Extended Calculation of Dark Matter-Electron Scattering in Crystal Targets

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References:
- \texttt{arXiv: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 $\rightarrow$ Conduction Contributions
4. Summary
Direct Detection of Sub-GeV Dark Matter via $e^-$

Kinematics

Nuclear recoil is great at searching for WIMPs.

$$\omega = 2 \frac{\mu_{\chi N}^2}{m_N} v_X^2 \sim 2 m_N v_X^2$$

$$m_\chi \sim \text{TeV}$$

$$m_N \sim \text{GeV}$$
Direct Detection of Sub-GeV Dark Matter via $e^-$

Kinematics

However for light DM, nuclei are too heavy,

$m_\chi \sim \text{MeV} \quad m_N \sim \text{GeV}$

\[ \omega = 2 \frac{\mu_{\chi N}^2}{m_N} v_\chi^2 \sim \frac{m_\chi^2}{m_N^2} (2m_N v_\chi^2) \]

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

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

\[
R = \frac{\rho_\chi}{8 \rho_T V m_e^2 m_\chi^3} \sum_{I,F} \int \frac{d^3 q}{(2\pi)^3} g(q, E_F - E_I) \left| \int \frac{d^3 k}{(2\pi)^3} \mathcal{M}_{\text{free}} \tilde{\psi}_F^*(k + q) \tilde{\psi}_I(k) \right|^2 \\
g(q, \omega) = \int d^3 v f_\chi(v; v_e(t)) \delta(\omega - \omega_q)
\]
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.
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.

\[ \psi \sim e^{i\mathbf{p} \cdot \mathbf{x}} \]
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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**

\[
|\Psi_{i}^{AE}\rangle = \left(1 + \sum_{j} \left(|\phi_{j}^{AE}\rangle - |\phi_{j}^{PS}\rangle\right) \langle p_{j} | \right) |\Psi_{i}^{PS}\rangle
\]

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

High $q$ contributions can significantly affect the scattering rate

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

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

$ΔR_ω$ - rate per kg-year between $ω$ and $ω + Δω$. 

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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 → 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]+[arXiv:1607.01009], Lee et al. [arXiv:1508.07361].
Conclusion

- Extended DM-electron scattering rate calculation to include core $\rightarrow$ conduction, core $\rightarrow$ free and valence $\rightarrow$ 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

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\[ \frac{d \log F_{\text{med}}}{d \log q} = 2 \]

Graphs showing \( \Delta R_\omega \times \text{kg} \cdot \text{yr} \) as a function of \( \omega [\text{eV}] \) for Si and Ge, with different colors representing different mediations and a note for Derenzo et al.:
In-Medium Screening Effects

$$\frac{\Delta R_{\text{sc} \mid \omega}}{\Delta R_{\text{no sc} \mid \omega}}$$

$$\frac{d \log F_{\text{med}}}{d \log q} = 2$$

$$\frac{d \log F_{\text{med}}}{d \log q} = 0$$

$$\frac{R_{\text{sc} \mid m \chi}}{R_{\text{no sc} \mid m \chi}}$$

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