Extended Calculation of Dark Matter-Electron Scattering in Crystal Targets

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References:

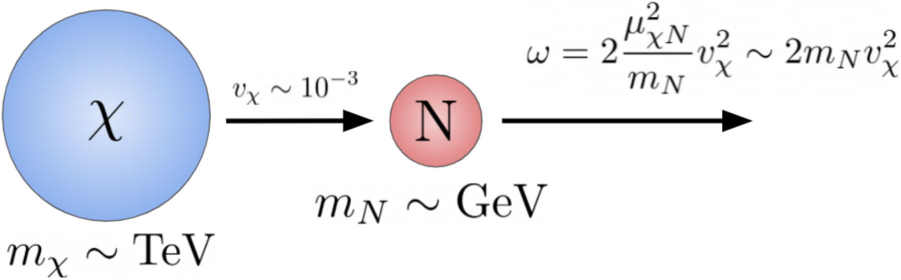
- arXiv:2105.05253: Extended Calculation of Dark Matter-Electron Scattering in Crystal Targets

Outline

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

Kinematics

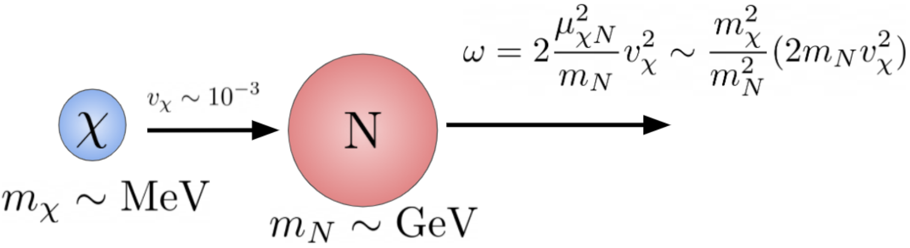
Nuclear recoil is great at searching for WIMPs.



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, arXiv:2009.13534, arXiv:2005.10256, arXiv:1910.08092, arXiv:1910.10716,arXiv:1905.13744.

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

Experiments

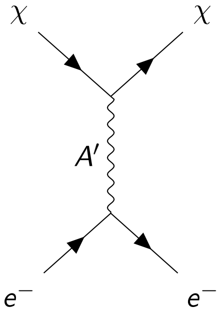
There is a **large** ongoing experimental program searching for DM-electron interactions:

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

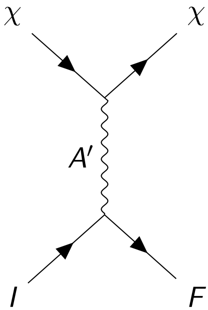
Important to have accurate theoretical predictions for DM-electron scattering rates to detect/constrain DM!

DM-Electron Scattering in Vacuum vs. Crystals

Vacuum



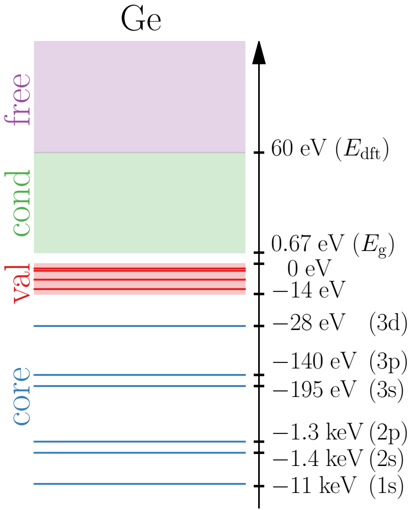
Crystals



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

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

Calculation Setup

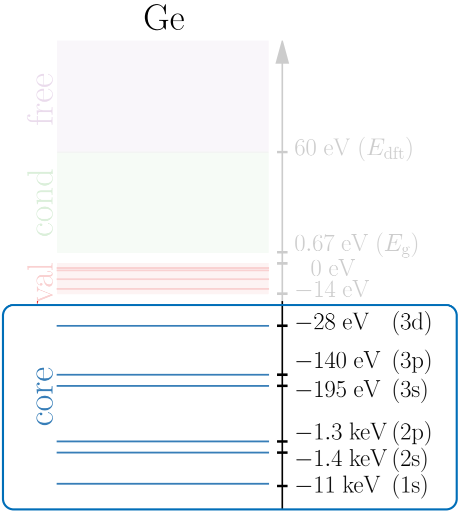


We extend the scattering rate calculation by including more states below the valence bands, and above the conduction bands.

- Most previous calculations focused on valence → conduction transitions.

Calculation Setup

Semi-analytic core states

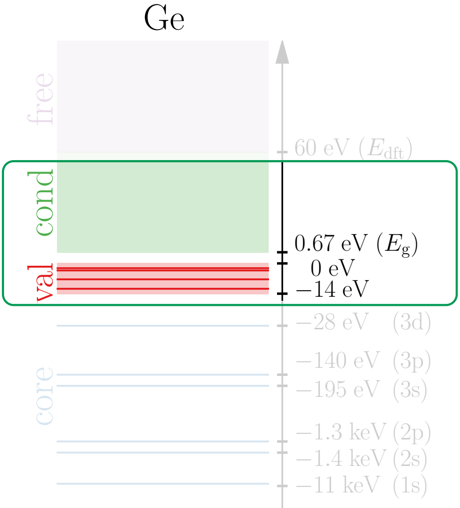


- Core electrons are tightly bound to the ionic sites, and less affected by the lattice environment.
- Wave functions are eigenstates of isolated atom Hamiltonians.
- Modelled **semi-analytically** with a linear combination of analytic functions.[a]

[a] Slater type orbitals (STO); common in atomic ionization calculations.

Calculation Setup

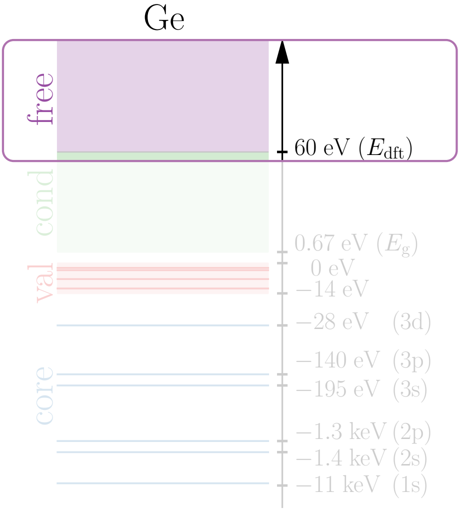
Valence and conduction states



- 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

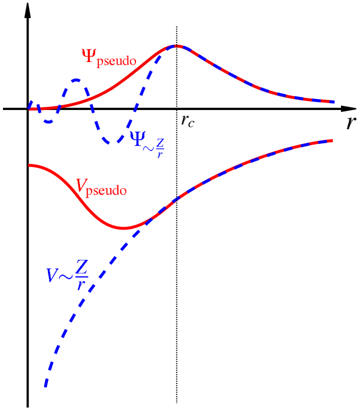


- Far from the band gap electrons are treated as **free** plane waves.

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

Outline

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



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

Pros

Focus on large r (small q) simplifies calculations.

Cons

Solution is not the complete wave function!

Certain DFT methods can add the high momentum contributions back in

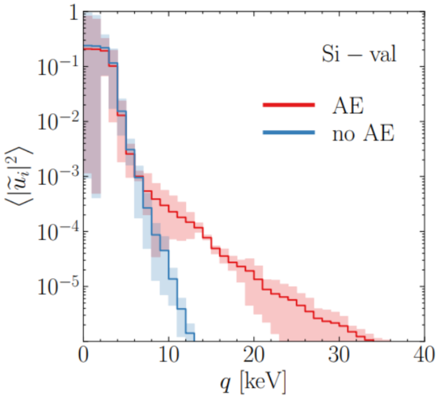
Projector Augmented Wave (PAW) Method

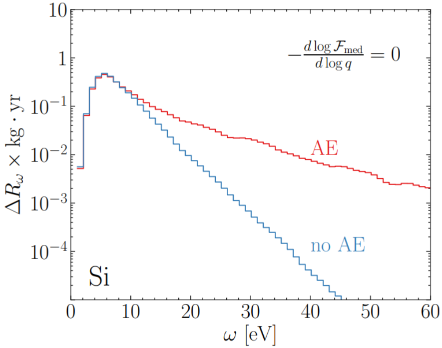
$$|\Psi_i^{\mathrm{AE}}\rangle = \left(1 + \sum_j \left(|\phi_j^{\mathrm{AE}}\rangle - |\phi_j^{\mathrm{PS}}\rangle\right)\langle p_j|\right)|\Psi_i^{\mathrm{PS}}\rangle$$

- ‘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 for more details.

High q contributions can significantly affect the scattering rate





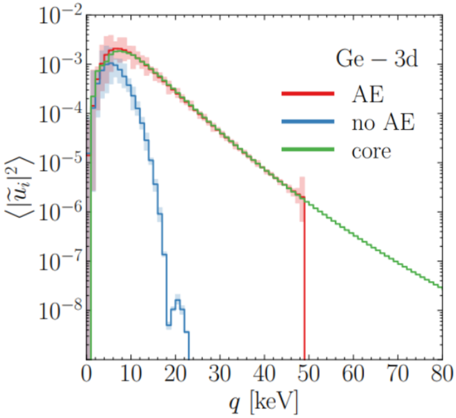
$\widetilde{u} \sim$ Fourier components of wave function.

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

See also Ref. arXiv:1810.13394 which discusses this effect.

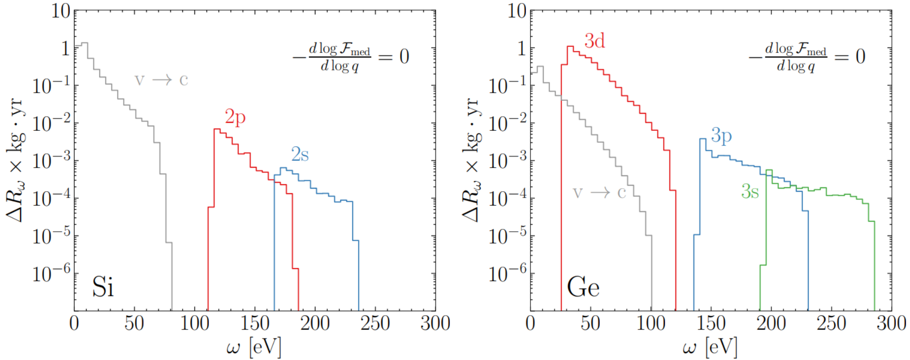
Outline

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 → 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.

Outline

Summary

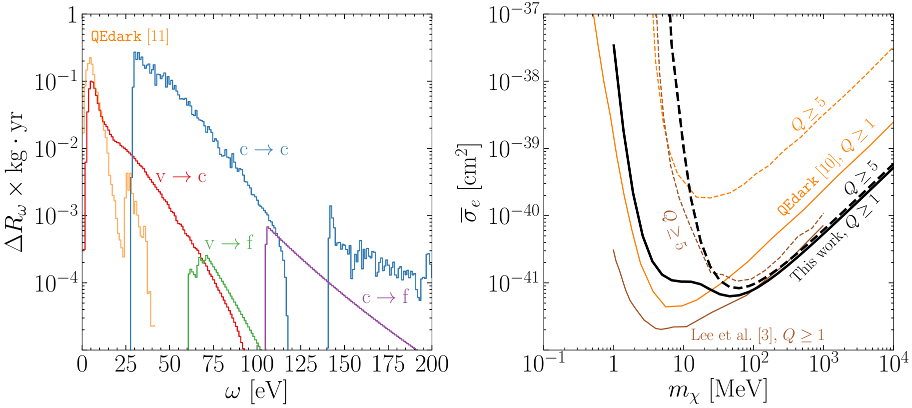
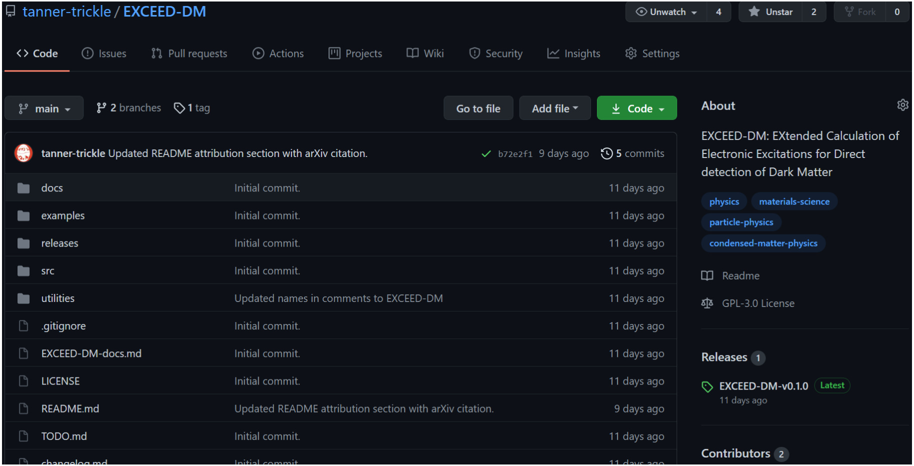


Figure: Ge target, heavy mediator, kg-year exposure, no backgrounds. Refs: QEdark arXiv:1509.01598+arXiv:1607.01009, Lee et al. arXiv:1508.07361.

Conclusion

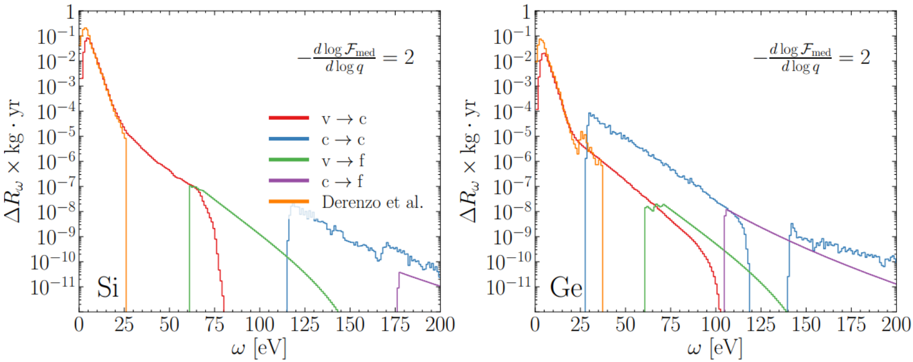
- Extended DM-electron scattering rate calculation to include **core → conduction**, **core → free** and **valence → free** transitions.
- High q components of the wave functions can change detection prospects by orders of magnitude for heavy ($m_{A'} \gg m_\chi v_\chi$) mediator models/higher thresholds.
- 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 !



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

Light Mediator Comparison



In-Medium Screening Effects