Leptophilic Dark Matter in Direct Detection Experiments and in the Sun

Joachim Kopp

Theoretical Physics Department, Fermilab

IDM 2010, 30 Jul 2010

in collaboration with Viviana Niro, Thomas Schwetz-Mangold and Jure Zupan
based on arXiv:0907.3159 (Phys. Rev. D **80** (2009) 083502)

Fermilab

Outline

1. Leptophilic Dark Matter

2. Signals of leptophilic WIMPs

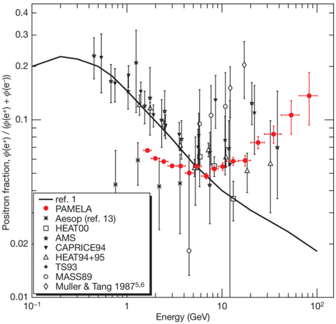
3. Fitting direct detection experiments

4. Leptophilic Dark Matter in the Sun

5. Conclusions

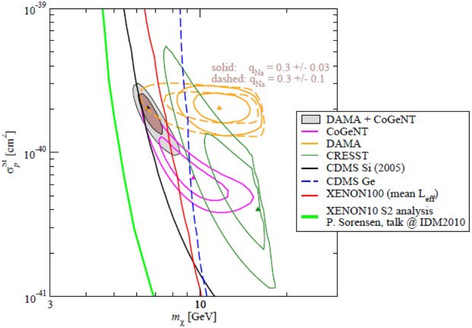
Outline

Why leptophilic Dark Matter?



Anomalies in cosmic e^+ and e^- fluxes (but not in $\bar{p}$ flux).

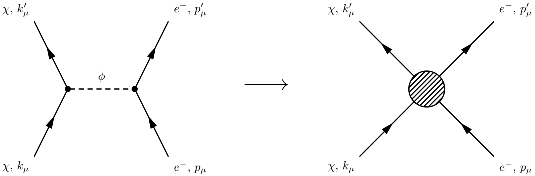
DM coupling predominantly to leptons?



Conflict between DAMA (electron & nuclear recoils) and other experiments (nuclear recoils only).

plots from PAMELA 0810.4995 + Thomas Schwetz' talk

Leptophilic DM formalism



$$\mathcal{L}_{\text{eff}} = \sum_i G\,(\bar\chi\Gamma^i_\chi\chi)\,(\bar\ell\Gamma^i_\ell\ell) \qquad \text{with} \qquad G = \frac{1}{\Lambda^2}$$

Possible Lorentz structures:

scalar/pseudoscalar:	$\Gamma_\chi = c^\chi_S + ic^\chi_P\gamma_5,$	$\Gamma_\ell = c^\ell_S + ic^\ell_P\gamma_5,$
vector/axial vector:	$\Gamma^\mu_\chi = (c^\chi_V + c^\chi_A\gamma_5)\gamma^\mu,$	$\Gamma_{\ell\mu} = (c^\ell_V + c^\ell_A\gamma_5)\gamma_\mu,$
tensor/axial tensor:	$\Gamma^{\mu\nu}_\chi = (c_T + ic_{AT}\gamma_5)\sigma^{\mu\nu},$	$\Gamma_{\ell\mu\nu} = \sigma_{\mu\nu},$

Only $S \otimes S$, $V \otimes V$, $A \otimes A$, $T \otimes T$ not velocity-suppressed → neglect others.

Leptophilic DM model: Fox Poppitz 0811.0399

Outline

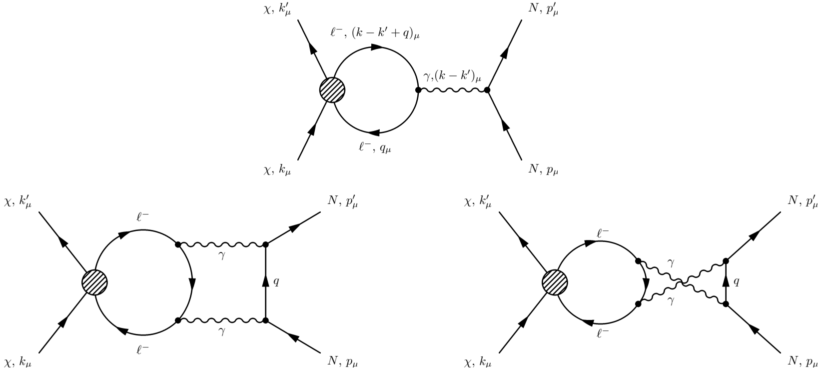
1. Leptophilic Dark Matter
2. **Signals of leptophilic WIMPs**
3. Fitting direct detection experiments
4. Leptophilic Dark Matter in the Sun
5. Conclusions

4 things a leptophilic WIMP can do in a detector

- Scattering on an electron
  - Outer-shell electrons can be kicked out (WIMP-electron scattering)
  - Inner-shell electrons will remain bound (elastic WIMP-atom scattering) → recoil transferred to nucleus
  - Electrons can be excited to an outer shell, but remain bound (inelastic WIMP-atom scattering) → recoil partly transferred to nucleus

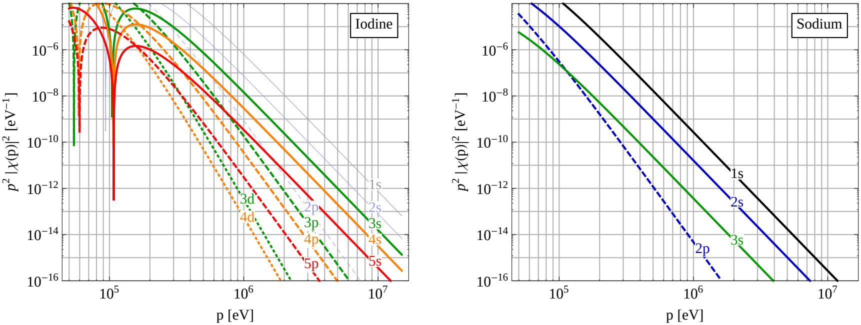
4 things a leptophilic WIMP can do in a detector

- Scattering on an electron
  - Outer-shell electrons can be kicked out (WIMP-electron scattering)
  - Inner-shell electrons will remain bound (elastic WIMP-atom scattering) → recoil transferred to nucleus
  - Electrons can be excited to an outer shell, but remain bound (inelastic WIMP-atom scattering) → recoil partly transferred to nucleus
- Loop-induced scattering on the nucleus



WIMP-electron scattering

- Bound electrons are in energy eigenstates, but not momentum eigenstates.
  → Include electron wave function $\chi_{nl}(p)$ in matrix element calculation
- For detectable recoil, need scattering on high-momentum tail of $\chi_{nl}(p)$

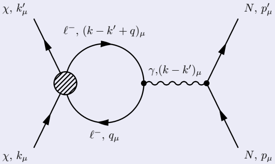


(approximate wave functions, neglecting relativistic corrections and multi-electron correlations)

Rate suppressed by $\frac{m_e}{m_N}$ (bound state kinematics) and by $|\chi_{nl}(p)|^2$ (wave function at $p \gtrsim 1$ MeV$/c$) compared to rate for "standard" nucleophilic WIMPs.

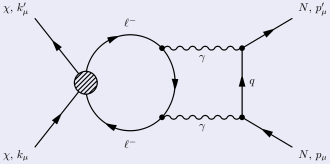
Loop-induced WIMP-nucleus scattering

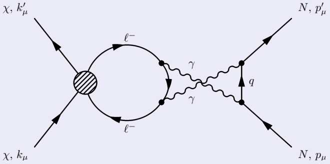
One-loop: Lowest order diagram for $V \otimes V$, $T \otimes T$



Rate suppressed by loop factor $\alpha Z/\pi$ compared to rate for "standard" nucleophilic WIMPs.
→ Loop-induced WIMP-nucleus scattering dominates when it is allowed.

Two-loop: Lowest order diagram for $S \otimes S$





$A \otimes A$ and $V \otimes V$ as representative cases

In the following, we will consider only

- $A \otimes A$ as an example for scenarios where WIMP-electron scattering dominates
- $V \otimes V$ as an example for scenarios where WIMP-nucleusn scattering dominates

All other Lorentz structures are phenomenologically equivalent to either $A \otimes A$ or $V \otimes V$.

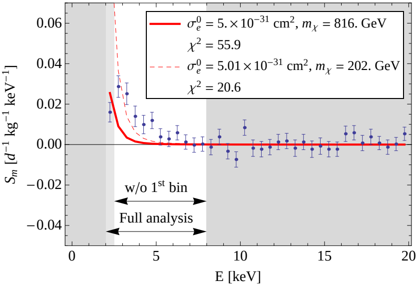
Outline

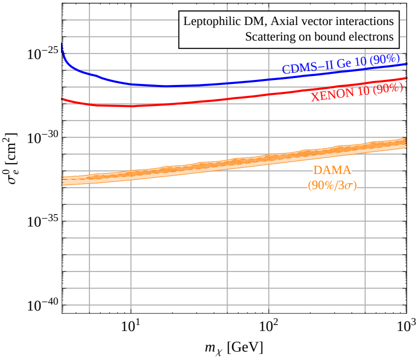
1. Leptophilic Dark Matter
2. Signals of leptophilic WIMPs
3. Fitting direct detection experiments
4. Leptophilic Dark Matter in the Sun
5. Conclusions

Annual modulation and *m*-σ exclusion plot for $A \otimes A$

(Dominated by WIMP-electron scattering)

Fit to DAMA modulation spectrum + total rates constraint



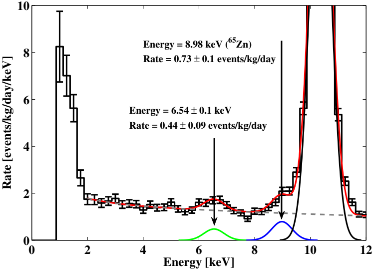


- Signal in DAMA from inelastic WIMP-electron scattering
- Signal in CDMS/XENON from inelastic WIMP-atom scattering
- $\Delta\chi^2$ fit formally yields allowed region, but poor quality of fit
- Required WIMP-electron cross sections very large → other constraints?

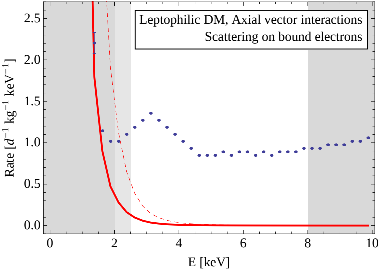
Conclusion: In the $A \otimes A$ case, leptophilic DM cannot explain DAMA

CDMS electron recoil analysis

CDMS data



DAMA, leptophilic DM, $A \otimes A$



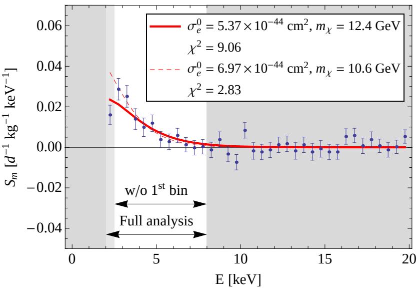
CDMS 0907.1438

e^- recoils in CDMS set tight constraint on $A \otimes A$ leptophilic DM.

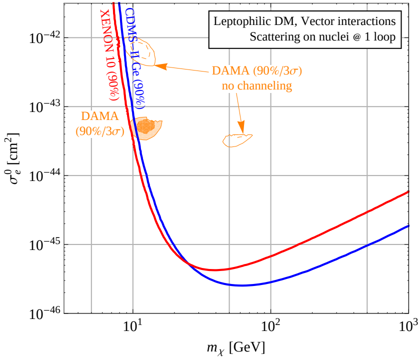
Assuming smooth background and Z^2 scaling of rate, the CDMS bound is close to the DAMA best fit, but does not rule it out yet.

Annual modulation and m-σ exclusion plot for $V \otimes V$

(Dominated by WIMP-nucleus scattering @ 1-loop)



Fit to DAMA modulation spectrum + total rates constraint



- Same spectrum as for conventional WIMPs
- Cannot explain the lowest DAMA bin
- Same situation as for conventional WIMPs:
  Conflict between DAMA and CDMS/XENON.

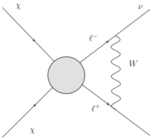
Conclusion: In the $V \otimes V$ case, leptophilic DM cannot explain DAMA

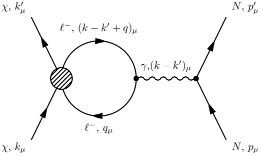
Outline

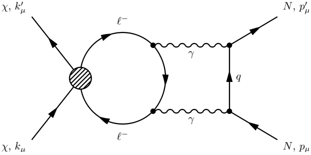
1. Leptophilic Dark Matter
2. Signals of leptophilic WIMPs
3. Fitting direct detection experiments
4. Leptophilic Dark Matter in the Sun
5. Conclusions

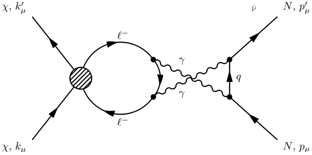
Scattering of leptophilic Dark Matter in the Sun

- Tree level scattering on *free* electrons
  → no suppression by wave function or atomic matrix elements
  → But energy loss in each scattering process is small since $m_e \ll m_\chi$.
  → Interesting feature: Strong temperature dependence
- Loop-induced scattering on heavy nuclei dominates if allowed (more efficient energy loss)
- Annihilation into neutrinos very likely in leptophilic models
  - $SU(2)$: Coupling to charged leptons accompanied by coupling to neutrinos (but: $SU(2)$ broken)
  - Loop level annihilation into neutrinos *unavoidable*
  - $V \otimes V$, $A \otimes V$, $T \otimes T$, $AT \otimes T$, $S \otimes S$, and $P \otimes S$: Loop level annihilation into all SM quarks and leptons







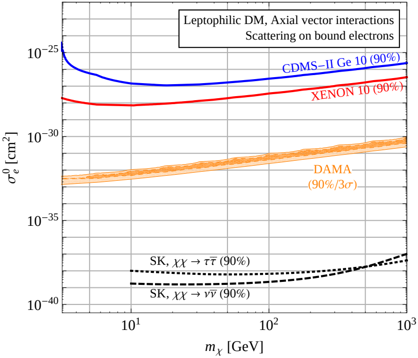


- One way to jeopardize interesting annihilation signals: χ-$\bar{\chi}$ asymmetry.

see e.g. Kaplan, Luty, Zurek, 0901.4117 for a recent work on asymmetric DM

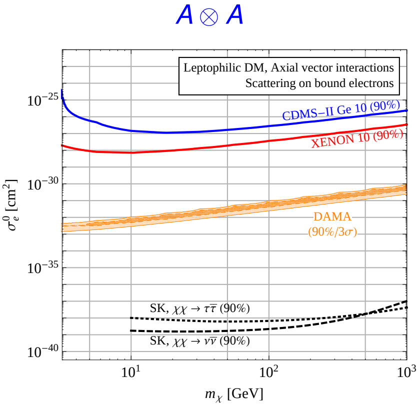
Resulting Super-K bounds

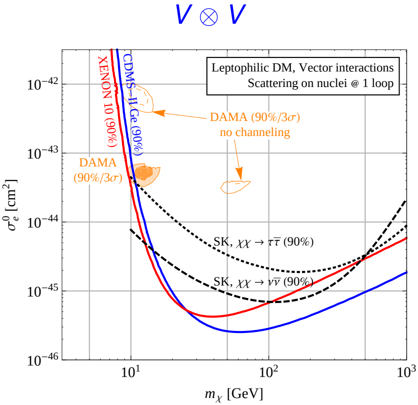
$A \otimes A$



- Super-K by far the most sensitive experiment
- Excludes DAMA-favored region

Resulting Super-K bounds





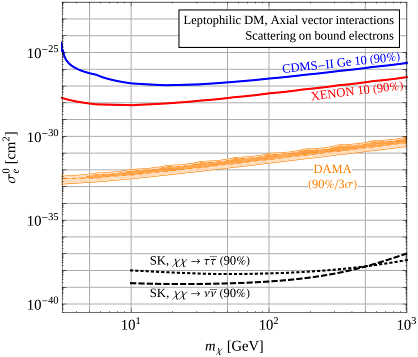
- Super-K by far the most sensitive experiment
- Excludes DAMA-favored region

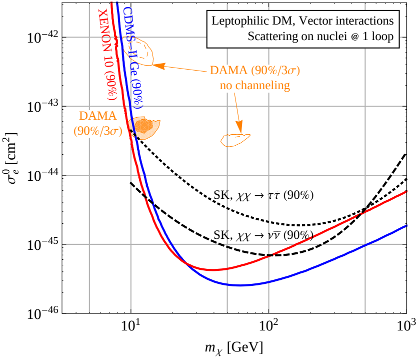
- Super-K competitive with CDMS/XENON
- Excludes DAMA-favored regions

Resulting Super-K bounds

$A \otimes A$

$V \otimes V$





- Super-K by far the most sensitive experiment
- Excludes DAMA-favored region

- Super-K competitive with CDMS/XENON
- Excludes DAMA-favored regions

but remember: Super-K not as model-independent as DAMA, CDMS, XENON

Outline

Summary

- Leptophilic Dark Matter is a well-motivated scenario

Summary

- Leptophilic Dark Matter is a well-motivated scenario
- Phenomenlogy of leptophilic Dark Matter in direct detection experiments
  - WIMP-electron scattering
    → strongly suppressed by smallness of e^- wave function at large p.
  - Elastic WIMP-atom scattering
    → Even stronger suppression from electronic matrix elements (sometimes completely absent due to cancellations)
  - Inelastic WIMP-atom scattering
    → Again, strong suppression from electronic matrix elements
  - WIMP-nucleus scattering → always dominant if allowed

Summary

- Leptophilic Dark Matter is a well-motivated scenario
- Phenomenlogy of leptophilic Dark Matter in direct detection experiments
  - WIMP-electron scattering
    → strongly suppressed by smallness of e^- wave function at large p.
  - Elastic WIMP-atom scattering
    → Even stronger suppression from electronic matrix elements (sometimes completely absent due to cancellations)
  - Inelastic WIMP-atom scattering
    → Again, strong suppression from electronic matrix elements
  - WIMP-nucleus scattering → always dominant if allowed
  - Result: Leptophilic DM constrained by CDMS, XENON
  - Cannot explain DAMA

Summary

- Leptophilic Dark Matter is a well-motivated scenario
- Phenomenlogy of leptophilic Dark Matter in direct detection experiments
  - WIMP-electron scattering
→ strongly suppressed by smallness of e^- wave function at large p.
  - Elastic WIMP-atom scattering
→ Even stronger suppression from electronic matrix elements (sometimes completely absent due to cancellations)
  - Inelastic WIMP-atom scattering
→ Again, strong suppression from electronic matrix elements
  - WIMP-nucleus scattering → always dominant if allowed
  - Result: Leptophilic DM constrained by CDMS, XENON
  - Cannot explain DAMA
- Leptophilic Dark Matter in the Sun
  - Neutrino signals almost unavoidable (except if there is a χ-$\bar{\chi}$ asymmetry)
  - Strong bounds from Super-K.

Thank you!

A leptophilic Dark Matter model

- $U(1)_{DS}$ dark sector
- Dark Matter is a Dirac fermion charged under $U(1)_{DS}$

$$\mathcal{L}_{DS} = -\frac{1}{4}F'^{2}_{\mu\nu} + \overline{\chi}\gamma^{\mu}D_{\mu}\chi + |D_{\mu}\phi|^{2} - M_{\chi}\overline{\chi}\chi - V_{DS}(\phi)\ .$$

- At least some SM leptons have small couplings to $U(1)_{DS}$.
- $U(1)_{DS}$ exchange provides Sommerfeld enhancement

Fox, Poppitz, 0811.0399

Phenomenology of different Lorentz structures

$\Gamma_\chi \otimes \Gamma_\ell$	$\sigma(\chi e \to \chi e)/\sigma^0_{\chi e}$
$S \otimes S$	1
$S \otimes P$	$\mathcal{O}(v^2)$
$P \otimes S$	$\mathcal{O}(v^2 m_e^2/m_\chi^2)$
$P \otimes P$	$\mathcal{O}(v^4 m_e^2/m_\chi^2)$
$V \otimes V$	1
$V \otimes A$	$\mathcal{O}(v^2)$
$A \otimes V$	$\mathcal{O}(v^2)$
$A \otimes A$	3
$T \otimes T$	12
$AT \otimes T$	$\mathcal{O}(v^2)$

Suppression factors:

v	WIMP velocity ($\mathcal{O}(10^{-3})$)
m_e/m_χ	Ratio of electron mass to WIMP mass (unique to leptophilic DM!)

see also: Momentum-dependent WIMP scattering: Chang, Pierce, Weiner, 0908.3192

Rate for WIMP-electron scattering

(Leptophilic DM, $A \otimes A$ interactions)

$$\frac{dR^{\text{WES}}}{dE_d} \simeq \frac{3\rho_0 G^2}{4\pi m_\chi} \frac{m_e}{m_N} \sum_{nl} \sqrt{2m_e(E_d - E_{B,nl})}\,(2l+1) \int \frac{dp\,p}{(2\pi)^3}\, |\chi_{nl}(p)|^2\, I(v_{\text{min}}^{\text{WES}})$$

where

$$I(v_{\text{min}}^{\text{WES}}) \equiv \int d^3v\, \frac{f_\oplus(\vec{v})}{v}\, \theta(v - v_{\text{min}}^{\text{WES}})\,, \qquad v_{\text{min}}^{\text{WES}} \approx \frac{E_d}{p} + \frac{p}{2m_\chi}$$

Rate for WIMP-electron scattering
(Leptophilic DM, $A \otimes A$ interactions)

$$\frac{dR^{\mathrm{WES}}}{dE_d} \simeq \frac{3\rho_0 G^2}{4\pi m_\chi} \frac{m_e}{m_N} \sum_{nl} \sqrt{2m_e(E_d - E_{B,nl})}\,(2l+1) \int \frac{dp\,p}{(2\pi)^3} \, |\chi_{nl}(p)|^2 \, I(v_{\min}^{\mathrm{WES}})$$

where

$$I(v_{\min}^{\mathrm{WES}}) \equiv \int d^3v \, \frac{f_\oplus(\vec{v})}{v} \, \theta(v - v_{\min}^{\mathrm{WES}}) \,, \qquad v_{\min}^{\mathrm{WES}} \approx \frac{E_d}{p} + \frac{p}{2m_\chi}$$

Compare to the formula for standard WIMPs:

$$\frac{dR^0}{dE_d} \simeq \frac{3\rho_0 G^2}{2\pi m_\chi} \, I(v_{\min}^0) \qquad \text{with} \qquad v_{\min}^0 = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2m_N}}$$

Rate for loop-induced WIMP-nucleus scattering

($V \otimes V$ case, one loop)

$$\frac{dR^{\text{WNS}}}{dE_d} = \frac{\rho_0 G^2}{18\pi\, m_\chi} \left(\frac{\alpha Z}{\pi} \right)^2 F^2(q) \left[\log \left(\frac{m_\ell^2}{\mu^2} \right) \right]^2 I(v_{\text{min}}^{\text{WNS}}) \,,$$

where

$$v_{\text{min}}^{\text{WNS}} = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2 m_N}}$$

Rate for loop-induced WIMP-nucleus scattering

($V \otimes V$ case, one loop)

$$\frac{dR^{\mathrm{WNS}}}{dE_d} = \frac{\rho_0 G^2}{18\pi\, m_\chi} \left(\frac{\alpha Z}{\pi}\right)^2 F^2(q) \left[\log\left(\frac{m_\ell^2}{\mu^2}\right)\right]^2 I(v_{\mathrm{min}}^{\mathrm{WNS}}),$$

where

$$v_{\mathrm{min}}^{\mathrm{WNS}} = \frac{m_\chi + m_N}{m_\chi}\sqrt{\frac{E_d}{2m_N}}$$

Compare to the formula for standard WIMPs:

$$\frac{dR^0}{dE_d} \simeq \frac{3\rho_0 G^2}{2\pi m_\chi} I(v_{\mathrm{min}}^0) \qquad \text{with} \qquad v_{\mathrm{min}}^0 = \frac{m_\chi + m_N}{m_\chi}\sqrt{\frac{E_d}{2m_N}}$$

Rate for loop-induced WIMP-nucleus scattering

($V \otimes V$ case, one loop)

$$\frac{dR^{\rm WNS}}{dE_d} = \frac{\rho_0 G^2}{18\pi\, m_\chi} \left(\frac{\alpha Z}{\pi}\right)^2 F^2(q) \left[\log\left(\frac{m_\ell^2}{\mu^2}\right)\right]^2 I(v_{\rm min}^{\rm WNS}),$$

where

$$v_{\rm min}^{\rm WNS} = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2 m_N}}$$

Compare to the formula for standard WIMPs:

$$\frac{dR^0}{dE_d} \simeq \frac{3\rho_0 G^2}{2\pi m_\chi}\, I(v_{\rm min}^0) \qquad \text{with} \qquad v_{\rm min}^0 = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2 m_N}}$$

→ Suppressed only by α^2

→ Loop-induced scattering on the nucleus will dominate whenever it is allowed!

Elastic WIMP-atom scattering

- Coherent scattering on all electrons
- Depends on atomic form factor, computable from the electron wave functions.

Rate for elastic WIMP-atom scattering

($A \otimes A$ case)

$$\frac{dR^{\rm WAS-el}}{dE_d} = \frac{3\rho_0 G^2}{2\pi\, m_\chi} \Big| \sum_{nlms} \langle nlms | e^{i(\vec{k}-\vec{k}')\vec{x}} | nlms \rangle \Big|^2 \, I(v_{\rm min}^{\rm WAS-el}) \,,$$

where

$$v_{\rm min}^{\rm WAS-el} = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2m_N}}$$

Rate for elastic WIMP-atom scattering

($A \otimes A$ case)

$$\frac{dR^{\mathrm{WAS-el}}}{dE_d} = \frac{3\rho_0 G^2}{2\pi\, m_\chi} \left| \sum_{nlms} \langle nlms | e^{i(\vec{k}-\vec{k'})\vec{x}} | nlms \rangle \right|^2 I(v_{\mathrm{min}}^{\mathrm{WAS-el}})\,,$$

where

$$v_{\mathrm{min}}^{\mathrm{WAS-el}} = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2m_N}}$$

Compare to the formula for standard WIMPs:

$$\frac{dR^0}{dE_d} \simeq \frac{3\rho_0 G^2}{2\pi m_\chi} I(v_{\mathrm{min}}^0) \qquad \text{with} \qquad v_{\mathrm{min}}^0 = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2m_N}}$$

Rate for elastic WIMP-atom scattering

($A \otimes A$ case)

$$\frac{dR^{\mathrm{WAS-el}}}{dE_d} = \frac{3\rho_0 G^2}{2\pi\, m_\chi} \Big| \sum_{nlms} \langle nlms | e^{i(\vec{k}-\vec{k'})\vec{x}} | nlms \rangle \Big|^2 \, I(v_{\mathrm{min}}^{\mathrm{WAS-el}}) \,,$$

where

$$v_{\mathrm{min}}^{\mathrm{WAS-el}} = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2 m_N}}$$

Compare to the formula for standard WIMPs:

$$\frac{dR^0}{dE_d} \simeq \frac{3\rho_0 G^2}{2\pi m_\chi} \, I(v_{\mathrm{min}}^0) \qquad \text{with} \qquad v_{\mathrm{min}}^0 = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2 m_N}}$$

→ Suppression by smallnes of matrix elements $\langle nlms | e^{i(\vec{k}-\vec{k'})\vec{x}} | nlms \rangle$ at large $|\vec{k} - \vec{k'}|$ (as required for $E_d \sim$ keV)

Rate for elastic WIMP-atom scattering

($A \otimes A$ case)

$$\frac{dR^{\mathrm{WAS-el}}}{dE_d} = \frac{3\rho_0 G^2}{2\pi\, m_\chi} \left| \sum_{nlms} \langle nlms | e^{i(\vec{k}-\vec{k'})\vec{x}} | nlms \rangle \right|^2 I(v_{\mathrm{min}}^{\mathrm{WAS-el}}) \,,$$

where

$$v_{\mathrm{min}}^{\mathrm{WAS-el}} = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2m_N}}$$

Compare to the formula for standard WIMPs:

$$\frac{dR^0}{dE_d} \simeq \frac{3\rho_0 G^2}{2\pi m_\chi} I(v_{\mathrm{min}}^0) \qquad \text{with} \qquad v_{\mathrm{min}}^0 = \frac{m_\chi + m_N}{m_\chi} \sqrt{\frac{E_d}{2m_N}}$$

→ Suppression by smallnes of matrix elements $\langle nlms | e^{i(\vec{k}-\vec{k'})\vec{x}} | nlms \rangle$ at large $|\vec{k} - \vec{k'}|$ (as required for $E_d \sim$ keV)

→ For the $A \otimes A$ case, $\sum_s \bar{u}_e^s \gamma^\mu \gamma^5 u_e^s$ vanishes

Inelastic WIMP-atom scattering

- Electrons contribute incoherently
- Requires computation of electron transition matrix elements

Rate for inelastic WIMP-atom scattering

($A \otimes A$ case)

$$\frac{dR^{\mathrm{WAS-in}}}{dE_d} = \frac{3\rho_0 G^2}{2\pi\, m_\chi} \sum_{nlm} \sum_{n'l'm'} |\langle n'l'm'| e^{i(\vec{k}-\vec{k'})\vec{x}} |nlm\rangle|^2 \, I(v_{\mathrm{min}}^{\mathrm{WAS-in}})\,,$$

where

$$v_{\mathrm{min}}^{\mathrm{WAS-in}} = \frac{E_d(m_\chi + m_N) - m_N \delta E_B}{m_\chi \sqrt{2 m_N (E_d - \delta E_B)}}\,,$$

Rate for inelastic WIMP-atom scattering

($A \otimes A$ case)

$$\frac{dR^{\mathrm{WAS-in}}}{dE_d} = \frac{3\rho_0 G^2}{2\pi\, m_\chi} \sum_{nlm} \sum_{n'\,l'\,m'} |\langle n'\,l'\,m'|e^{i(\vec{k}-\vec{k'})\vec{x}}|nlm\rangle|^2\; I(v_{\mathrm{min}}^{\mathrm{WAS-in}})\,,$$

where

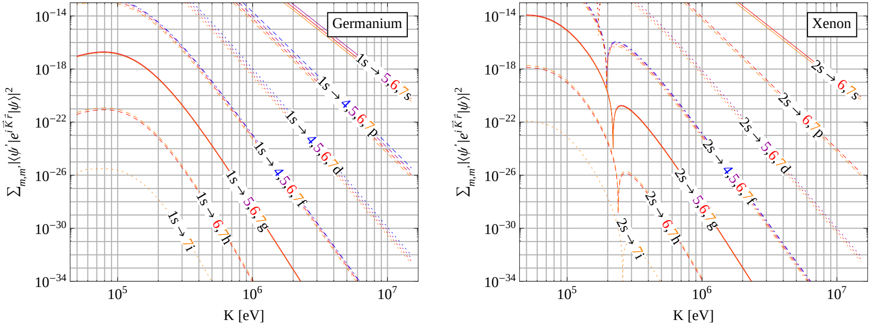
$$v_{\mathrm{min}}^{\mathrm{WAS-in}} = \frac{E_d(m_\chi + m_N) - m_N \delta E_B}{m_\chi \sqrt{2m_N(E_d - \delta E_B)}}\,,$$

Compare to the formula for standard WIMPs:

$$\frac{dR^0}{dE_d} \simeq \frac{3\rho_0 G^2}{2\pi m_\chi}\, I(v_{\mathrm{min}}^0) \qquad \text{with} \qquad v_{\mathrm{min}}^0 = \frac{m_\chi + m_N}{m_\chi}\sqrt{\frac{E_d}{2m_N}}$$

Discussion of inelastic WIMP-atom scattering

- Supression due to smallness of matrix elements $\langle n' l' m' | e^{i(\vec{k}-\vec{k'})\vec{x}} | nlm \rangle$ at large $|\vec{k}-\vec{k'}|$ (as required for $E_d \sim$ keV)



Computation of matrix elements $\langle n' l' m' | e^{i\vec{K}\vec{x}} | nlm \rangle$

- Expand $e^{i\vec{K}\vec{x}}$ in spherical harmonics and carry out angular integration:

$$\begin{aligned}\langle n' l' m' | e^{i\vec{K}\vec{x}} | nlm \rangle = 4\pi \int dr\, r^2 R_{nl}(r)\, R_{n'l'}(r) \sum_{L,M} j_L(Kr)\, Y_{LM}(\theta_K, \phi_K) \\ \times \frac{(-1)^m}{\sqrt{4\pi}} \sqrt{(2l+1)(2l'+1)(2L+1)} \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & L \\ m & m' & M \end{pmatrix}\end{aligned}$$

Computation of matrix elements $\langle n' l' m' | e^{i\vec{K}\vec{x}} | nlm \rangle$

- Expand $e^{i\vec{K}\vec{x}}$ in spherical harmonics and carry out angular integration:

$$\langle n' l' m' | e^{i\vec{K}\vec{x}} | nlm \rangle = 4\pi \int dr\, r^2 R_{nl}(r)\, R_{n'l'}(r) \sum_{L,M} j_L(Kr)\, Y_{LM}(\theta_K, \phi_K)$$

$$\times \frac{(-1)^m}{\sqrt{4\pi}} \sqrt{(2l+1)(2l'+1)(2L+1)} \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & L \\ m & m' & M \end{pmatrix}$$

- Square this and use properties of Wigner-3j symbols

$$\sum_{mm'} \left| \langle n' l' m' | e^{i\vec{K}\vec{x}} | nlm \rangle \right|^2 = (2l+1)(2l'+1) \sum_L (2L+1) \left[\begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \right]^2$$

$$\times \left[\int dr\, r^2 R_{nl}(r)\, R_{n'l'}(r) j_L(Kr) \right]^2$$

Computation of matrix elements $\langle n'l'm'|e^{i\vec{K}\vec{x}}|nlm\rangle$

- Expand $e^{i\vec{K}\vec{x}}$ in spherical harmonics and carry out angular integration:

$$\langle n'l'm'|e^{i\vec{K}\vec{x}}|nlm\rangle = 4\pi \int dr\, r^2 R_{nl}(r)\, R_{n'l'}(r) \sum_{L,M} j_L(Kr)\, Y_{LM}(\theta_K, \phi_K) \times \frac{(-1)^m}{\sqrt{4\pi}} \sqrt{(2l+1)(2l'+1)(2L+1)} \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & L \\ m & m' & M \end{pmatrix}$$

- Square this and use properties of Wigner-3j symbols

$$\sum_{mm'} \left| \langle n'l'm'|e^{i\vec{K}\vec{x}}|nlm\rangle \right|^2 = (2l+1)(2l'+1) \sum_L (2L+1) \left[\begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \right]^2 \times \left[\int dr\, r^2 R_{nl}(r)\, R_{n'l'}(r) j_L(Kr) \right]^2$$

- Numerically tricky, but OK if done carefully (spherical Bessel transform)

Spherical Bessel transform: Sharafeddin et al., J. Comput. Phys. **100** (1992) 294
Radial wave functions $R_{nl}(r)$ taken from Bunge, Barrientos, Atom. Dat. Nucl. Dat. Tab. **53** (1993) 113