

Extended Calculation of Dark Matter-Electron Scattering in Crystal Targets

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References:

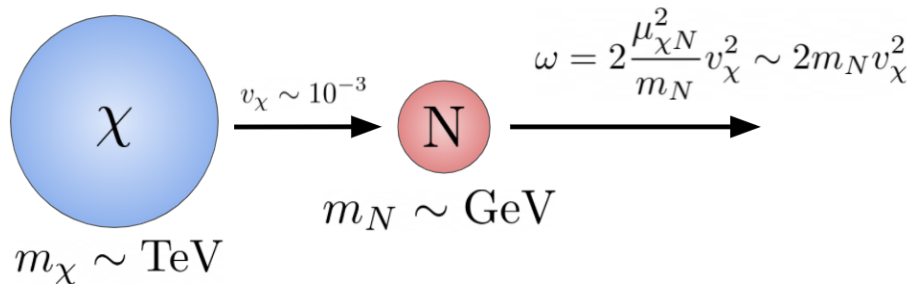
- [arXiv:2105.05253](https://arxiv.org/abs/2105.05253): Extended Calculation of Dark Matter-Electron Scattering in Crystal Targets

Outline

- 1 DM-Electron Scattering Overview
- 2 All Electron Reconstruction Effects
- 3 Core → Conduction Contributions
- 4 Summary

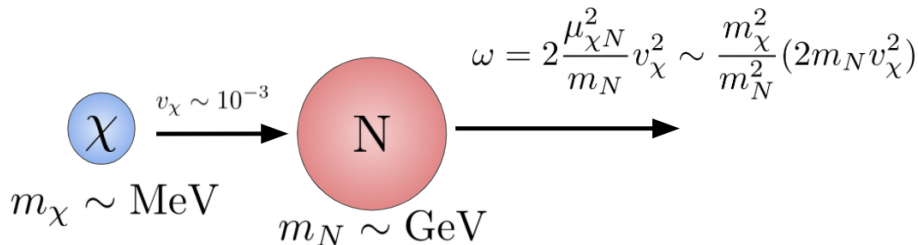
Direct Detection of Sub-GeV Dark Matter via e^- Kinematics

Nuclear recoil is great at searching for WIMPs.



Direct Detection of Sub-GeV Dark Matter via e^- Kinematics

However for light DM, nuclei are too heavy,



need to scatter off a lighter target, e.g. e^- .

Or more novel states such as phonons, polaritons, or magnons; see Refs. [arXiv:2102.09567](https://arxiv.org/abs/2102.09567), [arXiv:2009.13534](https://arxiv.org/abs/2009.13534), [arXiv:2005.10256](https://arxiv.org/abs/2005.10256), [arXiv:1910.08092](https://arxiv.org/abs/1910.08092), [arXiv:1910.10716](https://arxiv.org/abs/1910.10716), [arXiv:1905.13744](https://arxiv.org/abs/1905.13744).

Direct Detection of Sub-GeV Dark Matter via e^-

Experiments

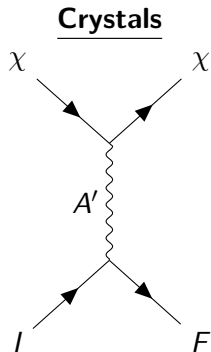
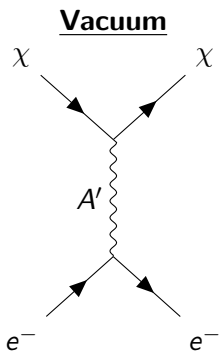
There is a **large** ongoing experimental program searching for DM-electron interactions:

- DAMIC - Si
- EDELWEISS - Ge
- SENSEI - Si
- SuperCDMS - Si and Ge



Important to have accurate theoretical predictions for DM-electron scattering rates to detect/constrain DM!

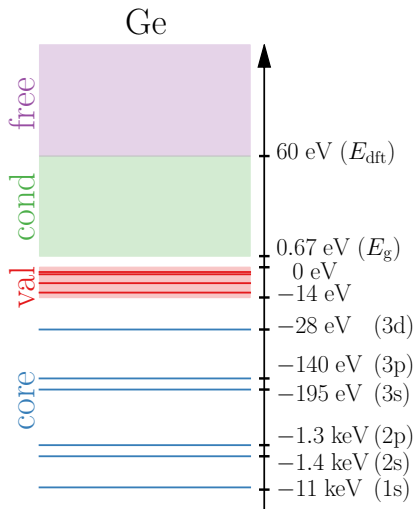
DM-Electron Scattering in Vacuum vs. Crystals



$$R = \frac{\rho_\chi}{8\rho_T V m_e^2 m_\chi^3} \sum_{I,F} \int \frac{d^3 q}{(2\pi)^3} g(\mathbf{q}, E_F - E_I) \left| \int \frac{d^3 k}{(2\pi)^3} \mathcal{M}_{\text{free}} \tilde{\psi}_F^*(\mathbf{k} + \mathbf{q}) \tilde{\psi}_I(\mathbf{k}) \right|^2$$

$$g(\mathbf{q}, \omega) = \int d^3 v f_\chi(\mathbf{v}; \mathbf{v}_e(t)) \delta(\omega - \omega_{\mathbf{q}})$$

Calculation Setup

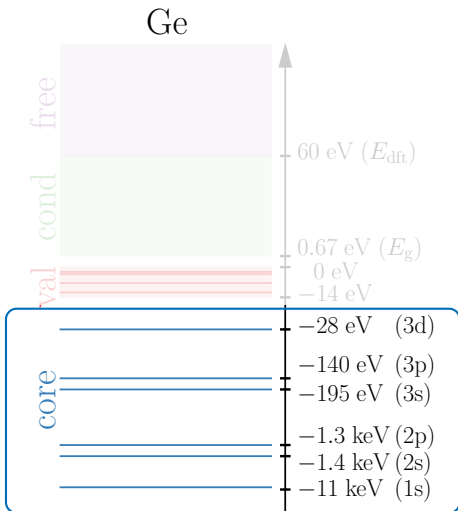


We extend the scattering rate calculation by including more states below the valence bands, and above the conduction bands.

- Most previous calculations focused on valence → conduction transitions.

Calculation Setup

Semi-analytic core states

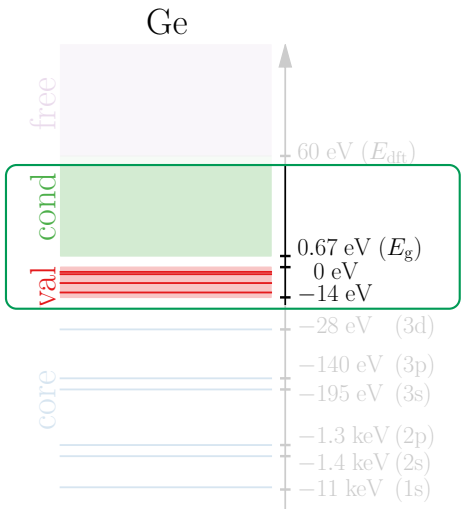


- Core electrons are tightly bound to the ionic sites, and less affected by the lattice environment.
- Wave functions are eigenstates of isolated atom Hamiltonians.
- Modelled **semi-analytically** with a linear combination of analytic functions.^a

^aSlater type orbitals (STO); common in atomic ionization calculations.

Calculation Setup

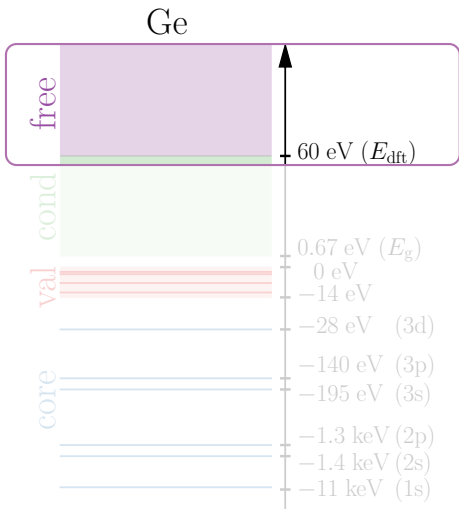
Valence and conduction states



- Valence e^- not bound to ionic cores (participate in bonding).
- Details of the band structure are important.
- Wave functions and energies calculated **numerically** using density functional theory (DFT).

Calculation Setup

Free states



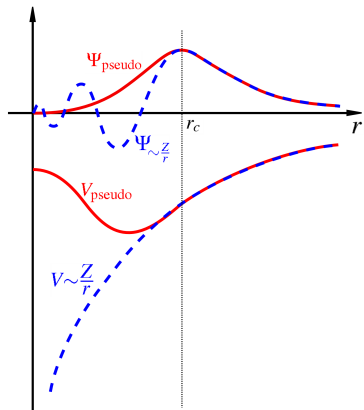
- Far from the band gap electrons are treated as **free** plane waves.

$$\psi \sim e^{i\mathbf{p}\cdot\mathbf{x}}$$

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DFT calculations typically use a 'pseudopotential' approximation to solve for the wave functions



Pros

Focus on large r (small q) simplifies calculations.

Cons

Solution is not the complete wave function!

<https://en.wikipedia.org/wiki/Pseudopotential>

Certain DFT methods can add the high momentum contributions back in

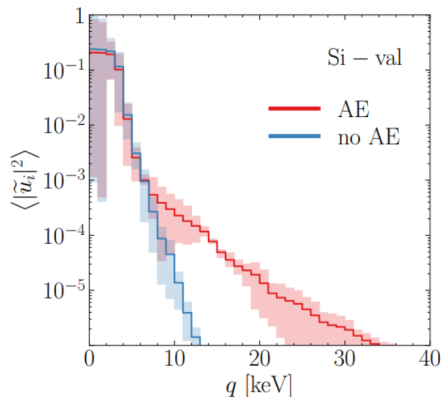
Projector Augmented Wave (PAW) Method

$$|\Psi_i^{\text{AE}}\rangle = \left(1 + \sum_j \left(|\phi_j^{\text{AE}}\rangle - |\phi_j^{\text{PS}}\rangle \right) \langle p_j | \right) |\Psi_i^{\text{PS}}\rangle$$

- 'All electron'/complete wave function (low q + high q)
- High q PS \leftrightarrow high q AE
- 'Pseudo' wave functions (low q), output of most DFT calculations

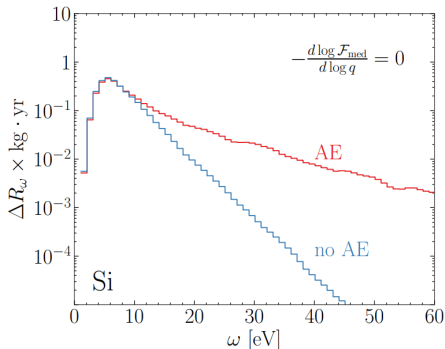
See Ref. [arXiv:0910.1921](https://arxiv.org/abs/0910.1921) for more details.

High q contributions can significantly affect the scattering rate



$\tilde{u} \sim$ Fourier components of wave function.

See also Ref. [arXiv:1810.13394](https://arxiv.org/abs/1810.13394) which discusses this effect.

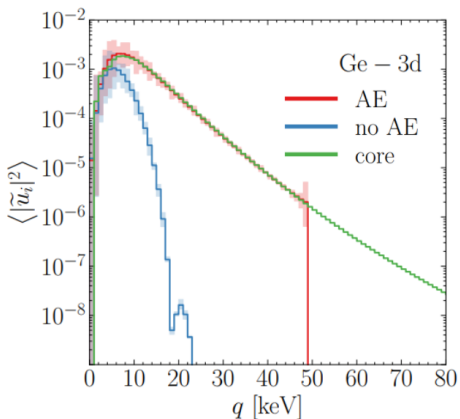


ΔR_ω - rate per kg-year between ω and $\omega + \Delta\omega$.

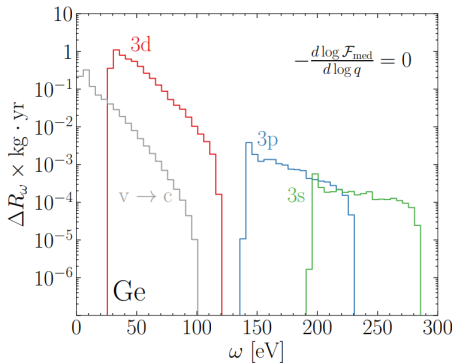
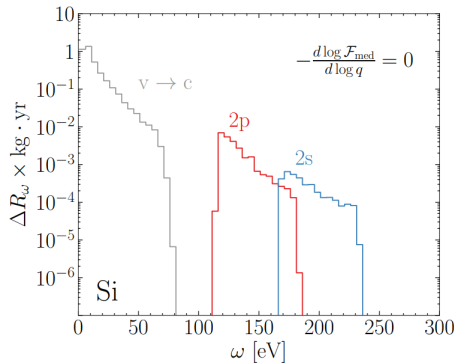
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3d electrons in Ge



- Example of how ‘core’ approximation is verified.
- Note that we only see agreement in the wave functions **after** the AE reconstruction is implemented.

Core \rightarrow conduction contributions can be dominant

- For a heavy mediator, 3d electrons in Ge dominate scattering rate even at low threshold.
- Transitions from 2p states in Si can be important for larger experimental thresholds.

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Summary

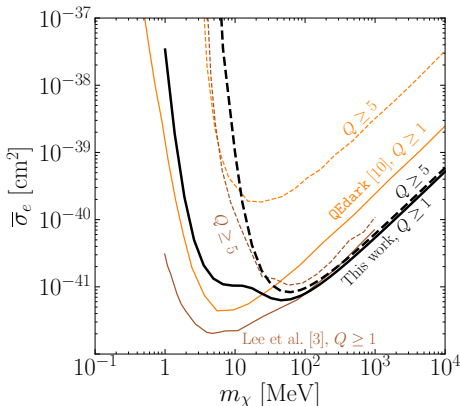
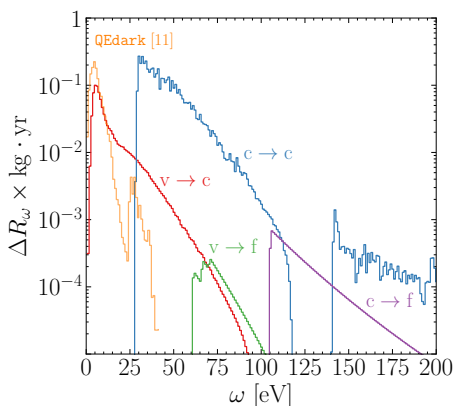
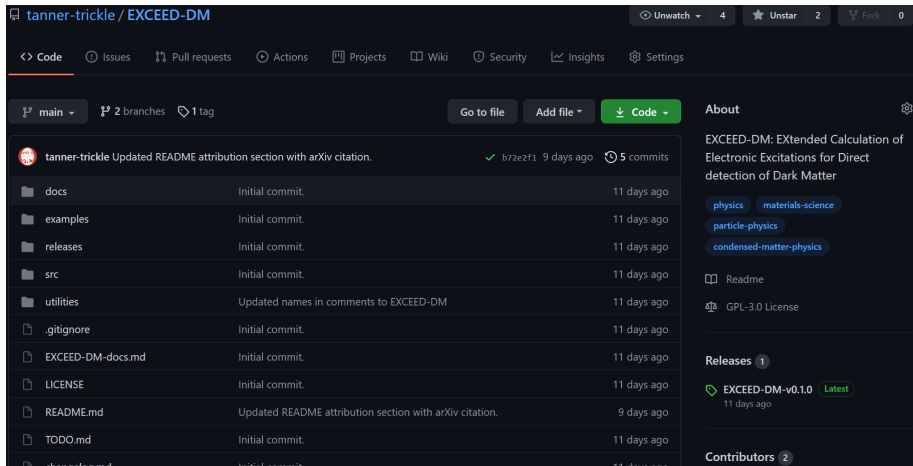


Figure: Ge target, heavy mediator, kg-year exposure, no backgrounds. Refs: QEdark [arXiv:1509.01598](https://arxiv.org/abs/1509.01598)+[arXiv:1607.01009](https://arxiv.org/abs/1607.01009), Lee et al. [arXiv:1508.07361](https://arxiv.org/abs/1508.07361).

Conclusion

- Extended DM-electron scattering rate calculation to include **core** → **conduction**, **core** → **free** and **valence** → **free** transitions.
- High q components of the wave functions can change detection prospects by orders of magnitude for heavy ($m_{A'} \gg m_\chi v_\chi$) mediator models/higher thresholds.
- Foundation for more general DM-electron scattering: general target, general DM-electron interactions, modulation signals (daily/annual), DFT calculator independent.
 - [Input](#) wave functions and [output](#) binned rates are publicly available.
 - EXCEED-DM: EXtended Calculation of Electronic Excitations for Direct detection of Dark Matter (beta version) is publicly available [here](#).

EXCEED-DM: Check out the project on !



The screenshot shows the GitHub repository page for `tanner-trickle / EXCEED-DM`. The repository is currently on the `main` branch, with 2 other branches and 1 tag. The repository has 4 unwatchers, 2 unstars, and 0 forks. The navigation bar includes links for Code, Issues, Pull requests, Actions, Projects, Wiki, Security, Insights, and Settings.

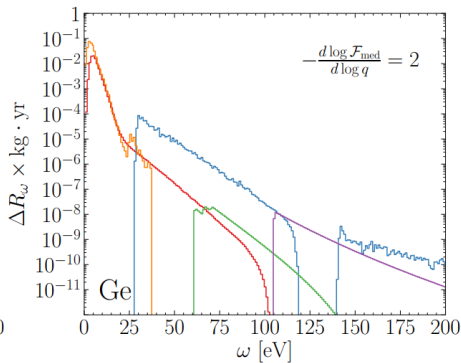
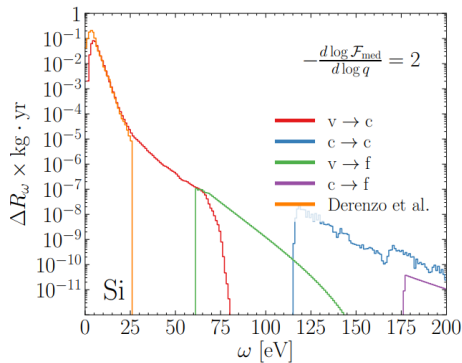
The commit history shows the following files and their commit details:

File	Commit Message	Commit Hash	Time Ago	Commits
docs	Initial commit.	b72e2f1	11 days ago	5
examples	Initial commit.		11 days ago	
releases	Initial commit.		11 days ago	
src	Initial commit.		11 days ago	
utilities	Updated names in comments to EXCEED-DM		11 days ago	
.gitignore	Initial commit.		11 days ago	
EXCEED-DM-docs.md	Initial commit.		11 days ago	
LICENSE	Initial commit.		11 days ago	
README.md	Updated README attribution section with arXiv citation.		9 days ago	
TODO.md	Initial commit.		11 days ago	
CHANGELOG.md	Initial commit.		11 days ago	

The repository description is: EXCEED-DM: Extended Calculation of Electronic Excitations for Direct detection of Dark Matter. It includes tags for `physics`, `materials-science`, `particle-physics`, and `condensed-matter-physics`. The repository has a Readme, a GPL-3.0 License, 1 release (EXCEED-DM-v0.1.0, Latest, 11 days ago), and 2 contributors.

<https://github.com/tanner-trickle/EXCEED-DM>

Light Mediator Comparison



In-Medium Screening Effects

