSHO_DEtimes0.99_OneHalf_16_10/Ag.d       -       -       ×         File       Edit       Format       View       Help         v_X\v_ex       104       105       106       107       108         127       0.28410       0.02376       0.01092       0.00432       0.00091         128       0.43894       0.44306       0.00016       0.00488       0.00092         129       0.06740       0.08971       0.62117       0.17570       0.00592         130       0.00655       0.01362       0.01996       0.09643       0.74363         131       0.00020       0.00042       0.00056       0.00296       0.00586       131         .       I31       0.00020       0.00042       0.00056       0.00296       0.00586       131         .       I31       0.00020       0.00042       0.00056       0.00296       0.00586       131         .       I31       0.00020       0.00042       0.00026       0.00296       0.00188       0.00196         .       I329       0.03193       0.00344       0.00240       0.00108       0.0019       130         .       I29       0.03193       0.00344       0	DissEng       -       ×         le       Edit       Format       View         27, -0.239036932508174       ^         28, -0.088042501821406       127       0.000         29, -0.0197678370221207       129       0.000         30, -0.000801889412685098       130       0.000         31, 0.000192059988259233       ×          DissEng       -       ×         Edit       Format       View       Help         >, -0.080801889412685098            DissEng       -       ×           Q0.00192059982532279             Q0.00743368499376608       130       0.0078           131       0.004	0.99_OneHalf_16_107Ag.dat       →         w Help       104       105       106       107       108         104       105       106       107       108       ▲         053       0.00000       0.00011       0.00001       0.00003         262       0.00352       0.00156       0.00019       0.00002         016       0.77771       0.15456       0.01661       0.00038         131       0.06071       0.17071       0.51624       0.21875         003       0.00084       0.00303       0.00278       0.06738         99_OneHalf_16_109Ag.dat - N       →       →       →         99_OneHalf_36       107       108       109       ▲         168       0.01045       0.00620       0.00246       0.00022         118       0.32866       0.00378       0.00167       0.00015         102       0.11302       0.56068       0.22130       0.00102         154       0.00967       0.01236       0.05989       0.90117	DissEng × File Edit Format View Help 127, -0.359021664074495 128, -0.151544304619359 129, -0.0458686700936669 130, -0.00609124005113412 131, 0.000110268275565008 × DissEn × File Edit Format View Help 128, -0.201460899388427 129, -0.0699349748339458 130, -0.0135749198226939 131, -0.00020277109698680
File       Edit       Format       View       Help         v_X\v_ex       104       105       106       107       108         127       0.28410       0.02376       0.01092       0.00432       0.00091         128       0.43894       0.44306       0.00016       0.00488       0.00091         128       0.43894       0.44306       0.00016       0.00488       0.00091         129       0.06740       0.08971       0.62117       0.17570       0.00059         130       0.00655       0.01362       0.01996       0.09643       0.74363         131       0.00020       0.00042       0.00056       0.00296       0.00586       v         I31       0.00020       0.00042       0.00056       0.00296       0.00586       v         I31       0.00020       0.00042       0.00056       0.00296       0.00586       v         I32       0.03193       0.0344       0.00240       0.00108       0.00106         I32       0.03193       0.03244       0.00277       0.00001         I32       0.00434       0.03519       0.00105       0.21734       0.70015         I33       0.00014       0.00	DissEng       —       →         Image: PCFs_XSHO_C6times0         FCFs_XSHO_C6times0         File       Edit       Format       View         P29, -0.0197678370221207       0.000       127       0.000         S0, -0.000801889412685098       129       0.000         S1, 0.000192059988259233       →          DissEng       —       →         DissEng       —       —         Left       Format       View       Help         V0.000192059988259233       →           DissEng       —       —           —       —           DissEng       —       —           —       —            —       —            —       —           <	0.99_OneHalf_16_107Ag.dat — □ × w Help 104 105 106 107 108 053 0.00000 0.00011 0.00011 0.00003 262 0.00352 0.00156 0.00019 0.00002 016 0.77771 0.15456 0.01661 0.00038 131 0.06071 0.17071 0.51624 0.21875 003 0.00084 0.00303 0.00278 0.06738 × 99_OneHalf_16_109Ag.dat - N — □ × w Help 05 106 107 108 109 168 0.01045 0.00620 0.00246 0.00022 118 0.32866 0.00378 0.00167 0.00015 102 0.11302 0.56068 0.22130 0.00102 154 0.00967 0.01236 0.65989 0.90117 146 0.00098 0.00120 0.00601 0.00078 ↓	DissEng × File Edit Format View Help 127, -0.359021664074495 128, -0.151544304619359 129, -0.0458686700936669 130, -0.00609124005113412 131, 0.000110268275565008 × File Edit Format View Help 128, -0.201460899388427 ^ 129, -0.0699349748339458 130, -0.0135749198226939 131, -0.00020277109698680 132, 0.000224064799013136 ×

# eEDM Constraint on Beyond-Standard-Model Theories Single-source interpretation (20??)<sup>29</sup>



<sup>29</sup>TF, D. DeMille, "Using Ultracold Assembled AgRa Molecules to Search for Time-Reversal Violation", to be submitted.

## Outline

### • Atomic EDMs : $^{129}$ Xe

 $|d_{Xe}| < 1.5 \times 10^{-27} e$  cm. Allmendinger *et. al.* (Mainz, Heidelberg), *Phys. Rev. A* **100** (2019) *022505*  $|d_{Xe}| < 4.81 \times 10^{-27} e$  cm. Sachdeva *et. al.* (Ann Arbor *et. al.*), arXiv:1902.02864 [physics.atom-ph] (2019) Sato *et. al.* (Tokyo *et. al.*), *Hyperfine Interact.* **230** (2015) *147* 

### **Tensor-Pseudotensor** $\mathcal{P}$ , $\mathcal{T}$ -odd Nucleon-Electron Interaction

Lagrangian density<sup>5</sup> for Ne neutral weak current  $(\sigma_{\rho\sigma} = \frac{i}{2} (\gamma^{\rho} \gamma^{\sigma} - \gamma^{\sigma} \gamma^{\rho}))$ :  $\mathcal{L}_{\text{Ne-TPT}} = \frac{1}{2} \frac{G_F}{\sqrt{2}} C_T \sum_N \varepsilon^{\mu\nu\rho\sigma} \overline{\psi}_N \Sigma_{N\mu\nu} \psi_N \ \overline{\psi} \sigma_{\rho\sigma} \psi$ 

Corresponding effective first-quantized Hamiltonian:

$$\hat{H}_{\text{Ne-TPT}}^{\text{eff}} = -\frac{1}{2} \frac{G_F}{\sqrt{2}} C_T \rho_N(\mathbf{r}) \gamma^0 \varepsilon^{\mu\nu\rho\sigma} \Sigma_{N\mu\nu} \sigma_{\rho\sigma}$$

Using 
$$\frac{1}{2} \varepsilon^{\mu\nu\kappa\lambda} \sigma_{\kappa\lambda} = -i\gamma^5 \sigma^{\mu\nu}$$
 we get:  
 $\hat{H}_{\text{Ne-TPT}}^{\text{eff}} = \frac{iG_F}{\sqrt{2}} C_T \rho(\mathbf{r}) \gamma^0 \Sigma_{N\mu\nu} \gamma^5 \sigma^{\mu\nu}$ 

Since 
$$\Sigma_{N\mu\nu}\gamma^5\sigma^{\mu\nu} = 2\gamma^0 \Sigma_N \cdot \gamma$$
 it follows that  
 $\hat{H}_{\text{Ne-TPT}}^{\text{eff}} = \imath G_F \sqrt{2} C_T \Sigma_N \cdot \gamma \rho(\mathbf{r})$ 

Nuclear state chosen as  $|I, M_I = I\rangle$  gives many-electron Hamiltonian:  $\hat{H}_{\text{Ne-TPT}}^{\text{eff}} = \imath G_F \sqrt{2} C_T \langle \Sigma_N \rangle_{\Psi_N} \sum_{j=1}^n (\gamma_j)^3 \rho_N(\mathbf{r}_j)$ 

<sup>&</sup>lt;sup>5</sup>K. Yanase, N. Yoshinaga, K. Higashiyama, N. Yamanaka *Phys. Rev. D* **99** (2019) 075021

### Scalar-Pseudoscalar $\mathcal{P}$ , $\mathcal{T}$ -odd Nucleon-Electron Interaction

via magnetic hyperfine interaction

Solve for  $K \in \mathbb{CI}$  STATES  $\left[\sum_{j}^{N} \left[c \, \boldsymbol{\alpha}_{j} \cdot \mathbf{p}_{j} + \beta_{j} c^{2} + \frac{Z}{r_{j}} \mathbb{1}_{4}\right] + \sum_{j,k>j}^{N} \frac{1}{r_{jk}} \mathbb{1}_{4} + \sum_{j} \mathbf{r}_{j} \cdot \mathbf{E}_{\text{ext}} \mathbb{1}_{4}\right] \left|\psi_{K}^{(0)}\right\rangle = \varepsilon_{K}^{(0)} \left|\psi_{K}^{(0)}\right\rangle$ 

First-order hyperfine-perturbed CI wavefunctions:

$$\left|\psi_{J}^{(1)}\right\rangle = \left|\psi_{J}^{(0)}\right\rangle + \sum_{K \neq J} \frac{\left\langle\psi_{K}^{(0)}\right| - \frac{1}{2c m_{p}} \frac{\mu \mathbf{I}}{I} \cdot \sum_{i=1}^{n} \frac{\boldsymbol{\alpha}_{i} \times \mathbf{r}_{i}}{r_{i}^{3}} \left|\psi_{J}^{(0)}\right\rangle}{\varepsilon_{J}^{(0)} - \varepsilon_{K}^{(0)}} \left|\psi_{K}^{(0)}\right\rangle$$

To leading order the SPS-ne energy shift is

$$\left(\Delta\varepsilon\right)_{J} = \frac{1}{\langle\psi_{J}^{(1)}|\psi_{J}^{(1)}\rangle} \left\langle\hat{H}_{\text{S-PS-ne}}\right\rangle_{\psi_{J}^{(1)}}$$

Atomic EDM due to Ne-SPS interaction  $d_a = \alpha_{C_S} C_S$  and so

$$\alpha_{C_{S}}(\psi_{J}) = \frac{-A\frac{G_{F}}{\sqrt{2}}}{E_{\text{ext}}\left\langle\psi_{J}^{(1)}\middle|\psi_{J}^{(1)}\right\rangle} \left[\sum_{K \neq J} \frac{\left\langle\psi_{K}^{(0)}\middle|\hat{H}_{\text{HF}}\middle|\psi_{J}^{(0)}\right\rangle\left\langle\psi_{J}^{(0)}\middle|i\sum_{e}\gamma_{e}^{0}\gamma_{e}^{5}\rho(\mathbf{r}_{e})\middle|\psi_{K}^{(0)}\right\rangle}{\varepsilon_{J}^{(0)} - \varepsilon_{K}^{(0)}} + h.c.\right]$$

## **Generalized Active Spaces**

#### Parameterization of the correlated wavefunction



Frontiers in Quantum Matter Workshop: Electric Dipole Moments, Canberra, 25-27 November 2019

# <sup>129</sup>Xe EDM

Leading<sup>31</sup> (and Subleading) Contributions

 $d_{\mathsf{Xe}} = \rho_Z^N d_N + \alpha_S S - \alpha_{C_T} C_T (+ \alpha_{C_S} C_S + \alpha_{d_e} d_e)$ 

- Atomic coefficients for leading contributions available  $(\alpha_{C_T})$  and in progress  $(\alpha_S)$
- Subleading contributions affect constraints obtained from global fits<sup>32</sup>



Example: Electron EDM and SPS-Ne coupling

- Measurements and calculations on systems with different ratios of atomic/molecular coefficients
- Global fit<sup>9</sup> constrains multiple possible EDM sources

<sup>31</sup>T. Chupp, M. Ramsey-Musolf, *Phys. Rev. C* **91** (2015) *035502*<sup>32</sup>W. Dekens, J. de Vries, M. Jung, K.K. Vos, *J. High En. Phys.* **1** (2019) *069*<sup>9</sup>T. F., M. Jung, *J. High En. Phys.* **7** (2018) *012*

## A digression on the TI EDM

Leading contributions to EDM of a paramagnetic atom

 $d_a = R \, d_e + \alpha_{C_S} \, C_S \qquad \qquad \alpha_{C_S} = S \, A \, \frac{G_F}{\sqrt{2}}$ 

Enhancement factor and  $\boldsymbol{S}$  ratio:

$$R := \frac{\left\langle \sum_{j} \gamma_{j}^{0} \boldsymbol{\Sigma}_{j} \cdot \mathbf{E}_{j} \right\rangle_{\Psi}}{E_{\text{ext}}} \qquad \qquad S := -\frac{\left\langle i \sum_{j} \gamma_{j}^{0} \gamma_{j}^{5} \rho_{N}(\mathbf{r}_{j}) \right\rangle_{\Psi}}{E_{\text{ext}}}$$

Model for <b>TI atom</b>	R	S [a.u.]
vDZ/SD18_CAS_3in3_SDT21/10au	-473	-331
vDZ/SD18_CAS_3in3_SDT21/20au	-479	-335
vDZ/SD8_SDT10_CAS_3in3_SDT21/10au	-471	-331
vDZ/SD18_CAS_3in3_SDTQ21/10au	-469	-329
vTZ/SD18_CAS_3in3_SDT21/20au	-541	-383
vQZ/SD18_CAS_3in3_SDT21/35au <sup>10</sup>	-562	-398
$CCSD(T) 53 + core corr. (Skripnikov)^{10}$	-557	
Literature values		
Porsev et al., Phys. Rev. Lett. 108 (2012) 173001	-573	-411
Nataraj et al., Phys. Rev. Lett. 106 (2011) 200403	-470	
Dzuba et al., Phys. Rev. A 80 (2009) 062509	-582	
Liu et al., Phys. Rev. A 45 (1992) R4210	-585	

<sup>10</sup>T. F., L.V. Skripnikov, (2019) in preparation.

## **Tensor-Pseudotensor** $\mathcal{P}$ , $\mathcal{T}$ -odd Nucleon-Electron Interaction

Results for  $^{129}$ Xe

Model/virtual cutoff (vDZ,vTZ,vQZ) [a.u.]	$R_T$ [10	$)^{-20} \langle \sigma_N \rangle$	$ angle \ e \ cm]$
		Basis set	
	vDZ	vTZ	vQZ
RPA/-	0.382	0.473	0.485
SD8/80,100,60	0.360	0.438	0.453
SDT8/80,100,60	0.360	0.435	0.450
SDTQ8/80,12,60	0.357	0.431	
SD16/80,100,60	0.406	0.481	0.496
SD8_SDT16/80,100,60	0.405	0.477	
SD18/80,100,60		0.453	
SD24/80,100,60	0.421	0.497	0.514
SD26/80,100,60		0.493	
S16_SD32/80,100,60		0.507	
SD32/80,100,60	0.431	0.508	0.525
SD36/80,100,60	0.417	0.499	
vQZ/SD32/60 $+\Delta$		0.536	
Mårtensson-Pendrill <sup>11</sup> RPA		0.52	
Dzuba $et \ al.^{12}$ RPA		0.57	
Singh $et \ al.^{13} \ CCSD_pT$		0.501	

<sup>11</sup>A.M. Mårtensson-Pendrill, *Phys. Rev. Lett.* **54** (1985) *1153* 

<sup>13</sup>Y. Singh, B.K. Sahoo, B.P. Das, *Phys. Rev. A* **89** (2014) 030502(*R*)

<sup>&</sup>lt;sup>12</sup>V.A. Dzuba, V.V. Flambaum, S.G. Porsev, *Phys. Rev. A* **80** (2009) *032120* 

## Scalar-Pseudoscalar $\mathcal{P}$ , $\mathcal{T}$ -odd Nucleon-Electron Interaction

Results for  $^{129}$ Xe

$\alpha_{C_S}(\psi_J) = \frac{-A \frac{G_F}{\sqrt{2}}}{E_{\text{ext}} \left\langle \psi_J^{(1)} \middle  \psi_J^{(1)} \right\rangle} \left[$	$\left[\sum_{K \neq J} - \right]$	$\left\langle \psi_{K}^{(0)} \Big  \hat{H}_{HF} \Big  \psi_{J}^{(0)} \right\rangle \left\langle \psi_{J}^{(0)} \Big  \imath \sum_{e} \gamma_{e}^{0} \gamma_{e}^{5} \rho(\mathbf{r}_{e}) \Big  \psi_{K}^{(0)} \right\rangle$	+ h.c.
		$arepsilon_J^{(0)} - arepsilon_K^{(0)}$	

Basis	# of CI states/X	$S \ [10^{-2} \ a.u.]$	$\alpha_{C_S} \ [10^{-22}  e \; \mathrm{cm}]$
cvTZ/40 a.u.	8/S8	0.059	0.063
cvTZ/7 a.u.	8/6s6p	0.055	0.059
cvTZ/14 a.u.	8/6s6p	0.055	0.059
cvTZ/7 a.u.	8/6s6p5d	0.060	0.065
cvTZ/7 a.u.	8/6s6p5d7p	0.067	0.072
cvTZ/7 a.u.	8/6s6p5d7p7s	0.069	0.074
cvTZ/7 a.u.	8/6s6p5d7p7s6d	0.070	0.075
cvTZ/7 a.u.	8/6s6p5d7p7s6d4f	0.070	0.075
cvTZ/7 a.u.	8/6s6p5d7p7s6d4f7d5f8p8s	0.067	0.072
cvTZ/7 a.u.	20/6s6p5d7p7s	0.055	0.059
cvTZ/S10-SDT8-SD18/7au	20/6s6p5d7p	0.05	0.05
cvQZ/100 a.u.	8/S8	0.059	0.064
cvQZ/50 a.u.	1000/S8	0.050	0.053
cvQZ/50 a.u.	8/6s6p	0.048	0.052
cvQZ/50 a.u.	8/6s6p5d7p7s	0.071	0.076
$\textbf{vQZ/1281/S8/100} + \Delta S_{corr}$		0.073	0.078

## Scalar-Pseudoscalar $\mathcal{P}, \mathcal{T}$ -odd Nucleon-Electron Interaction Results for <sup>129</sup>Xe

• Two major contributions in the sum over states:

$$\begin{split} C_{1} &= \frac{\langle 5p \rightarrow 6s \ 0, 0 | \hat{H}_{\mathsf{HF}} | 0, 0 \rangle \langle 0, 0 | \imath \sum_{e} \gamma_{e}^{0} \gamma_{e}^{5} \rho(\mathbf{r}_{e}) | 5p \rightarrow 6s \ 0, 0 \rangle}{\varepsilon_{0,0}^{(0)} - \varepsilon_{5p \rightarrow 6s \ 0, 0}^{(0)}} \\ C_{2} &= \frac{\langle 5p \rightarrow 6p \ 1, 0 | \hat{H}_{\mathsf{HF}} | 0, 0 \rangle \langle 0, 0 | \imath \sum_{e} \gamma_{e}^{0} \gamma_{e}^{5} \rho(\mathbf{r}_{e}) | 5p \rightarrow 6p \ 1, 0 \rangle}{\varepsilon_{0,0}^{(0)} - \varepsilon_{5p \rightarrow 6p \ 1, 0}^{(0)}} \\ & | \text{hole spinor } \rightarrow \text{ particle spinor } J, M_{J} \rangle \end{split}$$

• ... and a large number of small contributions uncorrected for correlation effects.

Final values for  $\alpha_{C_T}$  and  $\alpha_{C_S}$  will lead to tighter constraints.<sup>38</sup>

<sup>&</sup>lt;sup>38</sup>T. F., M. Jung, (2019) in preparation.

## The induced fermion EDM

#### **Standard Model Picture**<sup>34</sup>

**BSM Picture** 



• Three-loop  $\mathcal{CP}$ -odd contributions zero in the absence of gluonic corrections  $^{35}$ 

 $d_e^{SM} \leq 10^{-38}\,e\,\,\mathrm{cm}$ 



• MSSM ("naïve SUSY") prediction<sup>36</sup>:  $d_e \leq 10^{-27} e \text{ cm}$ 

<sup>&</sup>lt;sup>34</sup>E.D. Commins, *Adv At Mol Opt Phys* **40** (1998) *1* 

<sup>&</sup>lt;sup>35</sup>M. Pospelov, I.B. Khriplovich, Sov J Nuc Phys **53** (1991) 638

<sup>&</sup>lt;sup>36</sup>J. Ellis, J.S. Lee, A. Pilaftsis, J High Energy Phys **10** (2008) 049

## **Radium excited states - Comparison with experiment**<sup>42</sup>



<sup>42</sup>NIST Atomic Spectra Database (ver. 5.5.1)