Dark matter induced atomic ionisation:

Calculations of atomic ionisation cross-sections

Benjamin M. Roberts, Ashlee R. Caddell

University of Queensland, Australia;

University of Melbourne
30 March 2022

Usually:

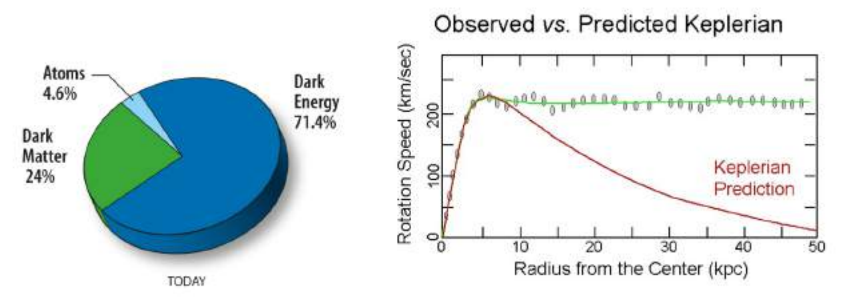
- High-precision atomic structure theory
- Applications: precision tests of fundamental physics
- Atomic parity violation, search for EDMs, exotic physics signatures in atomic experiments

This talk:

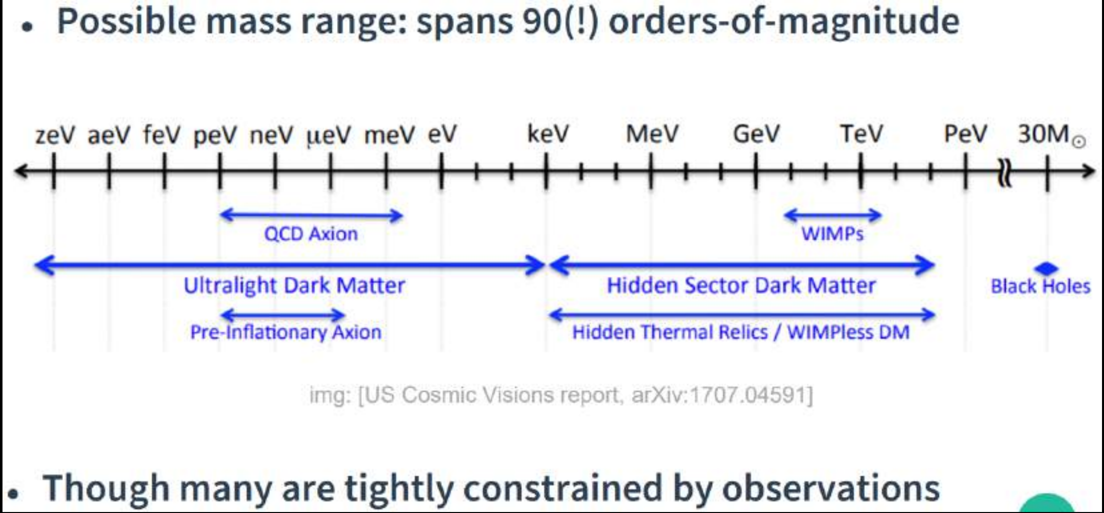
- Dark matter direct detection
- WIMP scattering on atomic electrons
- Modelling of atomic wavefunctions more important than expected

Dark Matter

- Rotation curves + velocity dispersion
- BAOs: Baryon acoustic oscillations
- Gravitational lensing
- Structure formation



What we don’t know about dark matter



- **Possible mass range: spans 90(!) orders-of-magnitude**

img: [US Cosmic Visions report, arXiv:1707.04591]

- **Though many are tightly constrained by observations**

Weakly Interacting Massive Particles:

- Theoretical: good motivation
- Experimental: "easy" (conceptually) to detect $m_\chi \gtrsim m_{\text{nucleus}}$

WIMP Miracle

- Neutron-like massive particles, only interact via weak force
- M $\sim$ 100 GeV + weak interaction $\Rightarrow \langle \sigma v \rangle \sim 10^{-26}$ cm^3/s
- Observed DM abundance $\Rightarrow$ annihilation: $\langle \sigma v \rangle \sim 10^{-26}$ cm^3/s

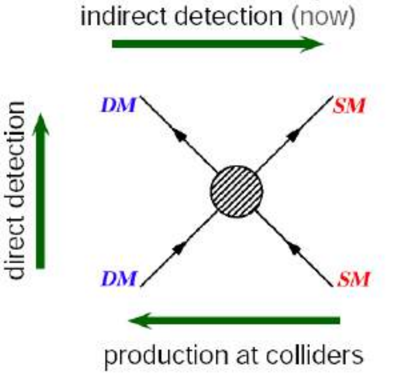
- Very weak dependence on mass, holds for 1 GeV – 10 TeV

(.....but large portions ruled out already)

Looking for Dark Matter

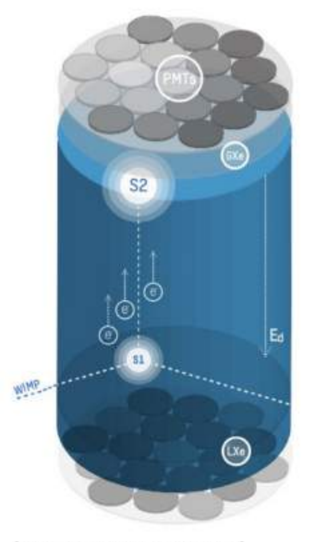
- Production: Missing energy + resonance searches as colliders **
- Decay: Astrophysics searches for annhilation/decay products
- Scattering: Directly detect DM–SM interactions ← This talk

** Also: DM-mediated processes: atomic physics, fifth-force, EDM searches, atomic parity violation



[https://www.mpi-hd.mpg.de]

Duel-Phase Time-Projection Chamber - S1 and S2



[http://www.xenon1t.org/]

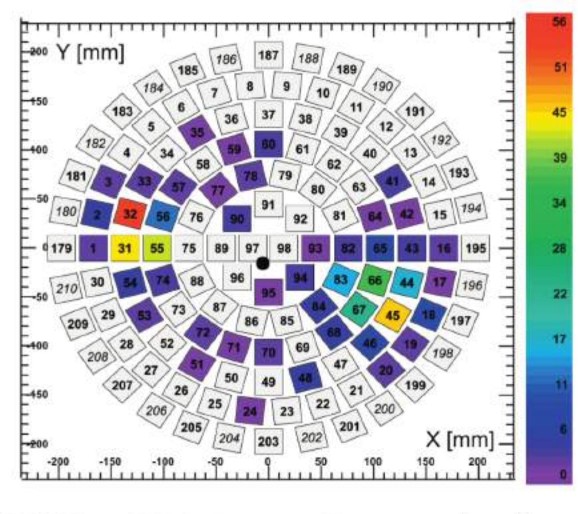
Duel-phase (Liquid & Gas) Scintillating liquid Xe

- Scattering event: excitations and ionisations
- De-excitation: prompt photons ("S1" signal)
  - PMTs give x, y positions

- Ionised electrons drifted upwards, accelerated through Xe gas: "S2" scintillation – like a neon (xenon) bulb
  - Drift time; re-construct z-position

- Reconstruct E_{recoil} from S1 and/or S2 (S1 better calibrated)

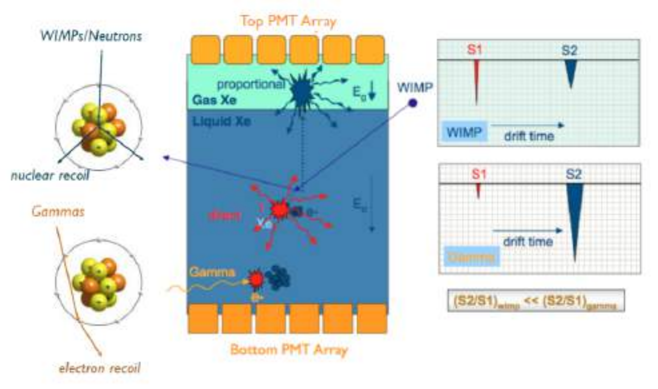
Duel-Phase Time-Projection Chamber - S1 and S2



[XENON100 Collab., Astropart. Phys. 54, 11 (2014)]

- Neutron/γ/charged particles: Probability of interaction drops quickly with length
- WIMP interactions: very rare:
  $\therefore$ flat probability
  - l-Xe Vito (only use middle)
  - e.g. Xe1T: 3 → 2 tonnes
- Also: Probability of double-scattering is negligible
  - Reject such events (e.g., left)

Time-projection Chamber - S1 and S2



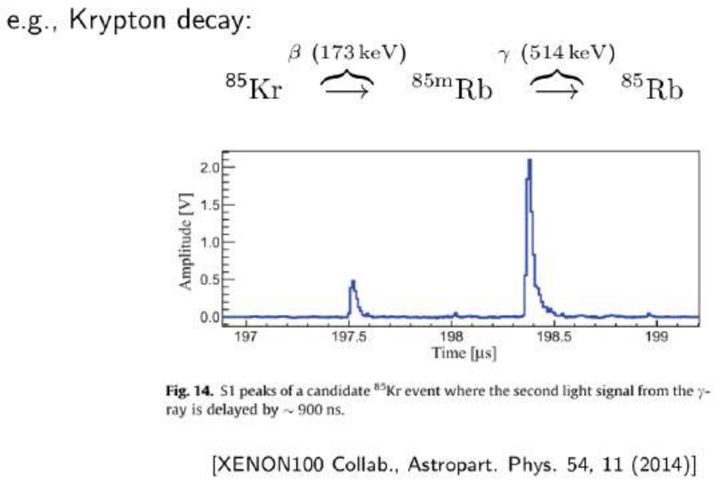
[E. Aprile (SUSY08)]

- Discrimination of nuclear recoils (WIMPs/*n*s) from electron recoils (γs/βs)

$$\frac{S2}{S1}_{\text{Nuclear Rec.}} \gg \frac{S2}{S1}_{\text{Electron Rec.}}$$

Time-projection Chamber - S1 and S2

- Also: background can be modelled/measured & rejected



e.g., Krypton decay:

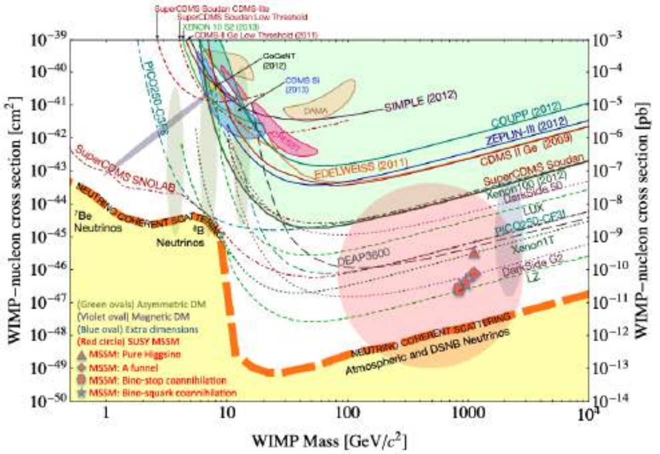
$$^{85}\mathrm{Kr} \xrightarrow{\beta\ (173\,\mathrm{keV})} {}^{85\mathrm{m}}\mathrm{Rb} \xrightarrow{\gamma\ (514\,\mathrm{keV})} {}^{85}\mathrm{Rb}$$

Fig. 14. S1 peaks of a candidate ^{85}Kr event where the second light signal from the γ-ray is delayed by ~ 900 ns.

[XENON100 Collab., Astropart. Phys. 54, 11 (2014)]

Point is: need/want both S1 and S2 to understand events

Limits/exclusions



[arXiv:1310.8327]

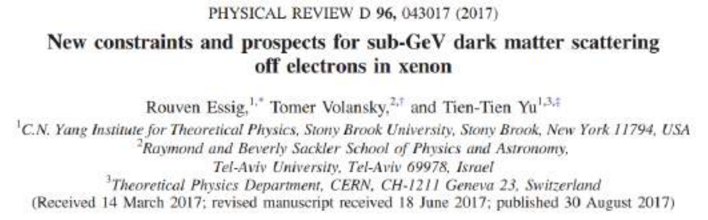
- Approaching Neutrino “floor”
- (From sun, annual modulation)
- Low-mass substantially less constrained

- Threshold vs. exposure

Lighter WIMPs

- $M_\chi \ll M_{\mathrm{Nuc.}}$: cannot cause appreciable nuclear recoil
- But can cause ionisations: assumed that S2$\gg$S1
- High background noise in these regime though
- Usually S2-only signal is excluded due to background

Other proposals (+constraints) to search using S2-only:



PHYSICAL REVIEW D **96**, 043017 (2017)

New constraints and prospects for sub-GeV dark matter scattering off electrons in xenon

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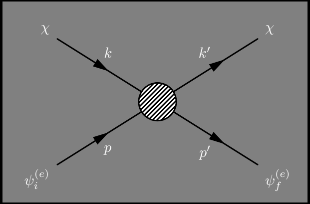
- $S1$ signal thought to be negligible
- In fact, it might be much larger than thought

WIMP-Electron ionisation



- Cause excitations, and **ionisations**
- q/E: momentum/energy transfer

$$dR = \frac{n_T \rho_{\rm DM}}{m_\chi c^2} \frac{{\rm d}\langle \sigma_{njl} v_\chi \rangle}{{\rm d}E} \, {\rm d}E$$

$$\frac{\langle {\rm d}\sigma v\rangle}{{\rm d}E} = \frac{\overset{\text{Particle Phys}}{\boxed{\bar{\sigma}_e}} c\alpha^2}{2E_H} \int {\rm d}v \overset{\text{Astrophys.}}{\boxed{\frac{f_\chi(v)}{v/c}}} \int_{q_-}^{q_+} a_0^2 q {\rm d}q \boxed{\left|F_\chi^\mu(q)\right|^2} \overset{\text{Atomic}}{\boxed{K(E,q)}}$$

- Free-electron cross-section, $\bar{\sigma}_e$, and DM form-factor:

$$\hbar q_\pm = m_\chi v \pm \sqrt{m_\chi^2 v^2 - 2 m_\chi E}$$

$$K_{njl} \equiv E_H \sum_m \sum_f \left| \langle f | e^{i\boldsymbol{q}\cdot\boldsymbol{r}} | njlm \rangle \right|^2 \varrho_f(E)$$

- Following: Essig, Manalaysay, Mardon, Sorensen, Volansky, Phys.Rev.Lett.**109**,021301('12).

S1 and S2

S1

$$R \propto \int_{E_{\mathrm{thresh.}}} \frac{\mathrm{d}\langle \sigma v \rangle}{\mathrm{d}E} \, \mathrm{d}E$$

- Low-energy threshold
- (hardware + software)
- Suppressed for electron recoils*
- Detector resolution very important

S2

$$R \propto \int_{0} \frac{\mathrm{d}\langle \sigma v \rangle}{\mathrm{d}E} \, \mathrm{d}E$$

- Electrons drifted upwards
- Scintillate in gaseous phase
- Energy agnostic: count electrons
- Secondary electrons

Why S1 thought to be small?

$$q_{\min} = m_\chi v - \sqrt{m_\chi^2 v^2 - 2 m_\chi E}$$

WIMP-induce ionisation:

- WIMP: $m_\chi \sim 10\,\text{GeV}$, $v_\chi \sim 10^{-3} c$
- Energy deposition: $\Delta E \sim \text{keV}$
- $\Rightarrow q \sim 1000\,\mathrm{a.u.} = 4\,\mathrm{MeV}$ momentum transfer
- $\therefore$ very suppressed

Simple Approach:

- Very large q: high-p tail of electron wavefunction: $r \sim q^{-1} \sim 10^{-3} a_B$
- Close to nucleus: s-states ($l = 0$) non-zero $\psi(0)$
- Close to nucleus: Oscillator-like wavefunctions: $\psi \sim A e^{-\beta r^2}$

$$\boxed{\langle f | e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} | i \rangle \propto e^{-q^2/8\beta}}$$

Coulomb wave-functions:

Smooth function: $\langle f|e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}|i\rangle \propto e^{-q^2/8\beta}$

Non-relativistic Coulomb Case:

$$\psi \sim Ar^l \left[1 - \frac{Z}{l+1} r + \dots\right]$$

- Coulomb wavefunctions contain a cusp, strongest $l = 0$:
- Lowest-order term: $\sim \int r^{l+l'+2} j_L(qr)\, dr$: Identically Zero
- Next term: $\sim \int r^{l+l'+3} j_L(qr)\, dr \propto Z\, q^{-(l+l'+4)}$
- $d\sigma \sim q^{-8}$ — s-waves dominate

Eighth power is still eighth power ..... but better than exponential

- BMR, V. Flambaum, and G. Gribakin, Phys. Rev. Lett. 116, 023201 (2016).

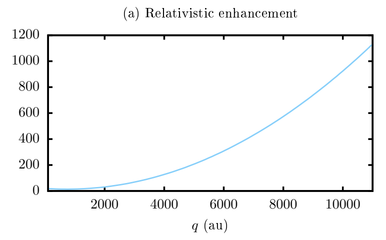
Dirac wave-functions

Relativistic Case is different:

$$\psi \sim A r^{\gamma-1}\left[\gamma - \kappa + B r + \ldots\right] \qquad : \qquad \gamma = \sqrt{\kappa^2 - (Z\alpha)^2} \approx 1 - (Z\alpha)^2$$

$\kappa = -1$ for s-states, 1 for $p_{1/2}$

- Lowest-order term: $\sim \int r^{\gamma+\gamma'} j_L(qr)\, dr$: Non-Zero!
- s, $p_{1/2}$-waves: $d\sigma \sim q^{-6+2(Z\alpha)^2} \simeq q^{-5.7\ldots}$ for Xe, I.


(a) Relativistic enhancement

$$e^{-q^2} \to q^{-8} \to q^{-6} \to q^{-6+2(Z\alpha^2)} \approx q^{-5.7..}$$

- Orders of magnitude enhancement

- BMR, V. Flambaum, and G. Gribakin, Phys. Rev. Lett. 116, 023201 (2016).

Outgoing electron wavefunction: Sommerfeld enhancement

For large p ($|p| = \sqrt{2m_e\varepsilon}$), plane waves should be OK?

$$\langle \boldsymbol{r}|\boldsymbol{p}\rangle = e^{i\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}, \qquad \int \frac{d^3\boldsymbol{p}}{(2\pi\hbar)^3}\langle \boldsymbol{p}|\boldsymbol{p}\rangle = 1.$$

But high q means low-r – close to nucleus.
Continuum *energy* eigenstates:

$$\boxed{\int_{\varepsilon-\delta\varepsilon}^{\varepsilon+\delta\varepsilon} \langle \varepsilon' jlm|\varepsilon jlm\rangle \, d\varepsilon' = 1.}$$

enhanced near origin for Coulomb potentials.
Approximate sommerfeld enhancement:

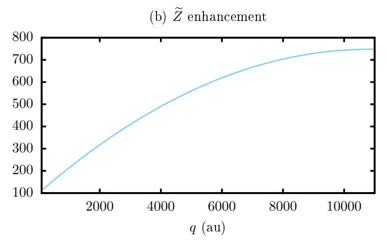
$$\left.\frac{K_{ns_{1/2}}}{K^{\rm pw}_{ns_{1/2}}}\right|_{r\to0} \approx \frac{8\pi Z}{\left[1-\exp(-\frac{2\pi Z}{|p'|})\right] n^3|p'|},$$

- Orders of magnitude enhancement

Low-r scaling

As well as Sommerfeld enhancement (enhance continuum wavefunction as low-r), same for bound states

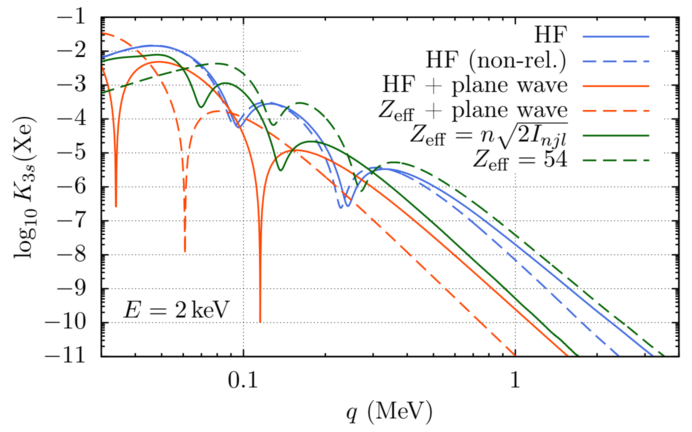
- Common approach: Use H-like wavefunctions with $Z_{\rm eff} = n\sqrt{|E|/R_y}$
- Works very well for many applications: fine at intermediate to large r
- Fails at low-r
- H-like functions: $\psi(0)^2 \sim Z_{\rm eff}^3$
- True wavefunctions: $\psi_{\rm inner}(0)^2 \sim Z^3$, $\psi_{\rm outer}(0)^2 \sim Z^1$



- Orders of magnitude "enhancement"

Different approximations

$$K = |\langle \mathrm{Xe}|e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}|\mathrm{Xe}^{+} + e^{-}\rangle|^{2}$$



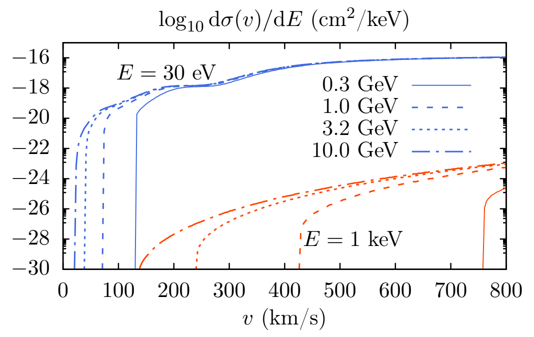
Very common to use: plane wave + Z_{eff} + non-relativistic functions

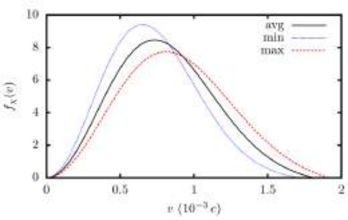
- $\sim$ 4 orders of magnitude too small at $\sim$1 MeV!

σ: Strong v dependence

$$\frac{\langle \mathrm{d}\sigma v\rangle}{\mathrm{d}E} = \frac{\bar{\sigma}_e c\alpha^2}{2E_H}\int \mathrm{d}v \boxed{\frac{f_\chi(v)}{v/c}\int_{q_-}^{q_+} a_0^2 q \mathrm{d}q \left|F_\chi^\mu(q)\right|^2} K(E,q)$$

$$\hbar q_\pm = m_\chi v \pm \sqrt{m_\chi^2 v^2 - 2m_\chi E}$$

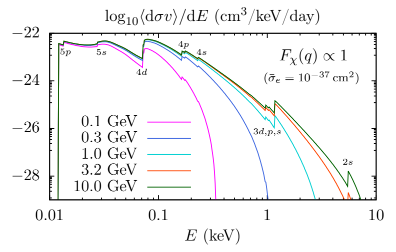




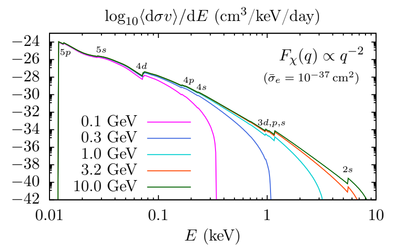
- Strong dependence on min q
- Strong dependence on v
- Assume standard halo model
- Account for uncertainties: v_{esc}, v_{rms} etc.

Calculated cross-section

Velocity-averaged cross-sections:



- Left: Heavy mediator (contact interaction)



- Right: Light mediator (Coulomb-like)

- Assume standard halo model:
- Above $\sim$ few keV - S1 suppressed cf S2
- Heavy mediator: If $E_{\rm thresh} \sim 0.5\,$keV: no suppression at all!
- Heavy mediator: S1 $\simeq$ S2

Detector response + resolution

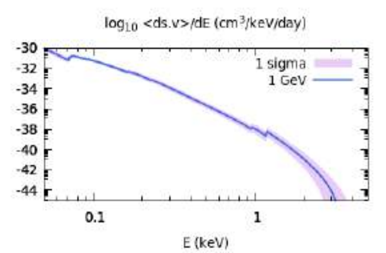
- Detector does not have perfect resolution: R (raw rate) vs S (observable rate)

$$\frac{dS}{dE} \approx \int \epsilon(E')\rho(E'-E)\frac{dR}{dE'}dE'$$

  - ϵ detector sensitivity + hardware threshold; E_{thresh}: software threshold
  - ρ: energy resolution of detector: often assumed Gaussian
  - Substantial part of rate can come from below threshold
  - Can be more precise: model number of produced photoelectrons etc.

Detectable rates:

- Hard-ware & software thresholds
- Detector resolution + efficiency
- *v*elocity error important



Low mass ($\sim$ GeV) WIMPs

- Substantially less constrained
- Look for deposited energy:
  low-mass too small
- Electron recoil instead of nuclear
- Can be advantage: large number

$$dR = \frac{n_T \rho_{\mathrm{DM}}}{m_\chi c^2} \frac{\mathrm{d}\langle \sigma_{njl} v_\chi \rangle}{\mathrm{d}E} \mathrm{d}E$$

- Look for low energy recoils: but high background

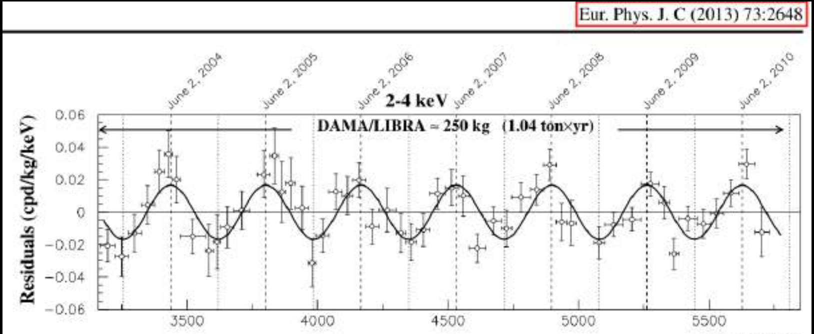
Annual modulation

- Yearly change in event rate:
- Sun + Earth velocities add
- $\Phi(t) = \Phi_0(1 + 5\%)\cos(\omega t + \phi_{\mathrm{June2}})$
- Rate *R* *not* necessarily cosine (non-linear *v* dependence)

DAMA/LIBRA

Annual modulation

- 250 kg highly radiopure NaI, $\sim$ 1 ton * yr
- Only “S1” (solid NaI, no gas phase)
- See significant ($> 9\sigma$) annual oscillation at low energy (correct phase, frequency)
- Other experiment see nothing: but comparison is model-dependent


Eur. Phys. J. C (2013) 73:2648

DAMA/LIBRA Phase II

Lower energy: down to 1 keV (from 2)

- phase II: 1.13 ton×yr (blue); phase I: 1.33 ton×yr (red);
- Expect exponential increase in low-*E* events (if χ-e)
- $\implies$ may have significant implications for χ-e

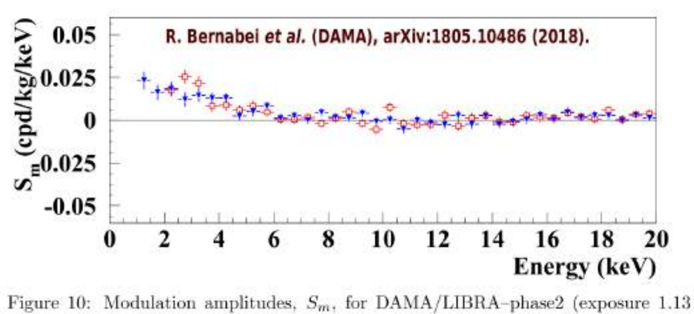
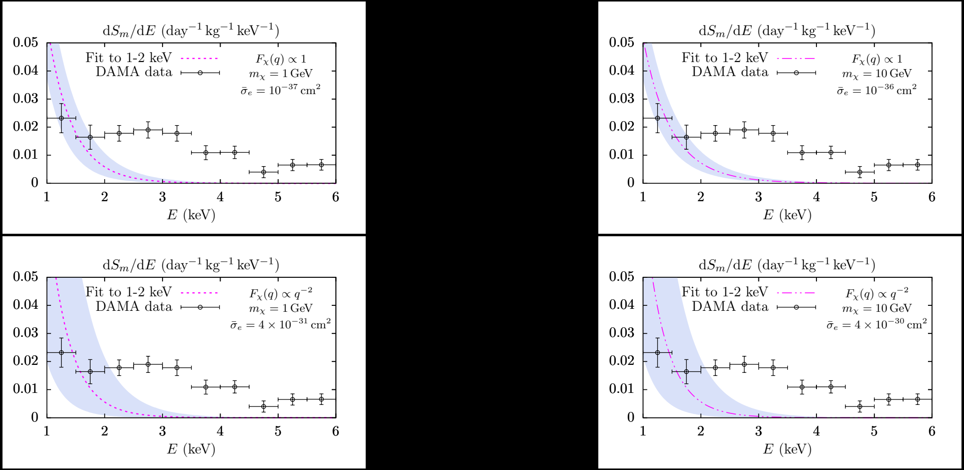


Figure 10: Modulation amplitudes, S_m, for DAMA/LIBRA–phase2 (exposure 1.13

Bernabei *et al.*, arXiv:**1805.10486** (2018). Bernabei *et al.*, J. Phys. Conf. Ser. **1056**, 012005 (2018).

Calculated rate: fit to DAMA II

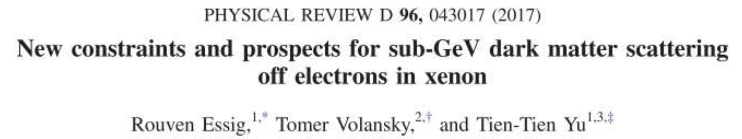


90% C.L. uncertainties. Include:

- Atomic physics errors (small), Velocity distribution (moderate), resolution + threshold (dominant)

- BMR and V. V. Flambaum, Phys. Rev. D **100**, 063017 (2019).

Existing constraints



PHYSICAL REVIEW D **96,** 043017 (2017)

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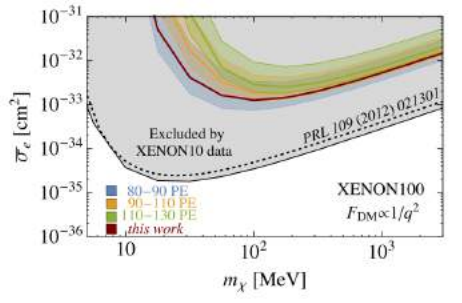
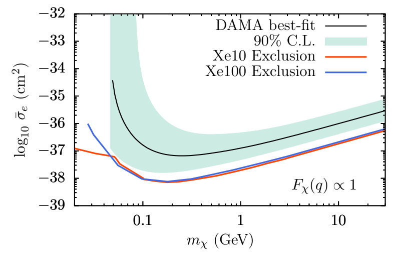
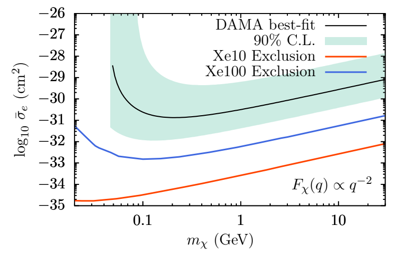


- Constraints from "S2"-only (just ionisations, no S1)
- Xe10 – 15 kg·days = 0.04 kg·yrs – finished 2011
- Xe100 – 30 kg·yrs – finished 2016
- Xe10: better constraints!?!

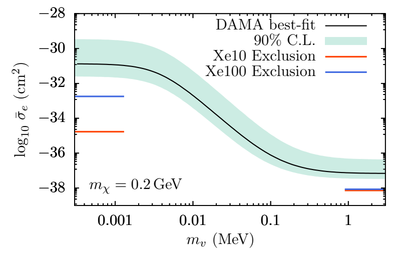
(— newer S2-only constraints coming from Xe1T)

Is DAMA electron-interacting DM? (No)

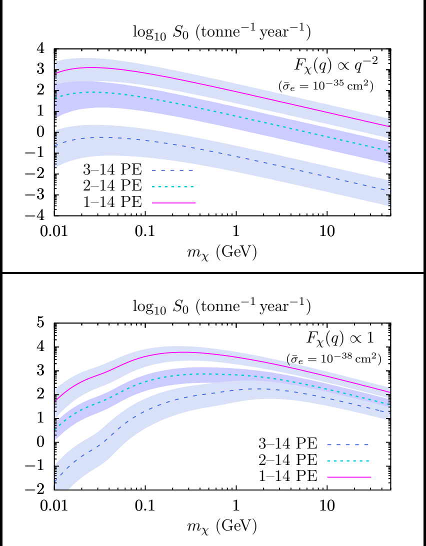




- Best-fit to 1-2 keV DAMA/LIBRA phase II
- Shaded green: 90% C.L.
- Ignore spectral fit
- Still: 100% excluded



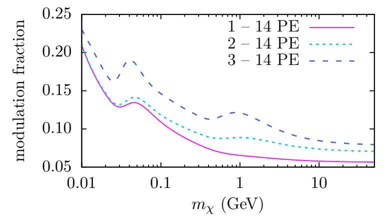
Looking forward: Xe1T



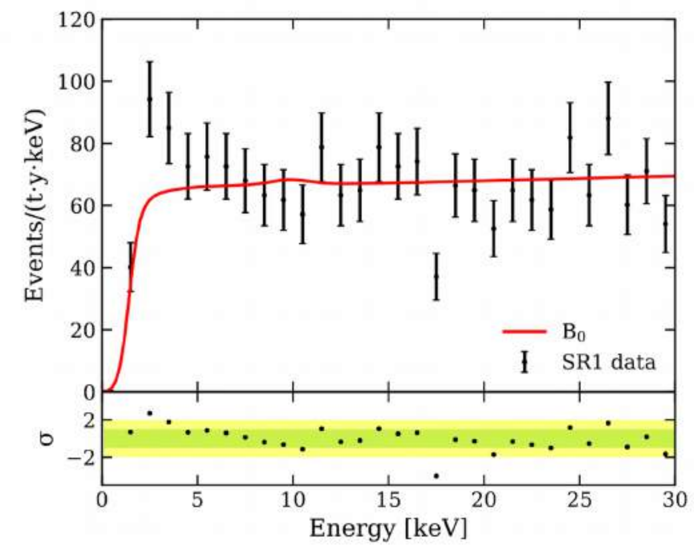
Potential rates

- Hypothetical event rates
- 1000kg Xe100-like detector
- for $\bar{\sigma}_e = 10^{-35}$ cm^2 – not excluded!

- Large Annual Modulation:∼10–20%



Xenon 1T excess



Phys. Rev. D 102, 072004 (2020)

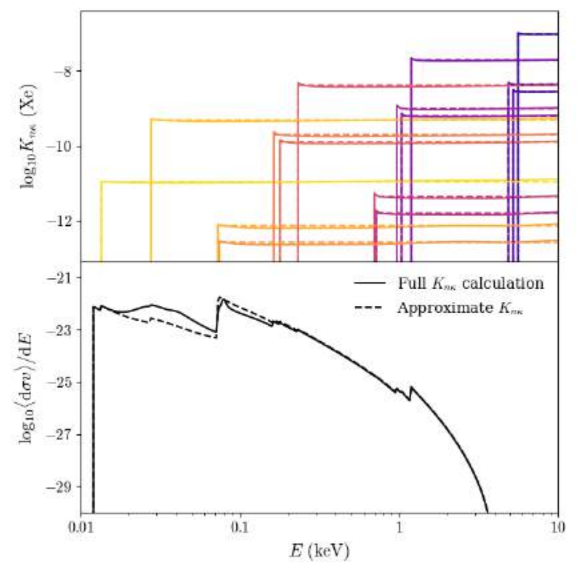
Tables of ionisation factors

- PhD Student: Ashlee Caddell

$$\left(T_k - \frac{Ze^2}{r} - \varepsilon\right)\psi = 0$$

- High p, low-r: $r \sim p^{-1} \sim 10^{-3} a_B$
- Low-r: $\frac{Ze^2}{r} \gg |\varepsilon|$
- At low r, ψ independent of ε
- Deepest shell always dominates
- Use 1D $K_n(q)$ instead of $K(E, q)$

$$K(E, q) = \sum_n K_n(q)\,\Theta(E - E_n)$$



Conclusion

- S1 (prompt scintillation signal) not very suppressed
- For heavy mediator, $m_\chi \gtrsim 0.1\,\text{GeV}$, $E_\text{thresh} \sim 0.5\,\text{keV}$ – no suppression
- S2 (ionization-only signal): good for placing constraints, not for detection
- Combined S1 and S2 possible for low-mass WIMPs – new discovery potential
- Tables of (mostly) model-independent ionisation factors made available
- Apply to your favourite DM model

Warnings

- Must use accurate atomic model for wavefunctions
- Highly dependent on modelling of low-energy detector response/resolution
- Highly velocity dependent: halo considerations more important than nuclear case