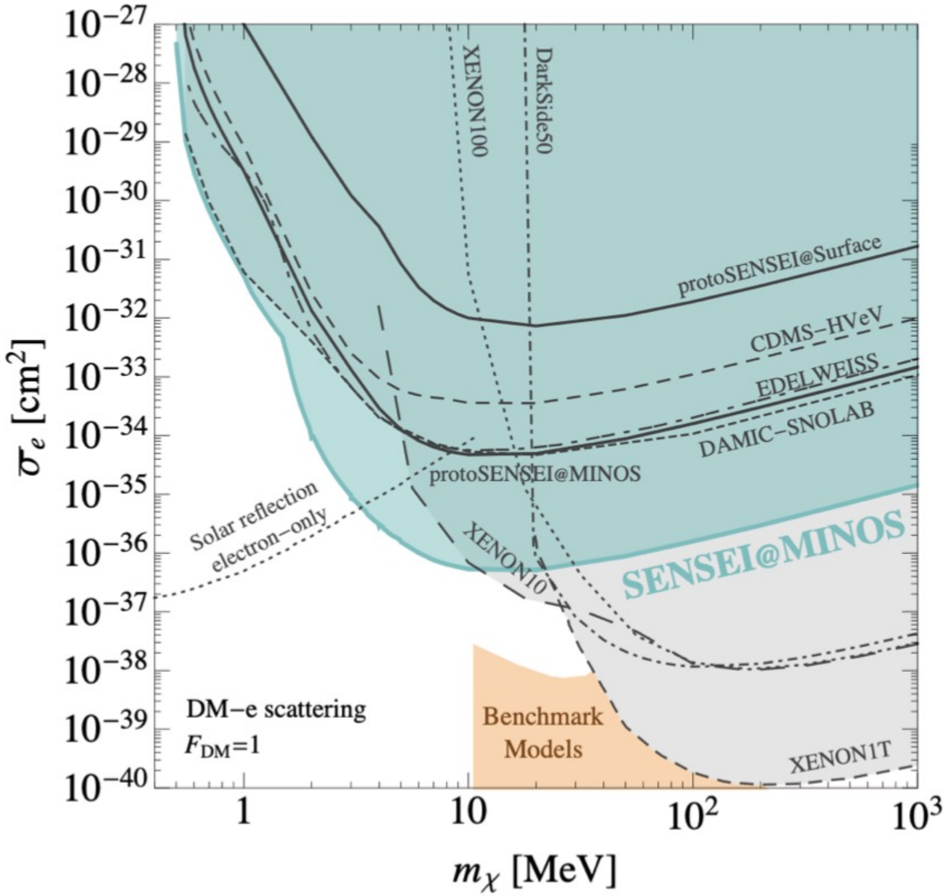
Fuelling the search for light DM-electron scattering

Louis Hamaide – DMUK Conference

Based on arxiv 2110.02985

Going To Lower DM Masses

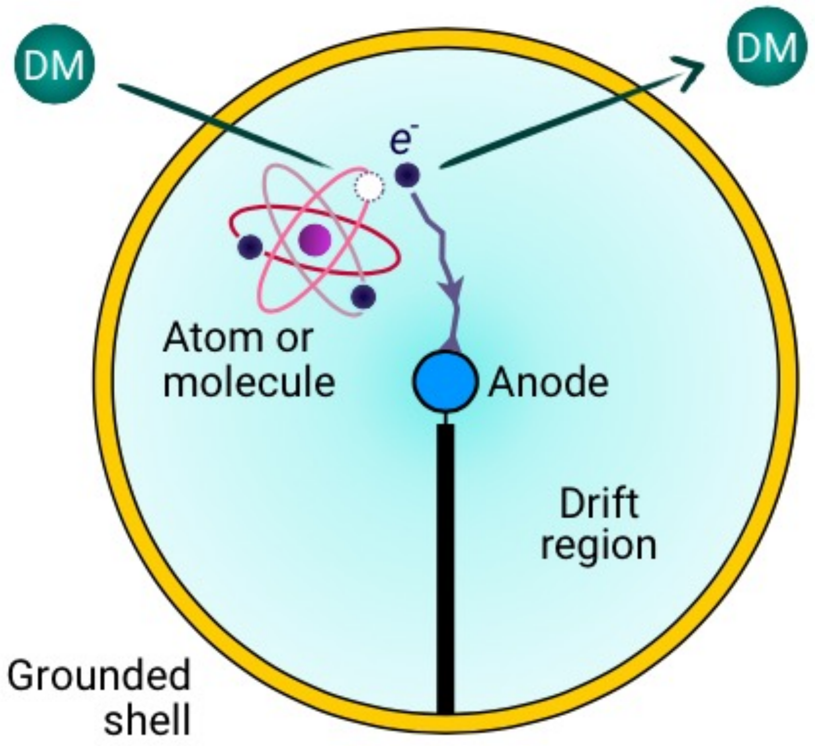
- DM-electron scattering opens searches for lighter DM (<1 GeV), but requires sensitivity to small number of electrons (<4e-)



arxiv 2004.11378

What Are Spherical Proportional Counters

- SPCs consist of gas in a sphere sensitive to 1e- events and exhibit low noise
- We study He and Ne (lighter), Xe (for comparison), CH_4 and C_4H_{10} (quenchers)

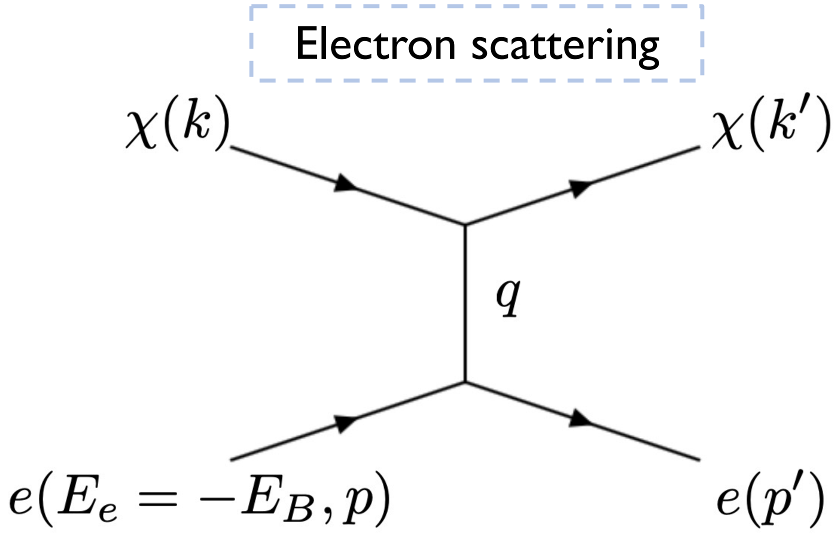


Ionization electrons drift to the anode where the initial energy can be reconstructed

Dark Matter Electron Scattering

- Dark matter transmits some energy to electron, ionizing atom/molecule
- Scattering rate depends on electronic bound and unbound wavefunction

→ Need to solve N-body atomic/molecular Hamiltonian



$$\mathcal{M}(n, l \to \text{free}\, e^-) = g_x g_y \frac{1}{q^2 - m^2} \int d^3x\, \tilde{\psi}^*_{p'l'm'}(\mathbf{x}) e^{i\mathbf{q}\cdot\mathbf{x}} \psi_{nlm}(\mathbf{x})$$

$F_{\mathrm{DM}}(q)$ $f^{nl}_{\mathrm{ion}}(q)$

where $\mathrm{d}R \;\alpha\; |\mathcal{M}|^2$

Bound Electron Wavefunctions

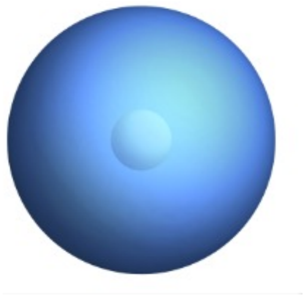
- Hartree-Fock approximation: mean field self consistent bound states:

$$-\frac{1}{2}\frac{d^2P_{n_al_a}}{dr^2} + \frac{l_a(l_a+1)}{2r^2}P_{n_al_a}(r) - \frac{Z}{r}P_{n_al_a}(r) + \sum_{n_bl_b}(4l_b+2)\left(v_0(n_bl_b,r)P_{n_al_a}(r) - \sum_{l}\Lambda_{l_all_b}v_l(n_bl_b,n_al_a,r)P_{n_bl_b}(r)\right)$$

$$= \epsilon_{n_al_a}P_{n_al_a}(r) + \sum_{n_b\neq n_a}\epsilon_{n_al_a,n_bl_a}P_{n_bl_a}(r)$$

- **PySCF** : Quantum chemistry package that solves HF eqs. for atoms and molecules:
  - HF equations solved self-consistently using gaussian basis
  - Includes relativistic treatments, molecular dipoles, and more
  - Expect accuracy of O(30%) in event rates/bounds

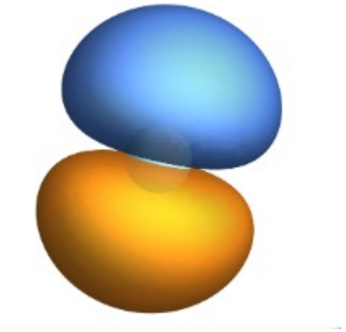
Bound Electron Wavefunctions - Results



1s orbital

HELIUM

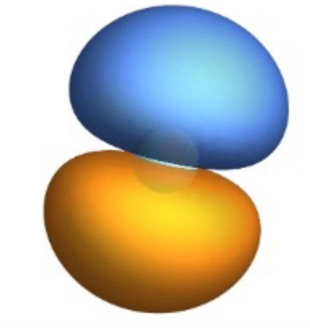
E_{ion} = -24.6 eV
→ events from 2 electrons



2p orbital

NEON

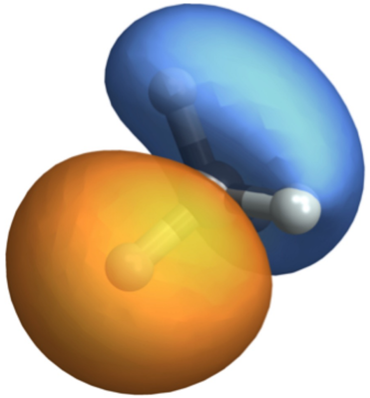
E_{ion} = -21.7 eV
→ events from 8 electrons



5p orbital

XENON

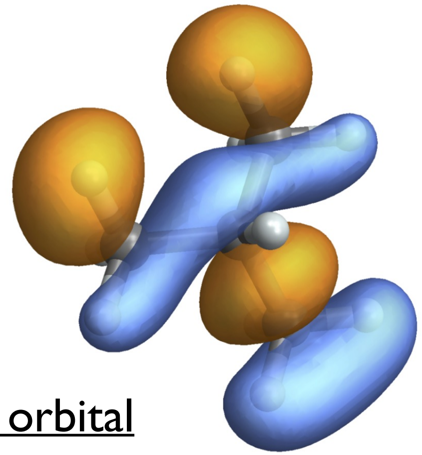
E_{ion} = -12.7 eV
→ events from 18 electrons



$2t_{2x}$ orbital

METHANE (CH_4)

E_{ion} = -13.6 eV
→ events from 8 electrons



$5e_y$ orbital

ISOBUTHANE (C_4H_{10}))

E_{ion}= -11.1 eV
→ events from 26 electrons

Unbound Electron Wavefunctions

- **Atoms:** Continuum limit: Hartree-Fock integrated, approximate the self-consistent piece of the potential + use frozen core:

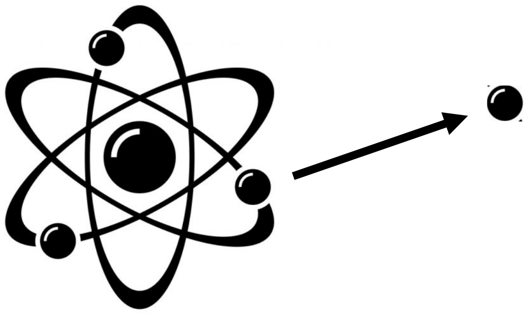
$$-\sum_{i\neq j} \frac{1}{|\mathbf{r_i}-\mathbf{r_j}|} = V_{dir}(r) + V_{exch}(r)$$

$$V_{dir}(r) = \sum_{n_b l_b} (4l_b + 2) \int_0^\infty \left(\frac{P^2_{n_b l_b}(r_1)}{\max(r_1, r)} \right) dr_1$$

$$V_{\text{exch}} = k_x \left(\frac{24\rho(r)}{\pi} \right)^{1/3}$$

- **Molecules:** Coulomb potential/wavefunction:

$$P_{kl}(r) = \frac{4\pi}{2k} \frac{\left|\Gamma\left(\ell + 1 - \frac{iZ}{k}\right)\right| e^{\frac{\pi Z}{2k}}}{(2\ell+1)!} (2kr)^{\ell+1} \times e^{-ikr}\, M\left(\ell + 1 + \frac{iZ}{k}, 2\ell+2; 2ikr\right)$$

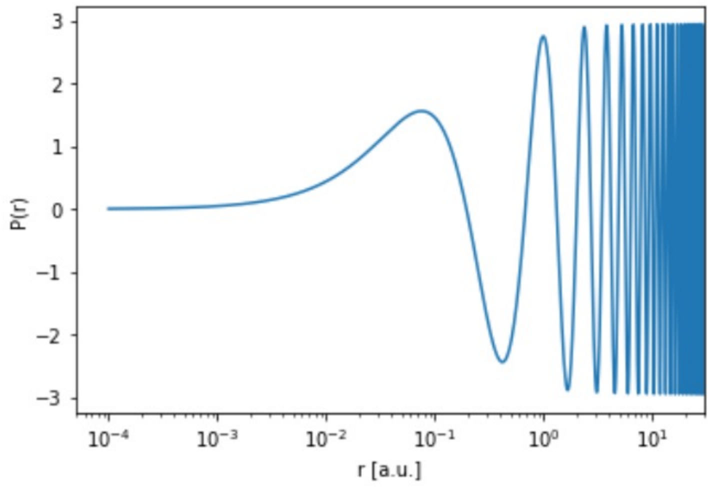


Potential:

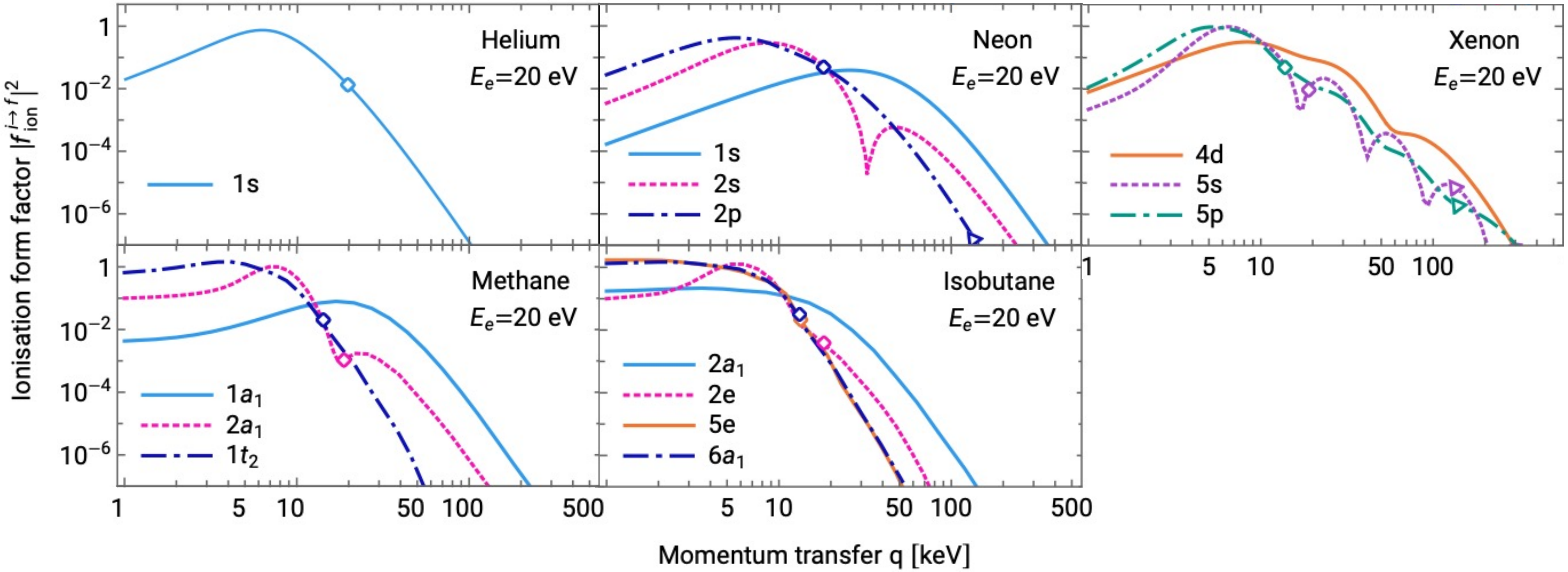
- Point nucleus : $-Z/r$
- Electron "cloud": $V_{dir}(r)$
- Electron "exchange": V_{exch}

→ 1/r at large r

Neon 2p → l_R=0, E = 250eV



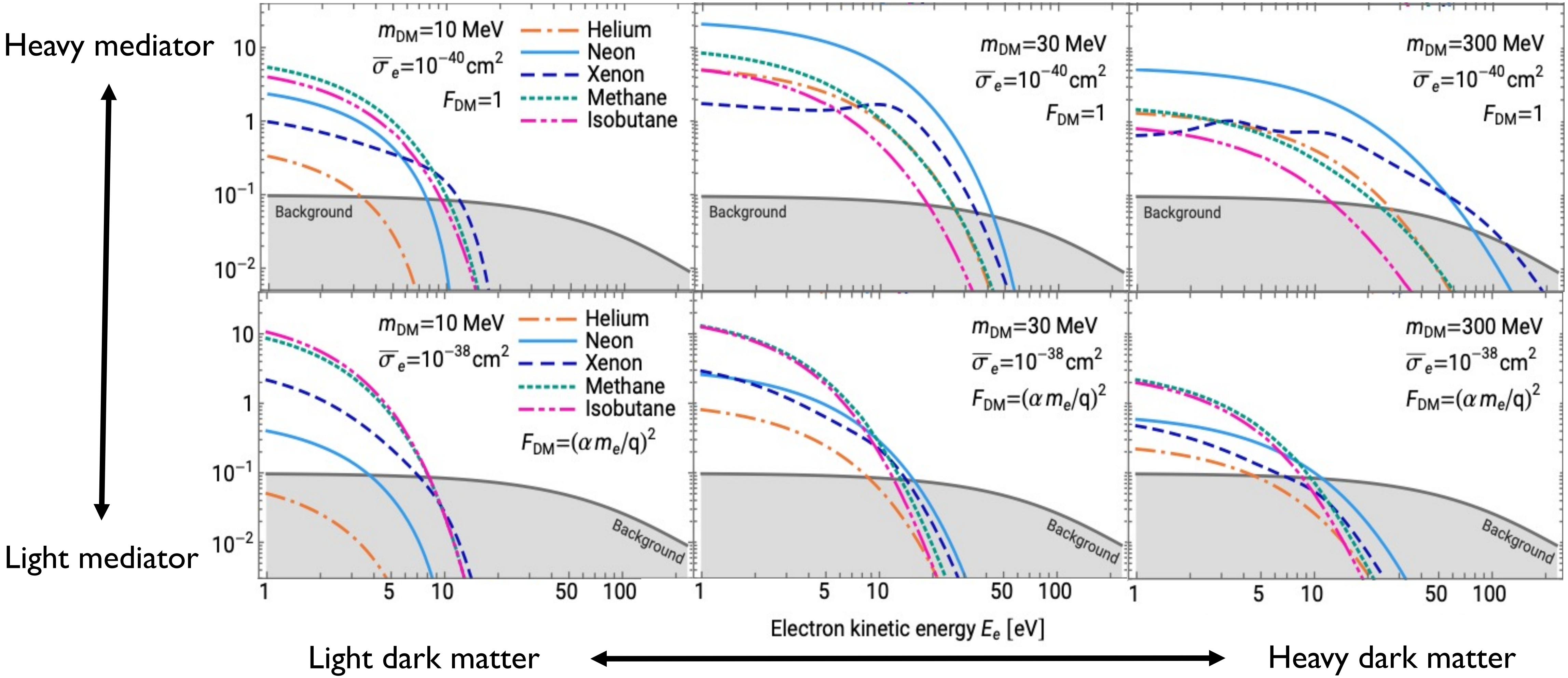
Form Factors



Form factor ($\alpha|\mathcal{M}|^2$): $$|f_{\rm ion}^{nl}(q)|^2 = \frac{(2m_e E_R)^{3/2}}{\pi^2} \sum_{\rm states:i,f} \left| \int d^3x\, \tilde{\psi}^*_{p'l'm'}(\mathbf{x}) e^{i\mathbf{q}\cdot\mathbf{x}} \psi_{nlm}(\mathbf{x}) \right|^2$$

Event Rates

arxiv 2110.02985



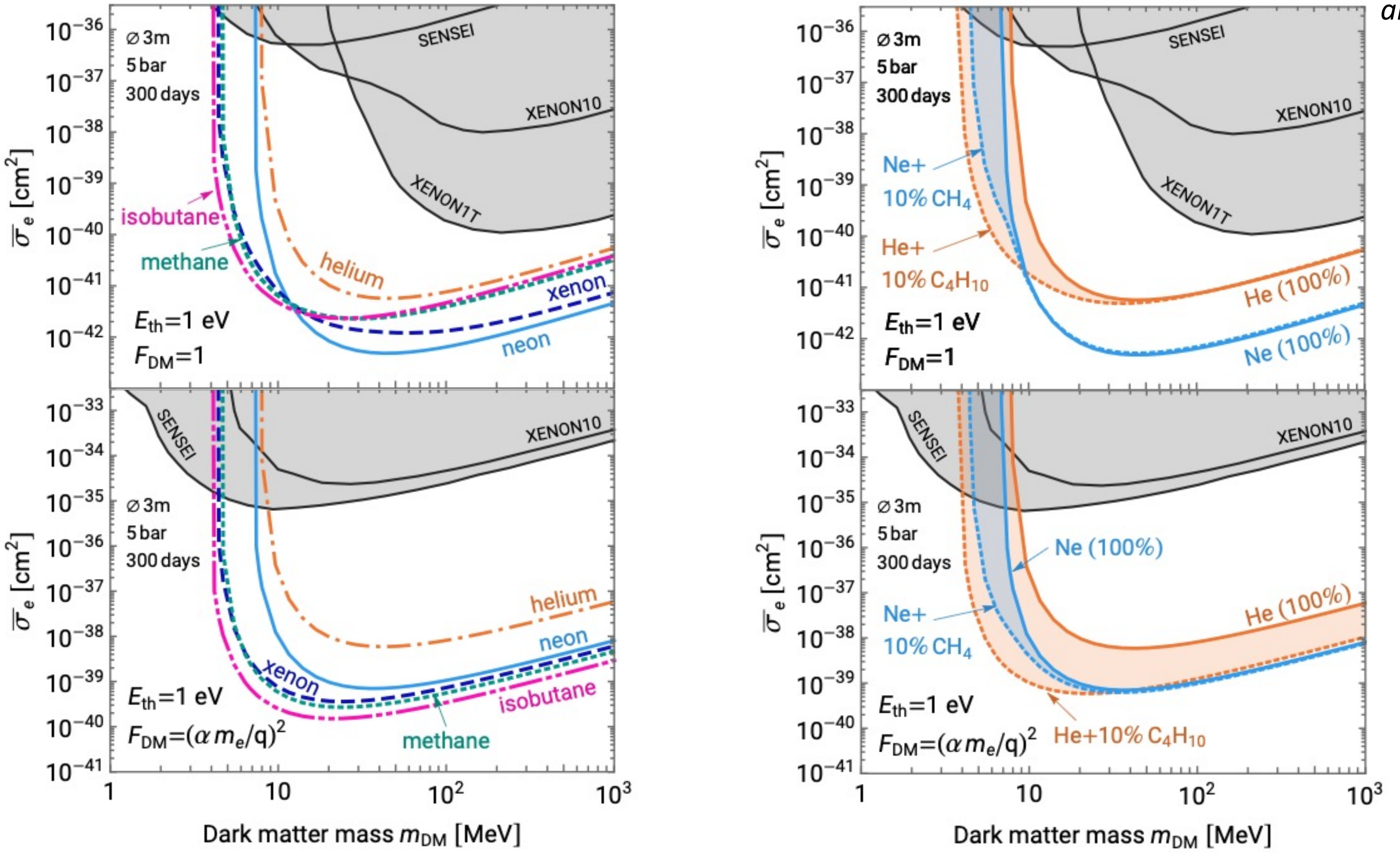
Louis Hamaide

Sensitivities

arxiv 2110.02985

Heavy mediator

Light mediator



Summary

- Dedicated direct detection of DM-electron scattering good probe of light DM (<1GeV)
- Atomic calculation under control – good accuracy & understanding (vs other HF & experiment)
- Molecular calculation more difficult (Coulomb approximation used), but can confidently be used to set bounds (i.e. with mixing)
- Seems promising → more sensitive than current bounds / comparable to other proposed experiments
- SPC good probe of light DM-electron scattering !
- Large scale experimental proposal coming soon: DARKSPHERE

Thank you!

Back up - Motivation for Light(er) Dark Matter

- Dark matter has many ways of appearing in the present day universe:

Thermal Production (e.g. freeze-out WIMP), Freeze-in (FIMP), Inflaton decay, Gravitino…

WIMPs annihilate until $T \sim m_\chi/20$, leaving relic density:

$$\Omega_\chi h^2 \approx \frac{3 \times 10^{-27} \text{cm}^3\text{s}^{-1}}{\langle \sigma_{\chi\chi} v_{rel} \rangle}$$

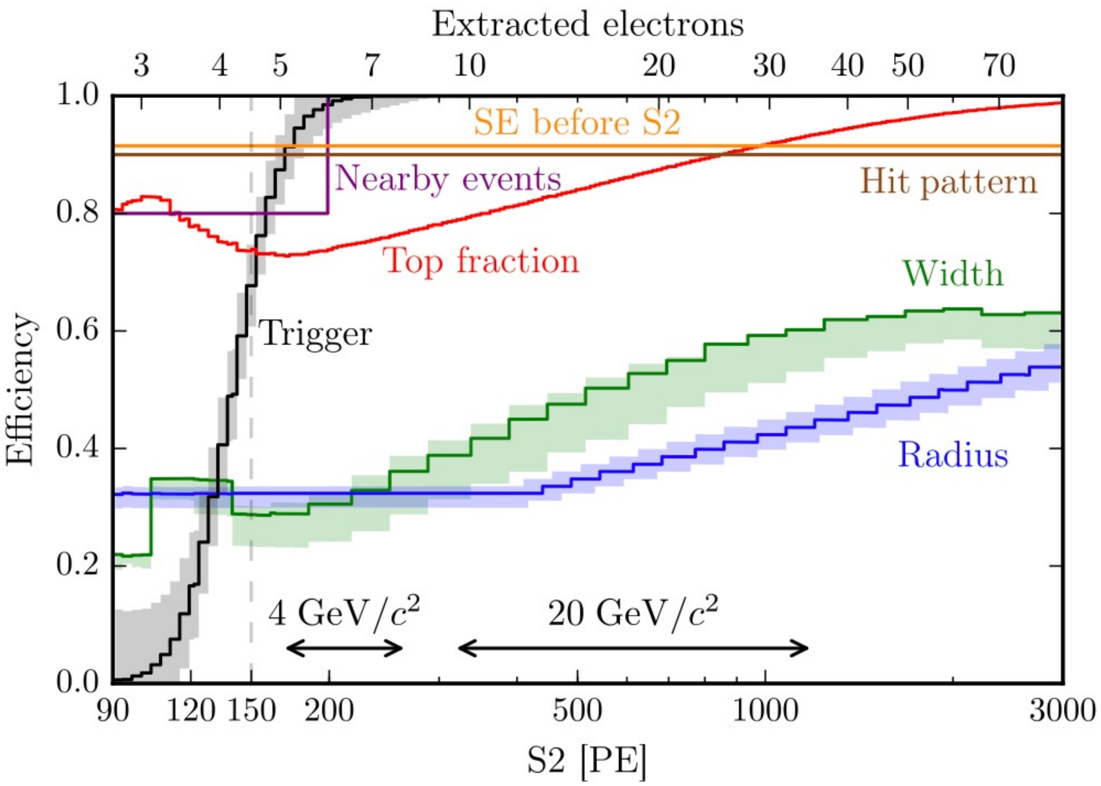
SM particles annihilate near $T \sim m_\chi$, leaving relic density:

$$\Omega_\chi h^2 \propto \langle \sigma_{\chi\chi} v_{rel} \rangle$$

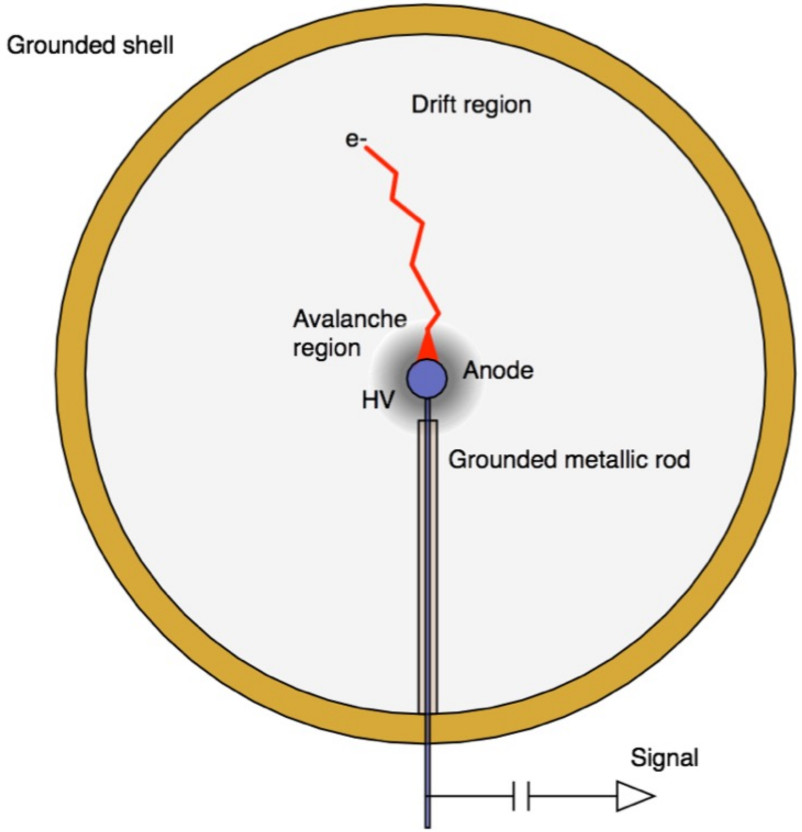
- Individual models of freeze-out and or freeze-in DM can be fully tested (even for unknown details of UV cosmology).
- Without knowledge of T_R, we cannot fully test inflaton decay or gravitino

Back up – More On Detector

(liquid) Xenon 1T threshold (>4.5e-)

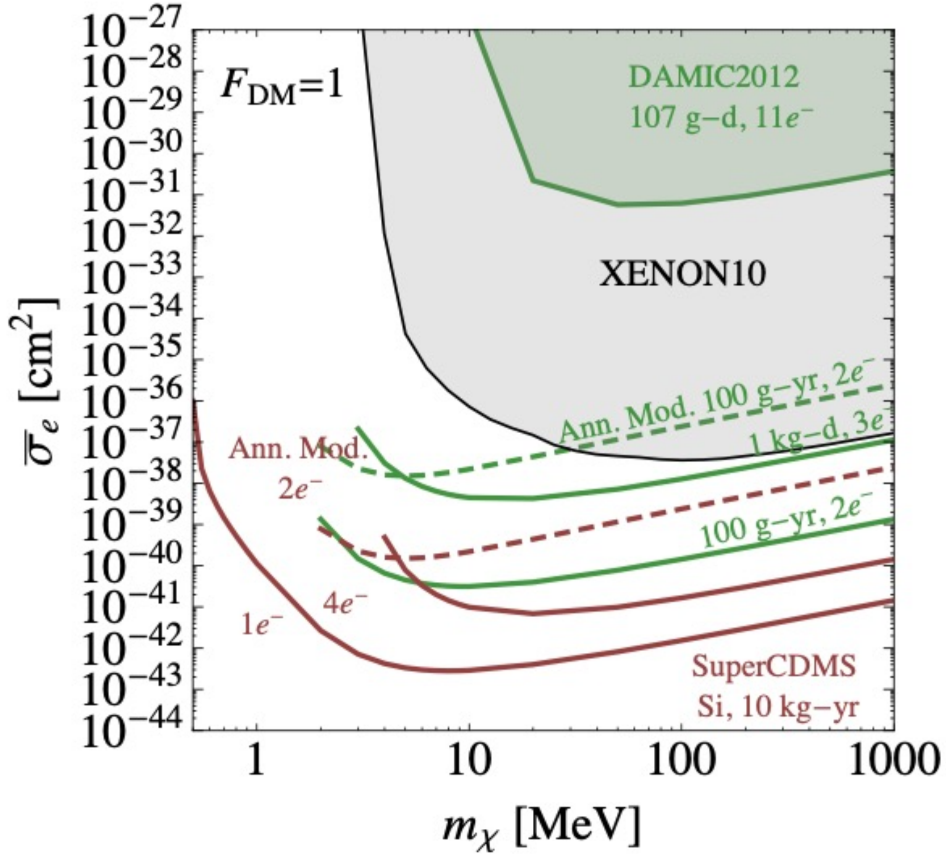


Spherical Proportional Counter (SPC, as proposed in DarkSPHERE)

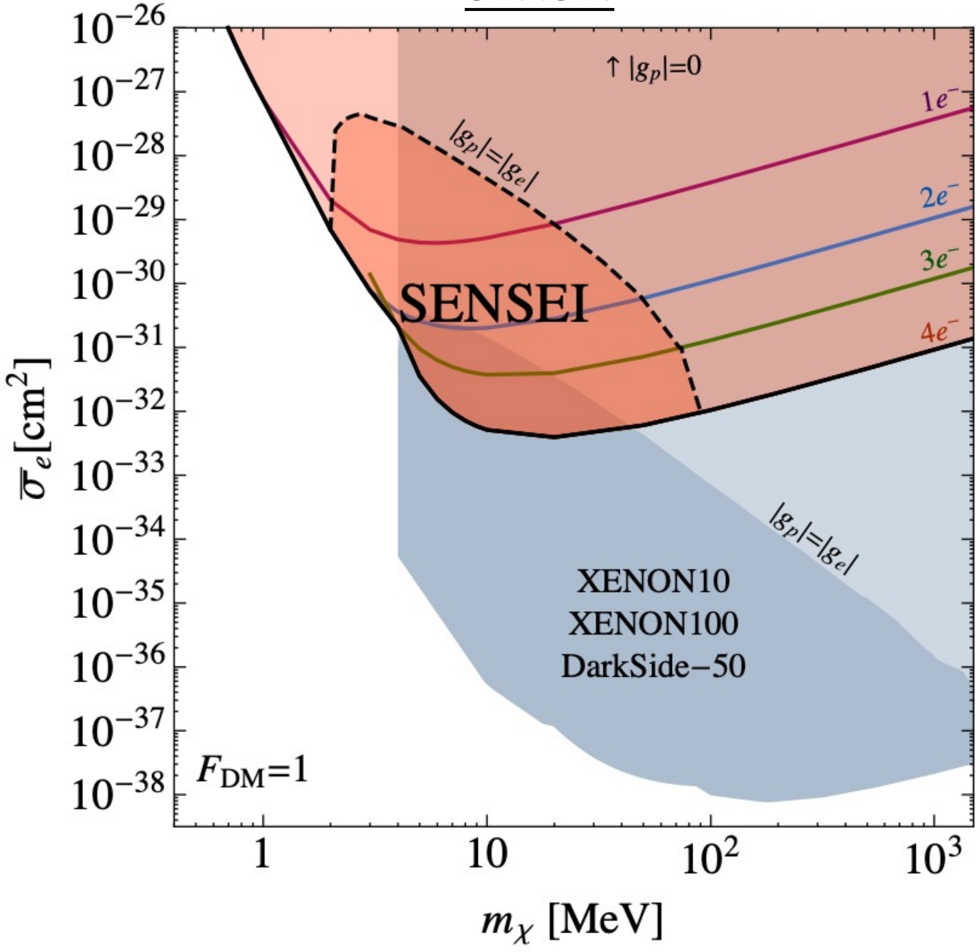


Back up – More On Constraints

Electron Recoil SuperCDMS projection (Essig et al.)



SENSEI



Back up – Hartree Fock choice

- Hartree-Fock approximation: self-consistent bound states with energies correct to first order:

$$
\begin{aligned}
&-\frac{1}{2}\frac{d^2 P_{n_a l_a}}{dr^2} + \frac{l_a(l_a+1)}{2r^2} P_{n_a l_a}(r) - \frac{Z}{r} P_{n_a l_a}(r) + \\
&\sum_{n_b l_b} (4l_b+2)\left(v_0(n_b l_b, r) P_{n_a l_a}(r) - \sum_l \Lambda_{l_a l l_b} v_l(n_b l_b, n_a l_a, r) P_{n_b l_b}(r) \right) \\
&= \epsilon_{n_a l_a} P_{n_a l_a}(r) + \sum_{n_b \neq n_a} \epsilon_{n_a l_a, n_b l_a} P_{n_b l_a}(r), \quad (3.71)
\end{aligned}
$$

Easy to solve Hamiltonians for full shell atoms	Non-Rel approx. good for q < 200keV	Accuracy of ~30% in event rates/bounds

- Sensitivities of bounds to choices:
  - ~30-50% Gaussian basis choice
  - ~50-100% exchange potential choice, orthogonalization
  - ~10-20% analysis of recoil energy profile vs. deposited energies
  - ~30% astrophysical parameter choices
  - Linear with background

Bound electron wavefunctions (3/4)

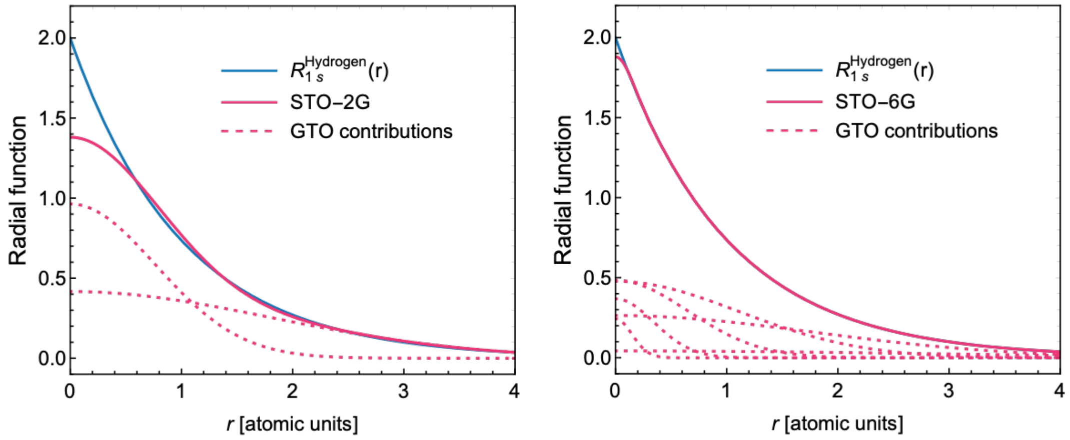
- Hartree-Fock approximation: mean field self consistent bound states:

$$-\frac{1}{2}\frac{d^2P_{n_al_a}}{dr^2}+\frac{l_a(l_a+1)}{2r^2}P_{n_al_a}(r)-\frac{Z}{r}P_{n_al_a}(r)+\sum_{n_bl_b}(4l_b+2)\left(v_0(n_bl_b,r)P_{n_al_a}(r)-\sum_{l}\Lambda_{l_all_b}v_l(n_bl_b,n_al_a,r)P_{n_bl_b}(r)\right)$$

$$=\epsilon_{n_al_a}P_{n_al_a}(r)+\sum_{n_b\neq n_a}\epsilon_{n_al_a,n_bl_a}P_{n_bl_a}(r)$$

Self-consistent approach required

Expect accuracy of O(30%) in event rates/bounds



Gaussian basis choice important at small/large r

$$AO_{nlm}\propto\sum_i c_i^n\exp(-\alpha_i^n r^2)Y_{lm}(\theta,\phi)$$

$$MO_{nlm}=\bar{v}_{nlm}AO_{nlm}$$

$$H_{ij}=\int AO_i(\mathbf{r})H_j(\mathbf{r})AO_j(\mathbf{r})\,d^3\mathbf{r}\ .$$

Treats atoms and molecules, relativistic treatments, molecular dipoles, and more.

Back up - Bound electron wavefunction symmetry

- Molecular orbitals are no longer eigenfunctions (spherical harmonics) of the SO(3) generators.

$$\psi(\mathbf{r}) = \frac{P(r)}{r} Y_{lm}(\theta, \phi) \quad \rightarrow \quad \psi(x, y, z)$$

- We need new classification of orbitals :

irreducible representations of SO(3) → irreducible representation of point group

$\mathbf{T_d}$	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$	xyz
A_2	+1	+1	+1	-1	-1	-	-	-
E	+2	-1	+2	0	0	-	$(2z^2-x^2-y^2, x^2-y^2)$	-
T_1	+3	0	-1	+1	-1	(R_x, R_y, R_z)	-	$[x(z^2-y^2), y(z^2-x^2), z(x^2-y^2)]$
T_2	+3	0	-1	-1	+1	(x, y, z)	(xy, xz, yz)	(x^3, y^3, z^3) $[x(z^2+y^2), y(z^2+x^2), z(x^2+y^2)]$

Tetrahedral group (Methane): T_d

Back-up - bound electron energies

Helium (He)			Neon (Ne)			Methane (CH_4)			Isobutane (C_4H_{10})			Xenon (Xe)		
Basis: aug-cc-pV5Z Total energy: -2.8616			Basis: aug-cc-pV5Z Total energy: -128.5467			Basis: 6-31G(d,p) Total energy: -40.2016			Basis: 6-31G(d,p) Total energy: -157.3123			Basis: Jorge-QZP Total energy: -7229.7195		
Orbital	I_{HF}	I_{exp}	Orbital	I_{HF}	I_{exp}	Orbital	I_{HF}	I_{exp}	Orbital	I_{HF}	I_{exp}	Orbital	I_{HF}	I_{exp}
$1s^2$	24.98	24.6	$2p^6$	23.14	21.7	$1t_2^6$	14.80	13.6	$6a_1^2$	12.34	11.13	$5p^6$	12.45	12.7
			$2s^2$	52.53	48.5	$2a_1^2$	25.66	22.9	$5e^4$	12.44	11.75	$5s^2$	25.54	23.3
			$1s^2$	891.79	870.2	$1a_1^2$	304.96	290.8	$1a_2^2$	13.86	12.85	$4d^{10}$	75.72	68.5
									$4e^4$	14.54	13.71	$4p^6$	163.56	146.1
									$3e^4$	16.04	15.03	$4s^2$	212.69	213.2
									$5a_1^2$	17.15	15.91	$3d^{10}$	711.26	682.7
									$4a_1^2$	20.62	18.58	$3p^6$	958.02	971.4
									$2e^4$	25.17	21.83	$3s^2$	1087.7	1149
									$3a_1^2$	29.44	24.83	$2p^6$	4839.8	4947
									$2a_1^2$	305.01	—	$2s^2$	5132.0	5453
									$1e^4$	305.01	—	$1s^2$	33321	34561
									$1a_1^2$	305.30	—			

Event rates – Back up

- The dark event rate can be calculated using:

$$\frac{dR}{dE_e} = \frac{1}{m_A}\frac{\rho_{DM}}{m_{DM}}\sum_{nl} w_{nl}\frac{d\langle\sigma_{ion}^{nl} v_{DM}\rangle}{dE_e}$$

, where

$$\frac{d\langle\sigma_{ion}^{nl} v\rangle}{d\ln E_e} = \frac{\sigma_e}{8\mu_e^2}\int_{q_-}^{q_+} q dq \left|f_{ion}^{nl}\right|^2 |F_{DM}|^2 g(v_{min}^{nl})$$

- Assume phenomenological background provided by NEWS-G, $F_{DM}=1$
- 10% Methane (plane wave) contribution

- Likelihood analysis: $\Lambda = \frac{\mathcal{L}(0)}{\mathcal{L}(\sigma_e)}$ $\quad -2\ln(\Lambda) \sim \chi^2_1$ $\quad \mathcal{L}(\sigma_e) = \prod_{i=0}^{N_{bins}} \mathcal{P}\left(N_{obs}^i \mid N_\chi^i(\sigma_e) + N_{bg}^i\right)$

- With exposure 5atm.300days in sphere of radius 1.5m DarkSPHERE sensitivity below Xenon 1T
- Molecular contribution seen as setting own bounds → potential for molecular bounds on DM-e scattering

Back-up – Sensitivities to higher threshold