

Dark matter scattering in dielectrics

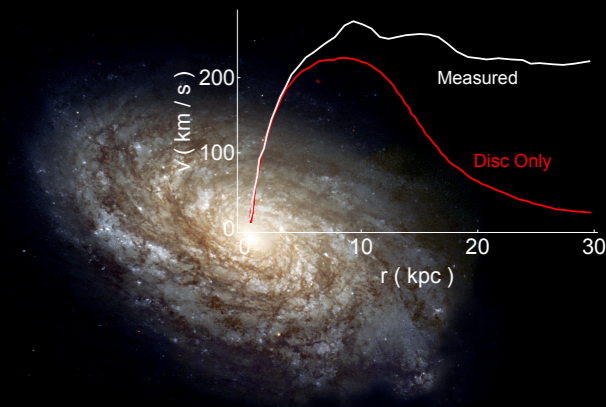
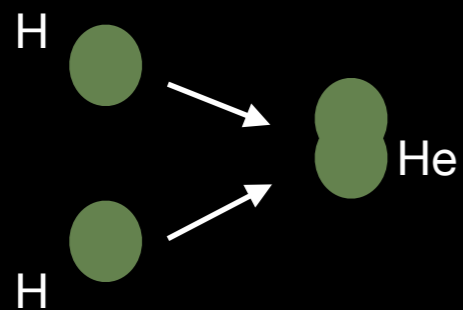
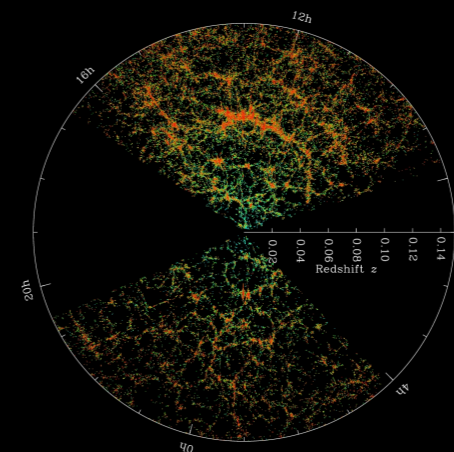
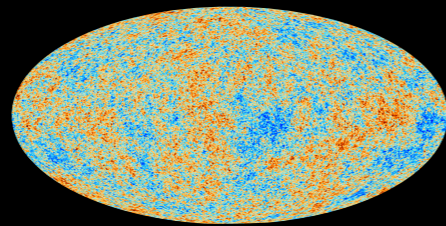
Simon Knapen

Lawrence Berkeley Lab



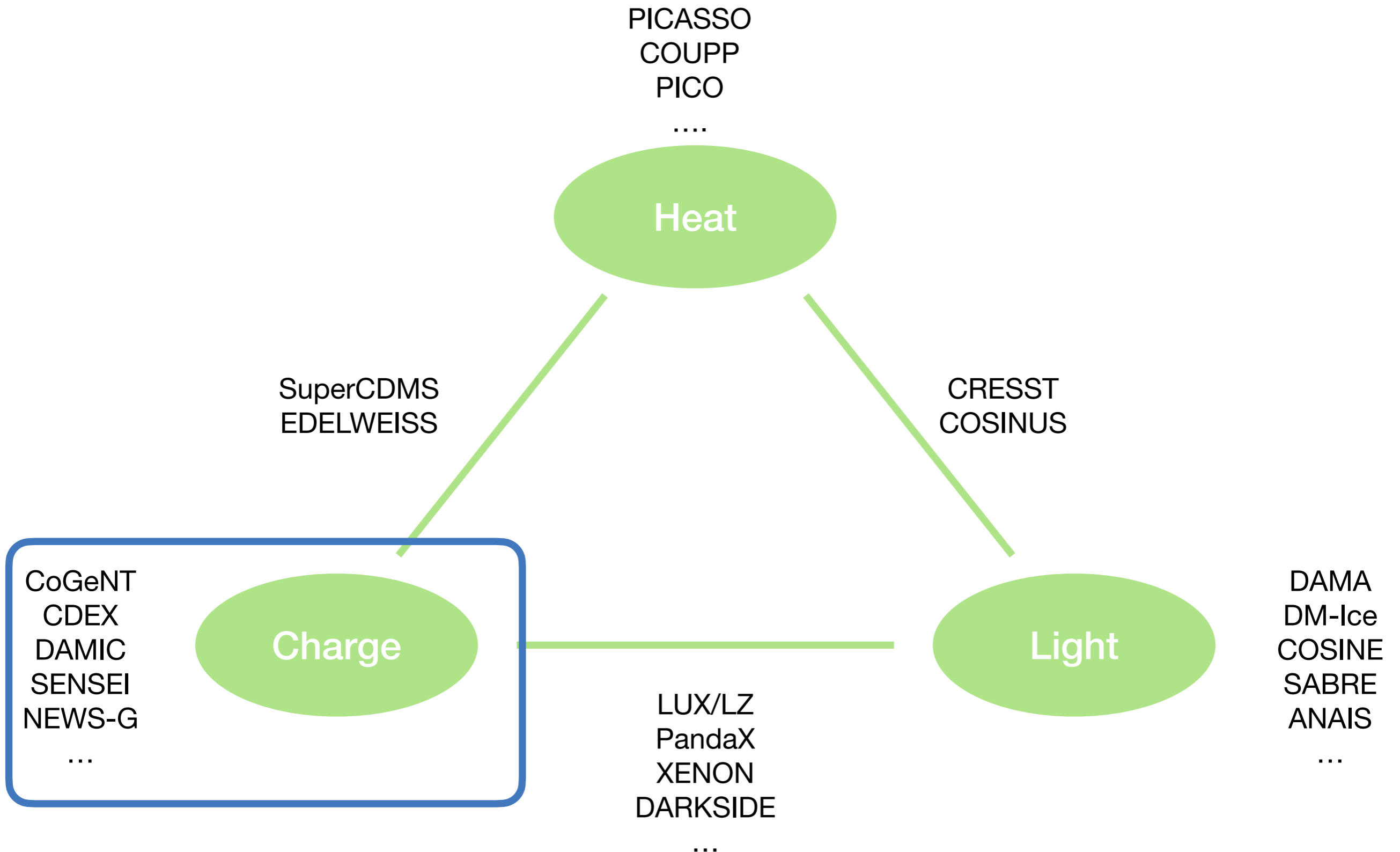
<http://dingercatadventures.blogspot.com/2012/08/>

A History of time



Evidence for cold dark matter from every epoch

Dark Matter direct detection

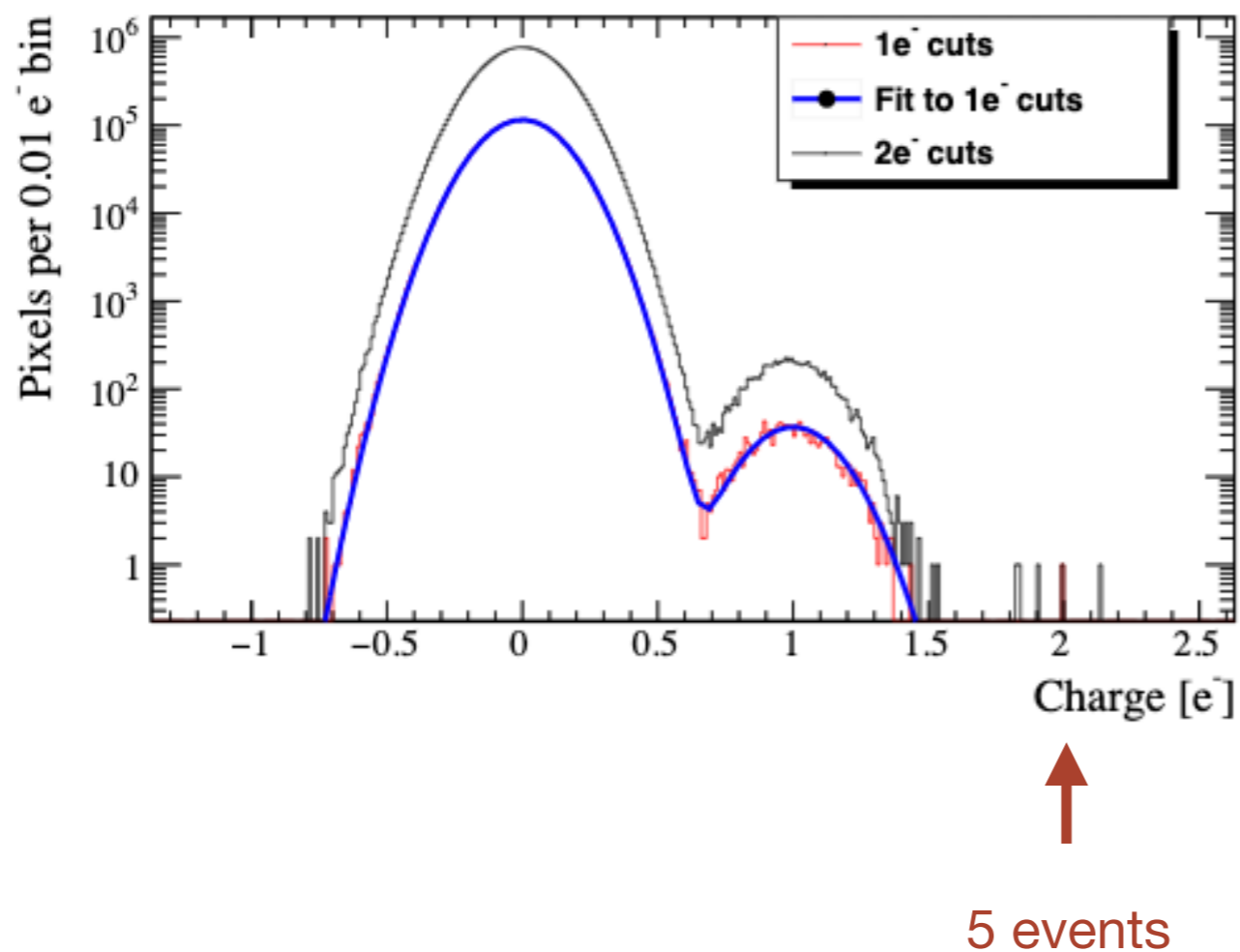


Impressive progress in lowering thresholds due to quantum sensor developments!

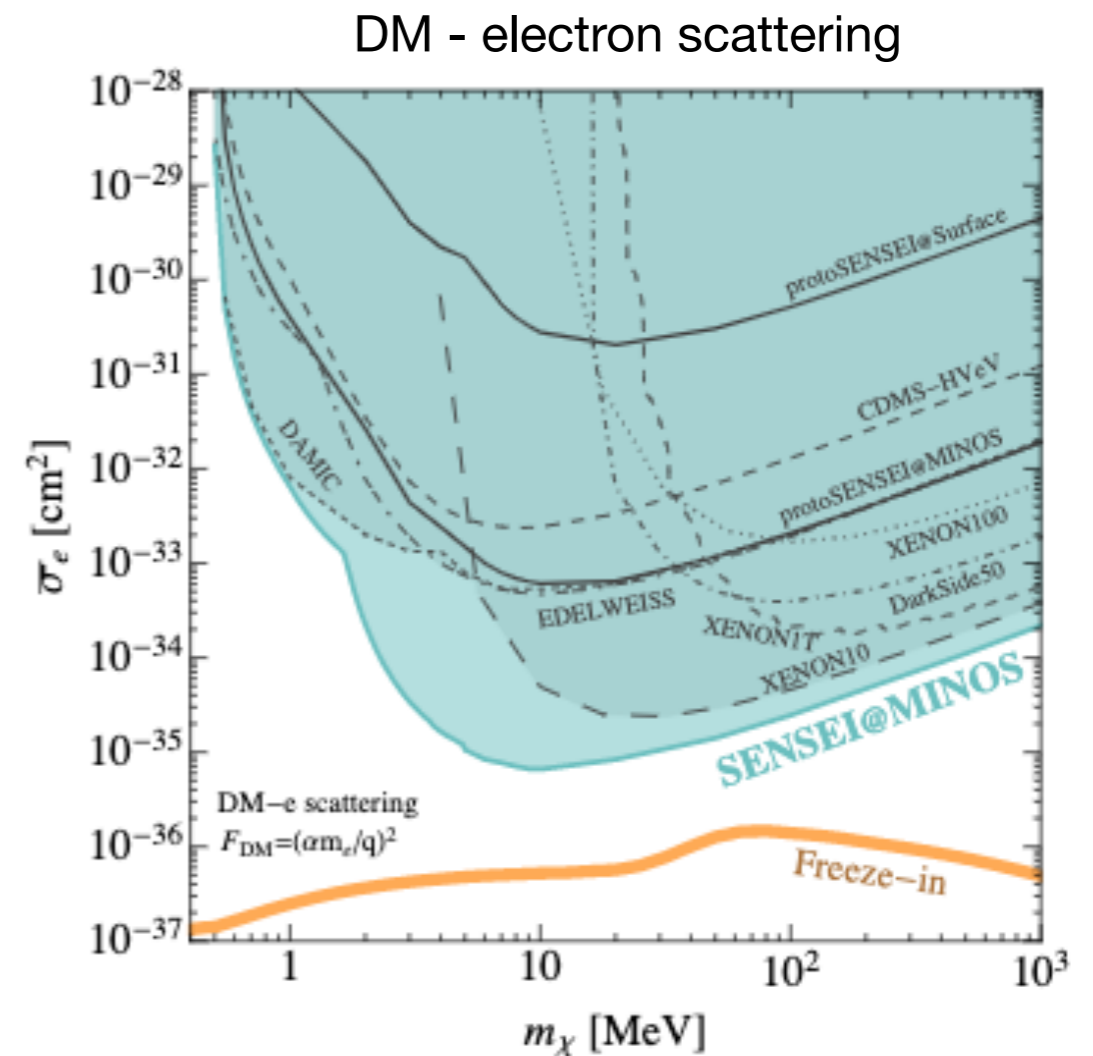
Single electron sensitivity

Example: SENSEI

- Skipper CCD (Si) → single charge sensitivity
- ~50 gram-days exposure (MINOS cavern)



SENSEI collaboration: arXiv 2004.11378



Similar results by superCMDS

Other applications

Migdal effect

Normal nuclear recoil:

$$E_R \leq \frac{v^2 m_X^2}{m_N} \approx 30 \text{ eV} \times \left(\frac{m_X}{\text{GeV}} \right)^2$$

Inelastic recoil:

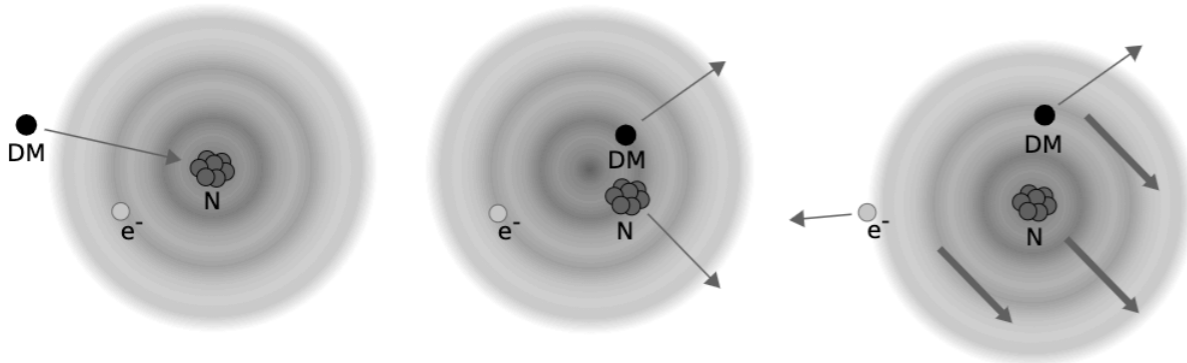


Figure from arXiv 1711.09906

Absorption processes

Light, bosonic DM can be absorbed

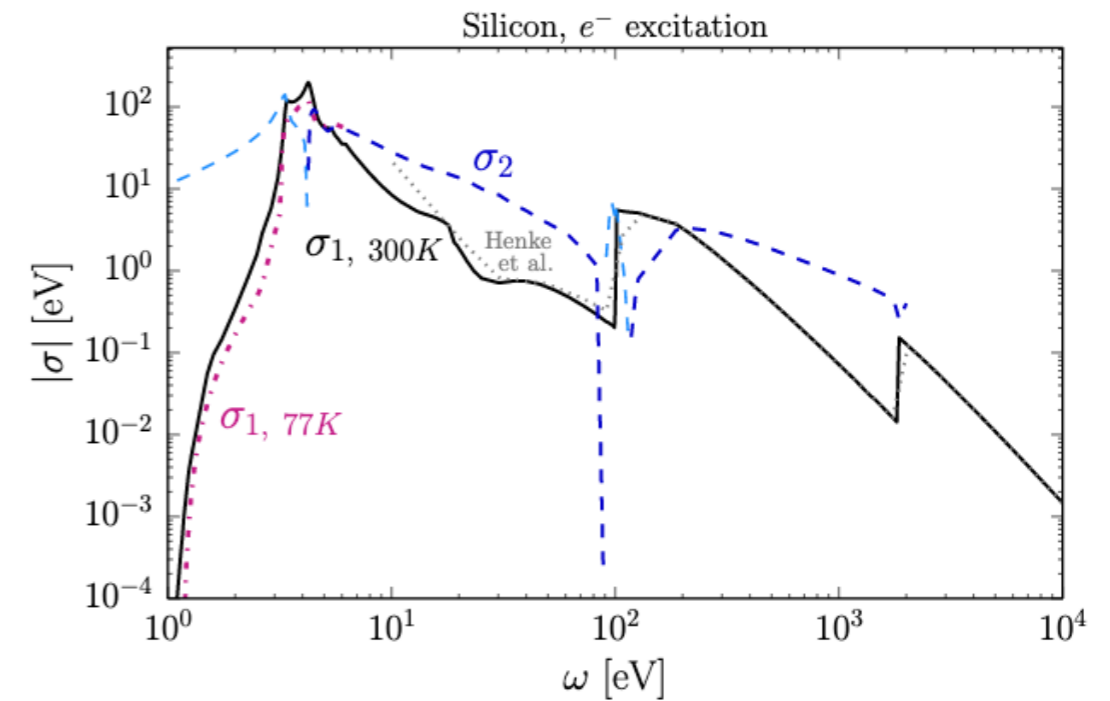


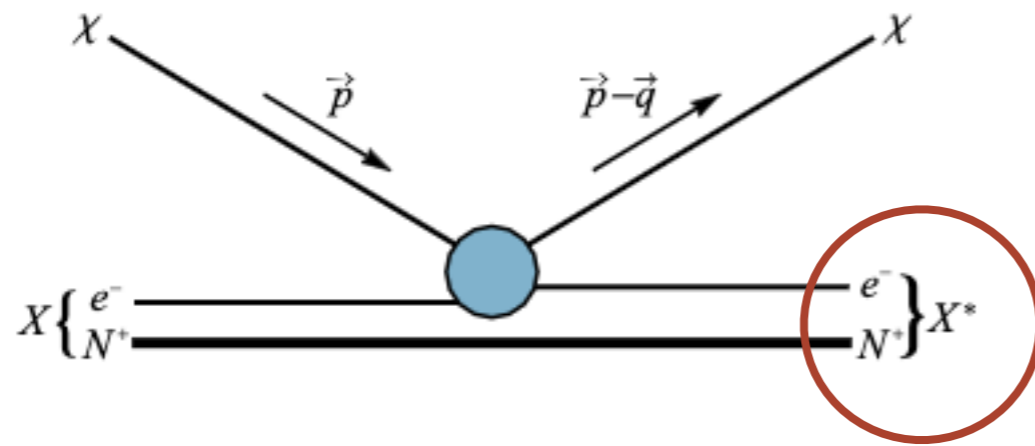
Figure from arXiv 1608.01994

Extract rate from photon absorption spectra

Collect e^- from DM absorption

Collect e^- from inelastic collision

Electronic signals are theoretically complicated



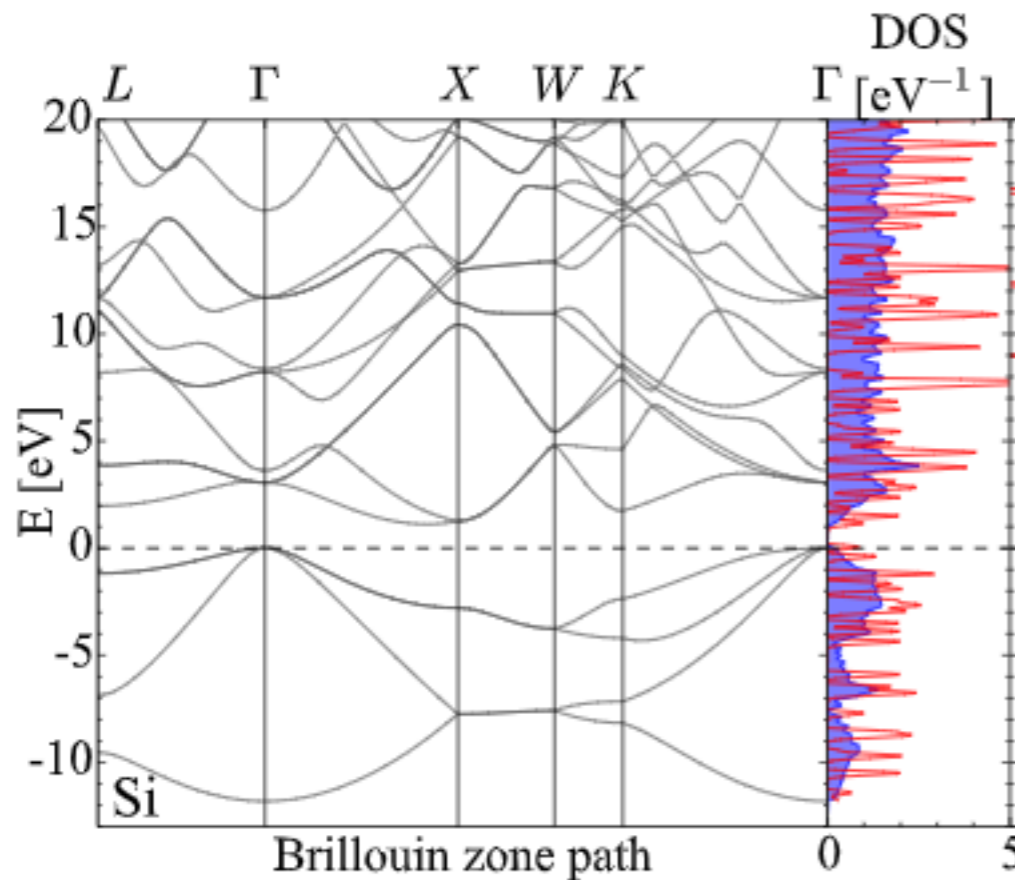
e^- are not free

e^- are not at rest

e^- are not localized

e^- are not alone

→ screening



Bloch wave functions

Obtain with density functional theory (DFT)

Outline

- Dark Matter - e^- scattering in semiconductors
- Migdal effect in semiconductors
- DarkELF package

Models

Scalar mediator: $g_\chi \phi \bar{\chi} \chi + g_e \phi \bar{e} e$

$$\rightarrow g_\chi \phi n_\chi + g_e \phi n$$

Vector mediator: $g_\chi V_\mu \bar{\chi} \gamma^\mu \chi + g_e V_\mu \bar{e} \gamma^\mu e$

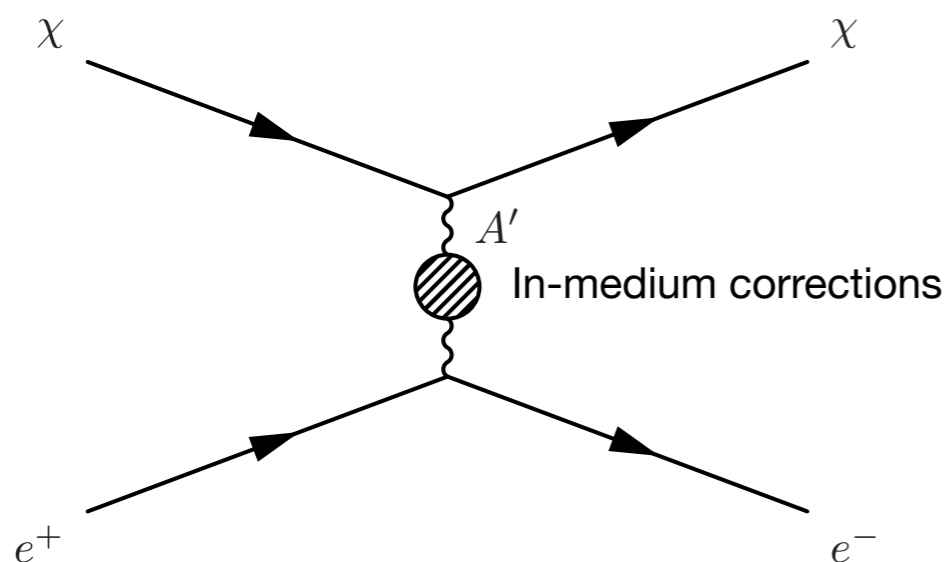
$$\rightarrow g_\chi V_0 n_\chi + g_e V_0 n$$

Both couple to the electron number density in the non-relativistic limit



The scattering rate should be the same

Old wisdom: “Interactions through a dark photon mediator are screened”



Replace:

$$\frac{1}{q^2} \rightarrow \frac{1}{\epsilon(q, \omega)} \frac{1}{q^2}$$

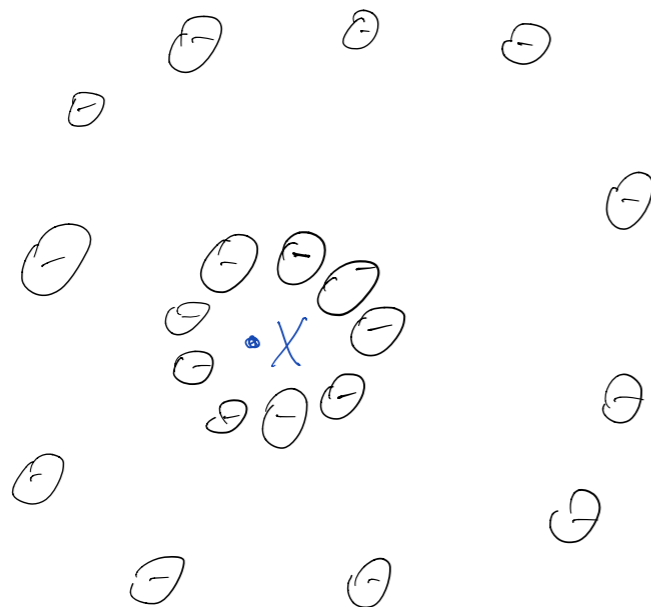
Dielectric function

Screening is mediator independent

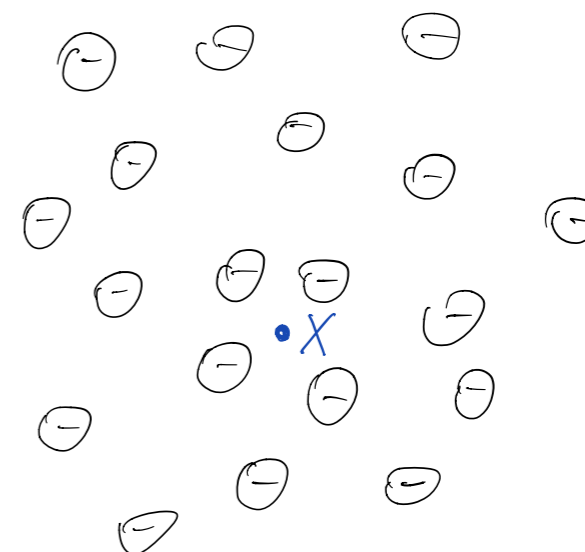
Consider a DM particle in the crystal, sourcing an external force

This creates a **local overdensity** in the electron number density

No screening



With screening



Density perturbations are suppressed because of Pauli blocking and electric repulsion

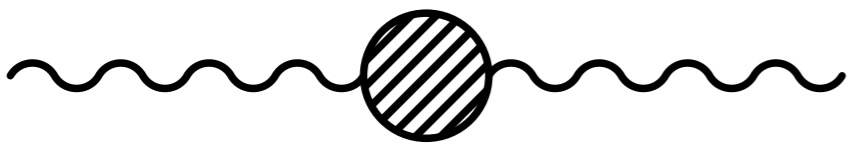
Purely standard model effect, and does not depend on the DM mediator

The energy loss function (ELF)

Coulomb potential in a dielectric:

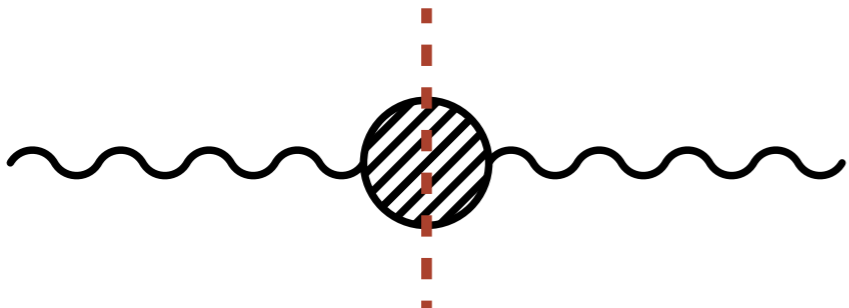
$$H = eQ_\chi \int \frac{d^3\mathbf{k}}{(2\pi)^2} \frac{1}{\epsilon(\mathbf{k}, \omega)} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{k^2}$$

In QFT language:



$$\sim \frac{1}{\epsilon(\mathbf{k}, \omega)} \frac{1}{k^2} \quad \text{(Non-relativistic limit)}$$

We are interested in energy dissipation:



$$\sim \text{Im} \left[\frac{-1}{\epsilon(\mathbf{k}, \omega)} \right]$$

“Energy Loss Function” (ELF)

Derivation (I)

Need to use *linear response theory*, essentially non-relativistic QFT

Susceptibility: how does the crystal respond to a density perturbation?

$$\chi(\omega, \mathbf{k}) = -\frac{i}{V} \int_0^\infty dt e^{i\omega t} \langle [n_{\mathbf{k}}(t), n_{-\mathbf{k}}(0)] \rangle$$

\downarrow
 Crystal
 volume

\downarrow
 Electron number
 density operator

This is the non-relativistic, retarded Green's function (fully dressed)

Now we use the *fluctuation-dissipation theorem*

$$\text{Im}\chi(\omega, \mathbf{k}) = -\frac{1}{2}(1 - e^{-\beta\omega})S(\omega, \mathbf{k}) \quad \beta \equiv \frac{1}{k_B T}$$

With the *dynamical structure factor* defined as

$$S(\omega, \mathbf{k}) \equiv \frac{2\pi}{V} \sum_{i,f} \frac{e^{-\beta E_i}}{Z} |\langle f | n_{-\mathbf{k}} | i \rangle|^2 \delta(\omega + E_i - E_f)$$

Fermi's golden rule

Derivation (II)

Now consider the response to an external electromagnetic perturbation.

The induced electron number density is

$$\begin{aligned} \langle \delta n(\mathbf{k}, \omega) \rangle &= \langle n(\mathbf{k}, \omega) H_{coul} \rangle & \text{with} & \quad H_{coul} = -e \int \frac{d^3 \mathbf{k}}{(2\pi)^2} \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{k^2} n(-\mathbf{k}, \omega) \rho_{ext}(\mathbf{k}, \omega) \\ &= -\frac{e}{k^2} \chi(\mathbf{k}, \omega) \rho_{ext}(\mathbf{k}, \omega) \end{aligned}$$

Using Maxwell's equations

$$\begin{aligned} i\mathbf{k} \cdot \mathbf{D}(\mathbf{k}, \omega) &= 4\pi \rho_{ext}(\mathbf{k}, \omega) \\ i\mathbf{k} \cdot \mathbf{E}(\mathbf{k}, \omega) &= 4\pi \rho_{ext}(\mathbf{k}, \omega) - 4\pi e \langle \delta n(\mathbf{k}, \omega) \rangle \end{aligned} \quad \text{with} \quad \mathbf{D}(\mathbf{k}, \omega) = \epsilon(\mathbf{k}, \omega) \mathbf{E}(\mathbf{k}, \omega)$$

Which results in the relation

$$\frac{1}{\epsilon(\omega, \mathbf{k})} = 1 + \frac{4\pi\alpha_{em}}{k^2} \chi(\omega, \mathbf{k}),$$

Now plugging this into the fluctuation-dissipation theorem

$$S(\omega, \mathbf{k}) = \frac{k^2}{2\pi\alpha_{em}} \frac{1}{1 - e^{-\beta\omega}} \text{Im} \left[\frac{-1}{\epsilon(\omega, \mathbf{k})} \right] \quad \text{Energy Loss Function (ELF)}$$

DM-electron scattering rate

Full formula

$$R = \frac{1}{\rho_T} \frac{\rho_\chi}{m_\chi} \frac{\bar{\sigma}_e}{\mu_{\chi e}^2} \frac{\pi}{\alpha_{em}} \int d^3v \boxed{f_\chi(v)} \int \frac{d^3\mathbf{k}}{(2\pi)^3} k^2 \boxed{F_{DM}(k)|^2} \int \frac{d\omega}{2\pi} \frac{1}{1 - e^{-\beta\omega}} \boxed{\text{Im} \left[\frac{-1}{\epsilon(\omega, \mathbf{k})} \right]} \delta \left(\omega + \frac{k^2}{2m_\chi} - \mathbf{k} \cdot \mathbf{v} \right).$$

↓
↓
↓

DM velocity distribution
DM form factor
ELF

What is the difference with earlier results?

We can write

$$\text{Im} \left[\frac{-1}{\epsilon(\omega, \mathbf{k})} \right] = \frac{\text{Im} \epsilon(\omega, \mathbf{k})}{|\epsilon(\omega, \mathbf{k})|^2}$$

Taking $\epsilon(q, \omega) \approx 1$ we reproduce the earlier results, using Lindhard's formula

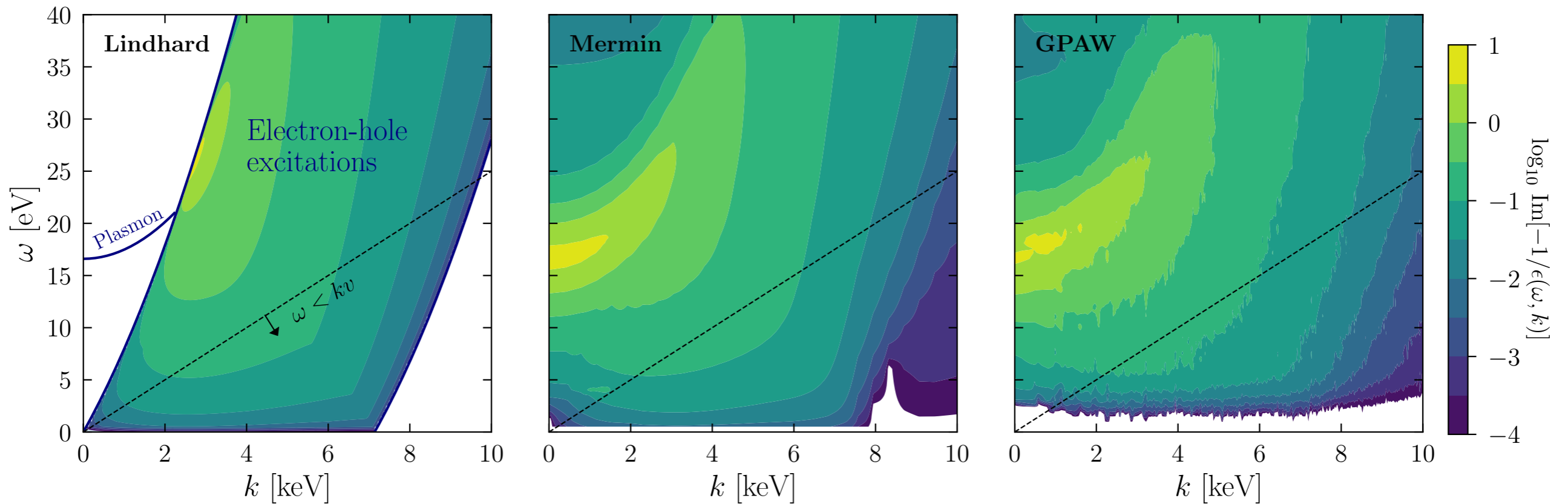
Advantages of using the ELF:

- Screening included automatically
- ELF has been measured and calculated extensively in the condensed matter literature

Calculating the ELF

Simple

Sophisticated



Free electron gas
approximation

100% analytic

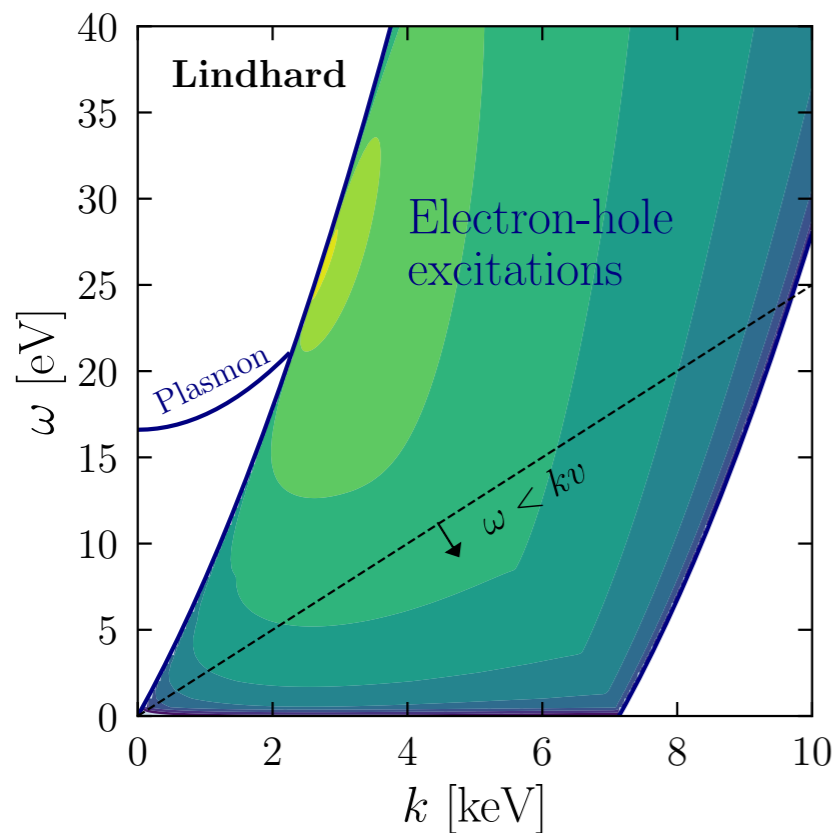
Phenomenological
model fit to data

semi-analytic

First principles DFT
calculation

Fully numerical

Lindhard model



Homogenous, free electron gas:

$$\epsilon_{\text{Lin}}(\omega, k) = 1 + \frac{3\omega_p^2}{k^2 v_F^2} \lim_{\eta \rightarrow 0} \left[f \left(\frac{\omega + i\eta}{k v_F}, \frac{k}{2m_e v_F} \right) \right]$$

with

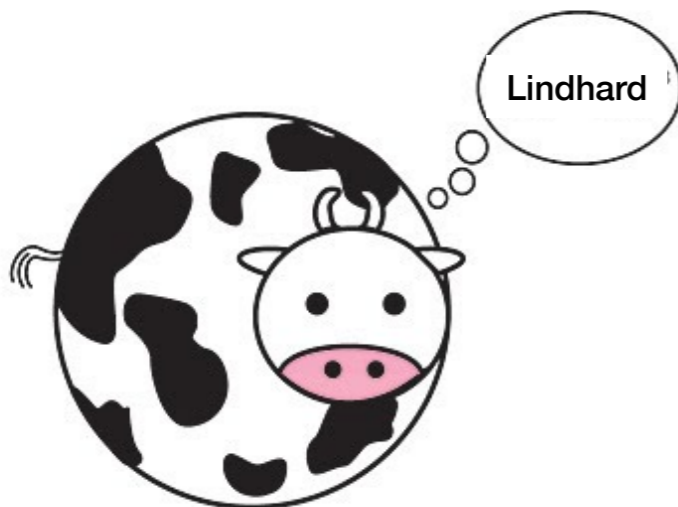
$$v_F = \left(\frac{3\pi\omega_p^2}{4\alpha m_e^2} \right)^{1/3} \text{ Plasmon frequency}$$

$$f(u, z) = \frac{1}{2} + \frac{1}{8z} [g(z - u) + g(z + u)]$$

$$g(x) = (1 - x^2) \log \left(\frac{1 + x}{1 - x} \right)$$

Features:

- Pauli blocking
- e-h pair continuum
- Plasmon width
- Low k region
- Bandgap



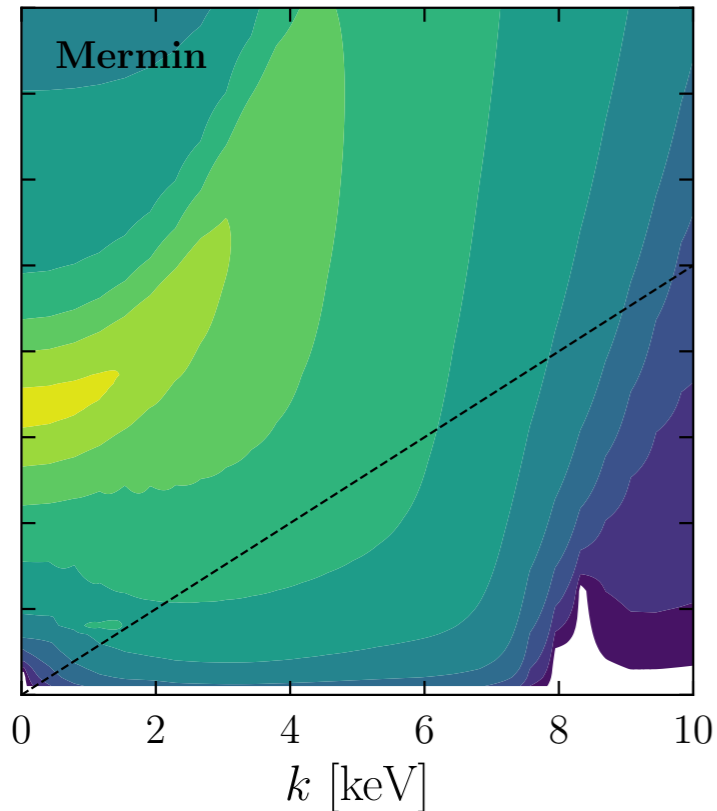
Mermin model

Homogenous, free electron gas with dissipation (Γ)

$$\epsilon_{\text{Mer}}(\omega, k) = 1 + \frac{(1 + i\frac{\Gamma}{\omega})(\epsilon_{\text{Lin}}(\omega + i\Gamma, k) - 1)}{1 + (i\frac{\Gamma}{\omega})\frac{\epsilon_{\text{Lin}}(\omega + i\Gamma, k) - 1}{\epsilon_{\text{Lin}}(0, k) - 1}}.$$

Fit a linear combination of Mermin oscillators to optical data:

$$\text{Im} \left[\frac{-1}{\epsilon(\omega, k)} \right] = \sum_i A_i(k) \text{Im} \left[\frac{-1}{\epsilon_{\text{Mer}}(\omega, k; \omega_{p,i}, \Gamma_i)} \right]$$

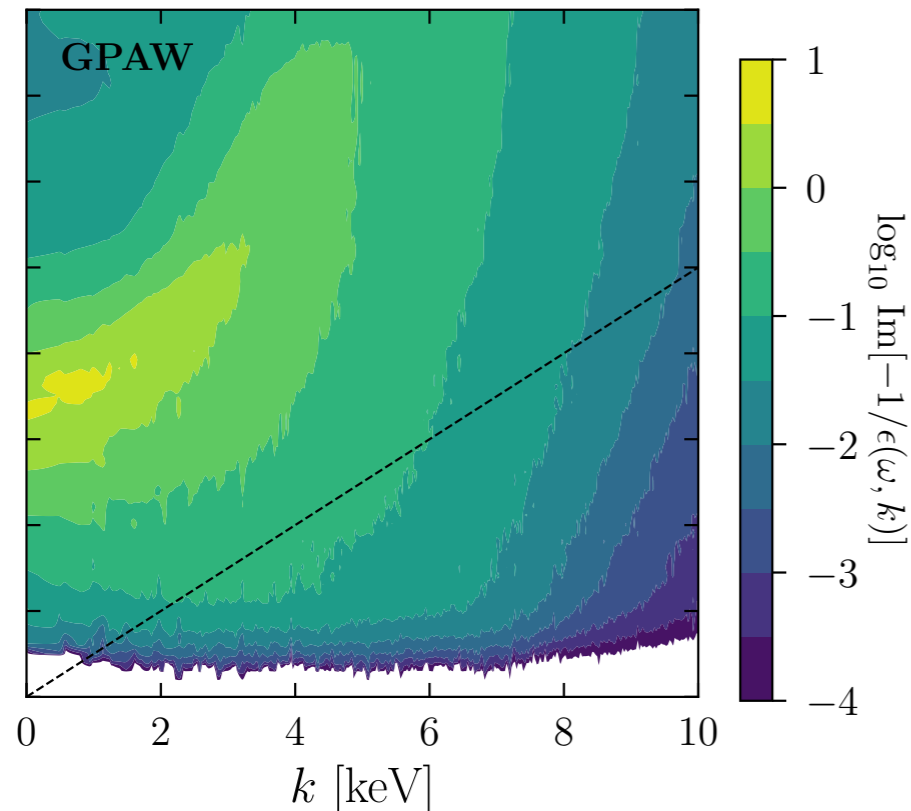


Features:

- Pauli blocking
- e-h pair continuum
- Plasmon width
- Low k region
- Bandgap

M. Vos, P. Grande: chapidif package
 Data from Y. Sun et. al. Chinese Journal of
 Chemical Physics 9, 663 (2016)

GPAW method



Compute the ELF from first principles with time-dependent Density Functional Theory methods (TD-DFT)

Puts atoms on periodic lattice and model interacting e^- as non-interacting e^- + effective external potential (Kohn-Sham method)

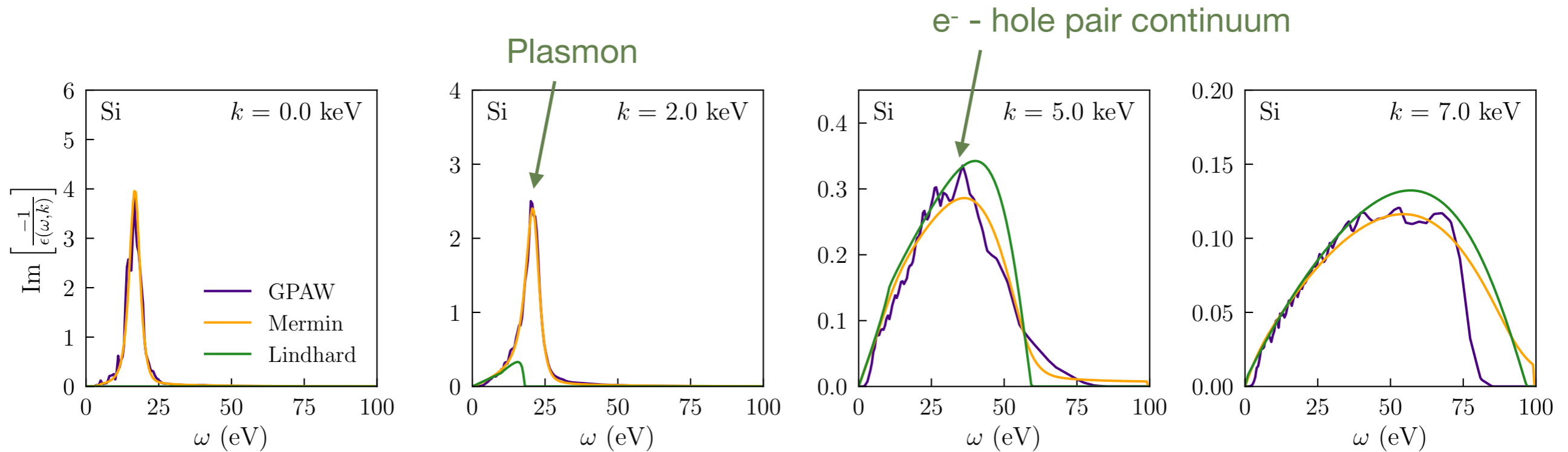
Inner shell e^- are treated as part of the ion (frozen core approximation)

Features:

- Pauli blocking
- e-h pair continuum
- Plasmon width
- Low k region
- Bandgap



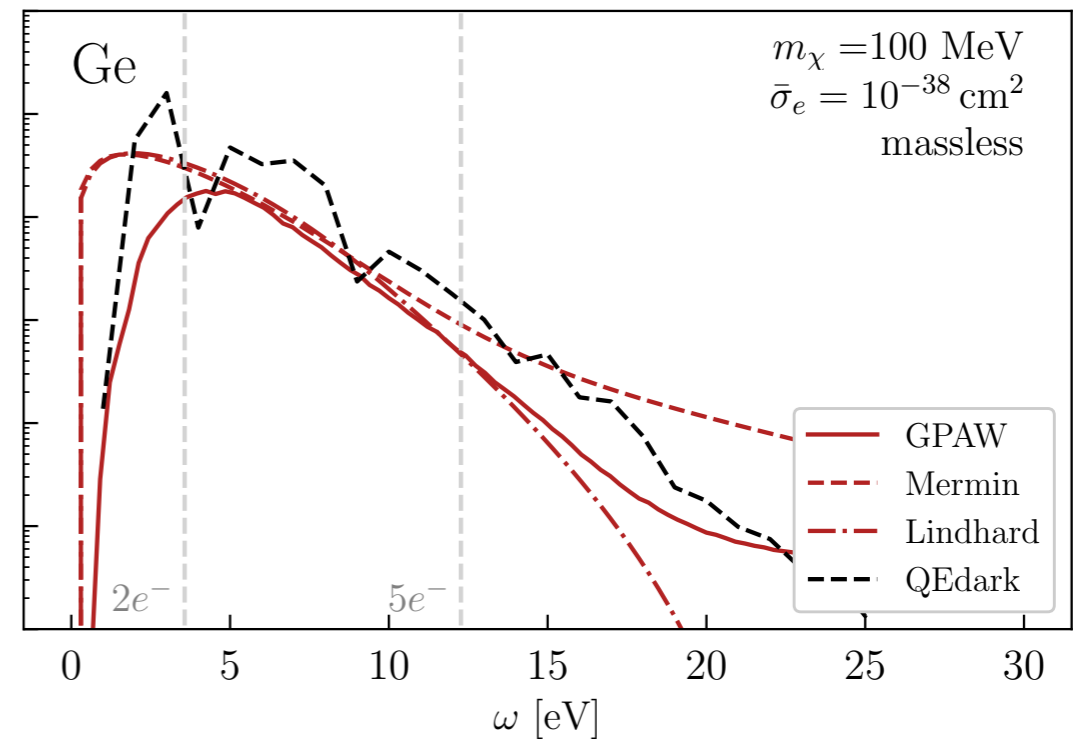
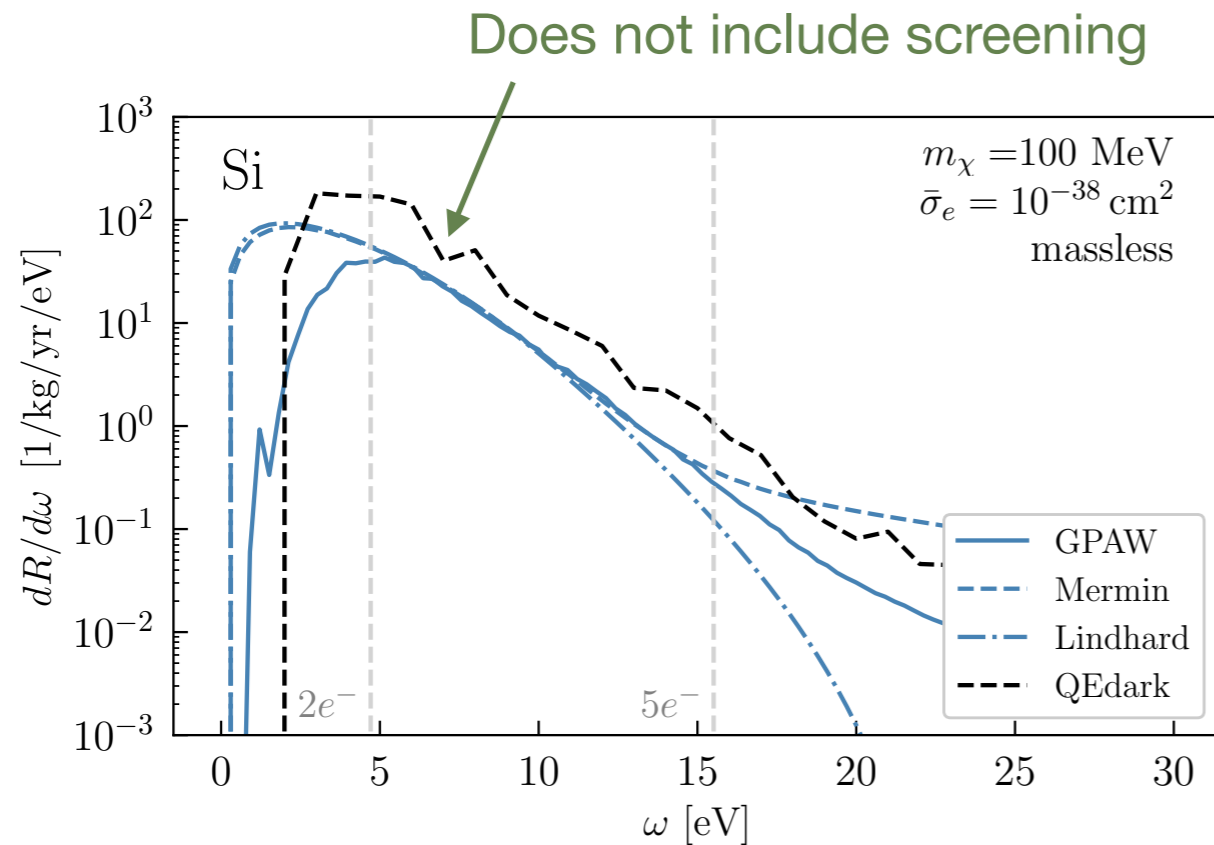
Comparing all three methods



TO BE UNDERSTOOD FURTHER

Generally very good agreement, especially between Mermin and GPAW!

Differential rate

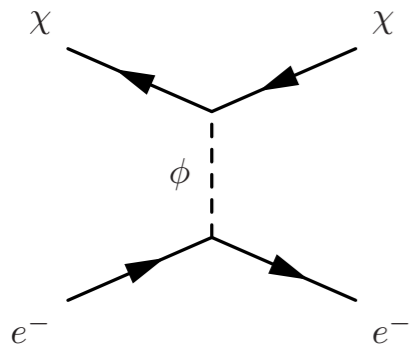


Mermin & GPAW in very good agreement except:

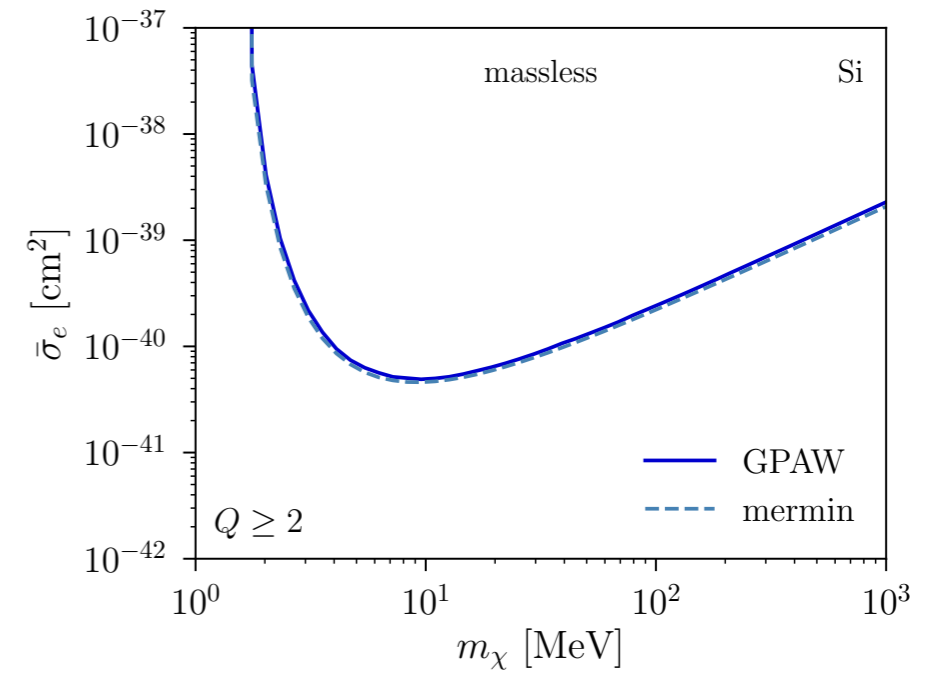
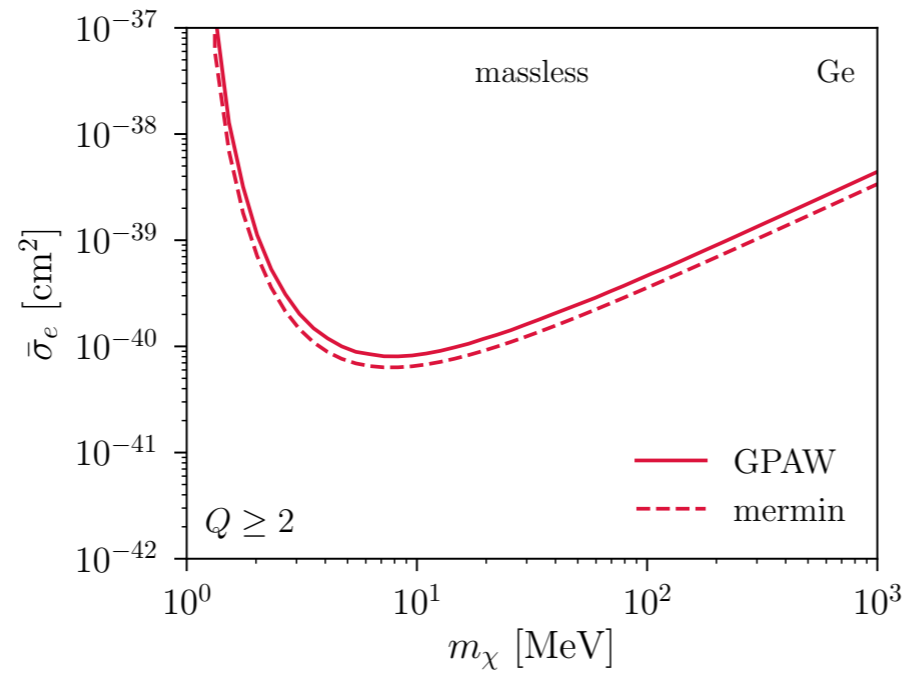
- Single ionization e⁻ region (background dominated)
- High energy region (subdominant)

(Agreement is less good in massive mediator case; work in progress)

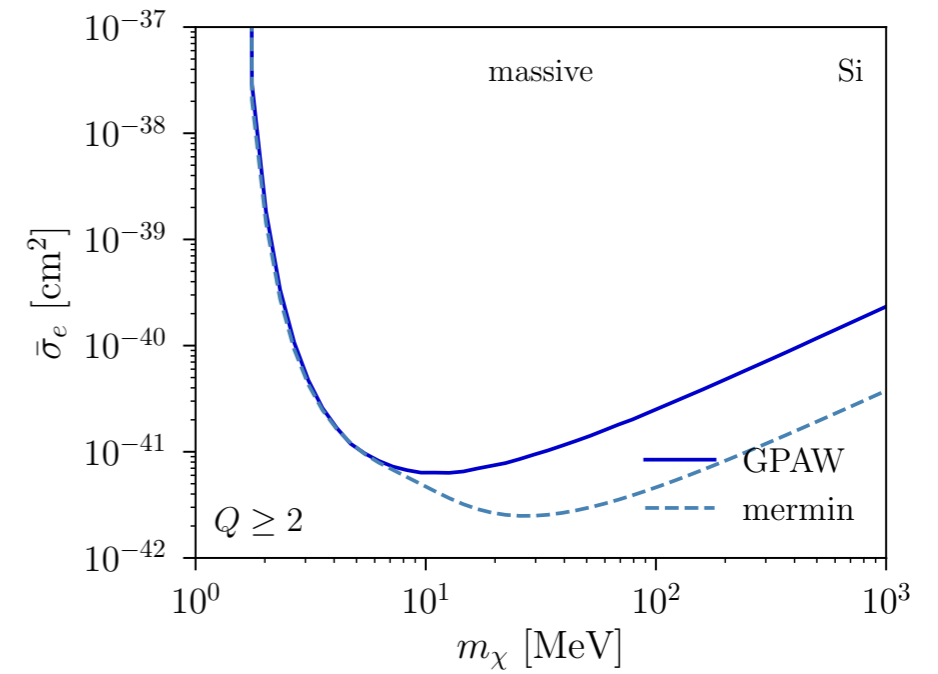
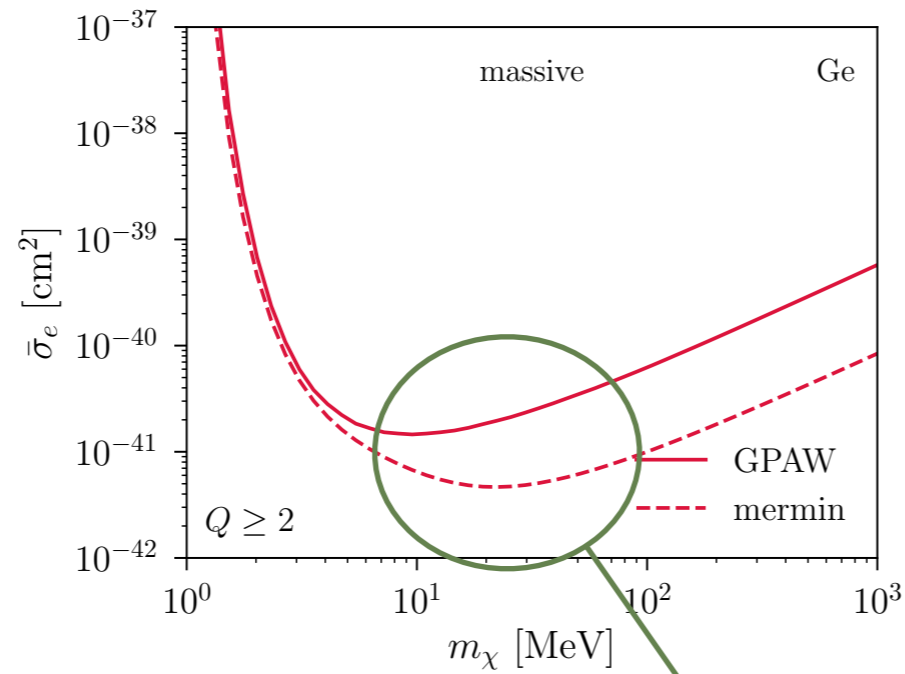
Integrated rate: Mermin vs GPAW



$$m_\phi \ll \alpha m_e$$



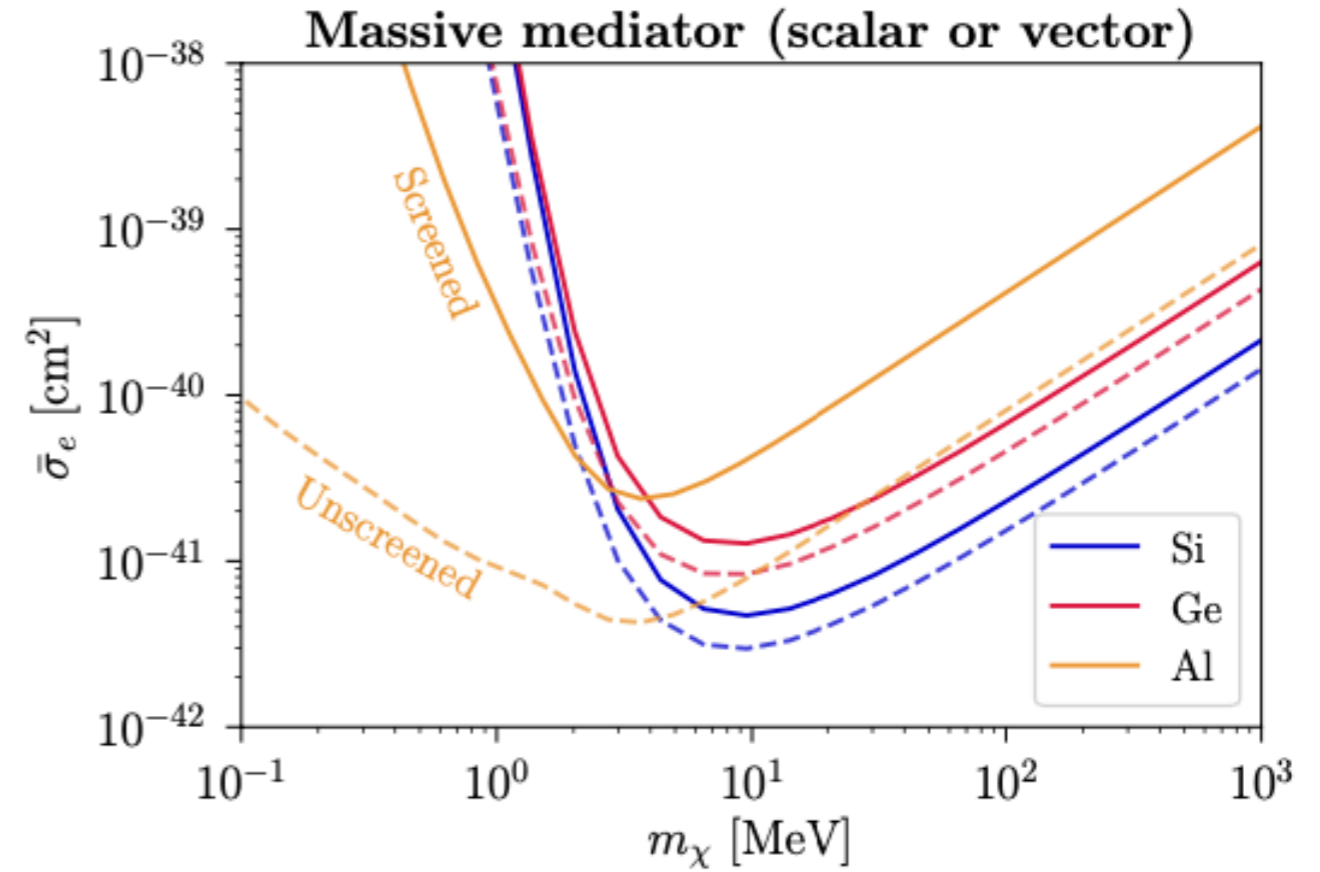
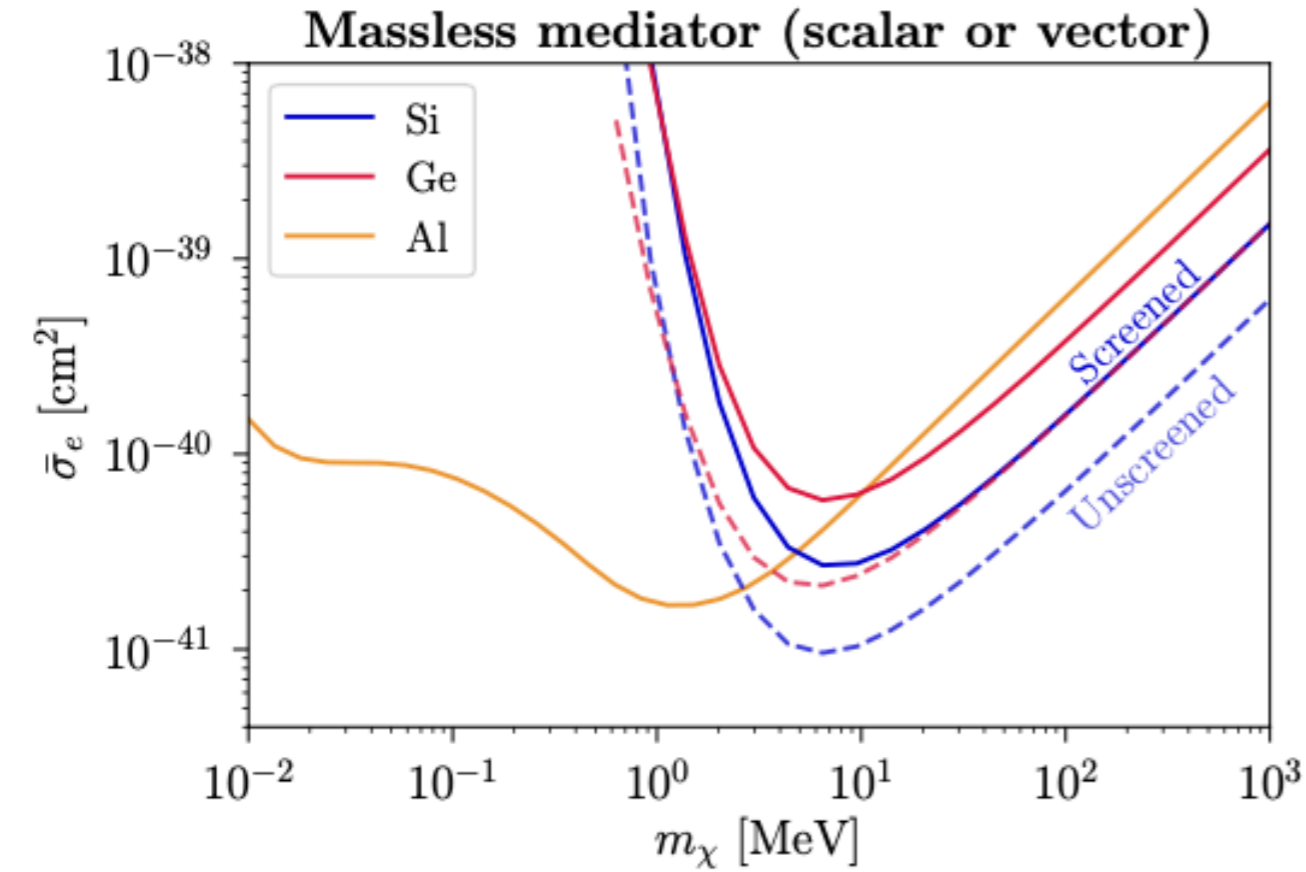
$$m_\phi \gg \alpha m_e$$



High k region of the ELF (work in progress)

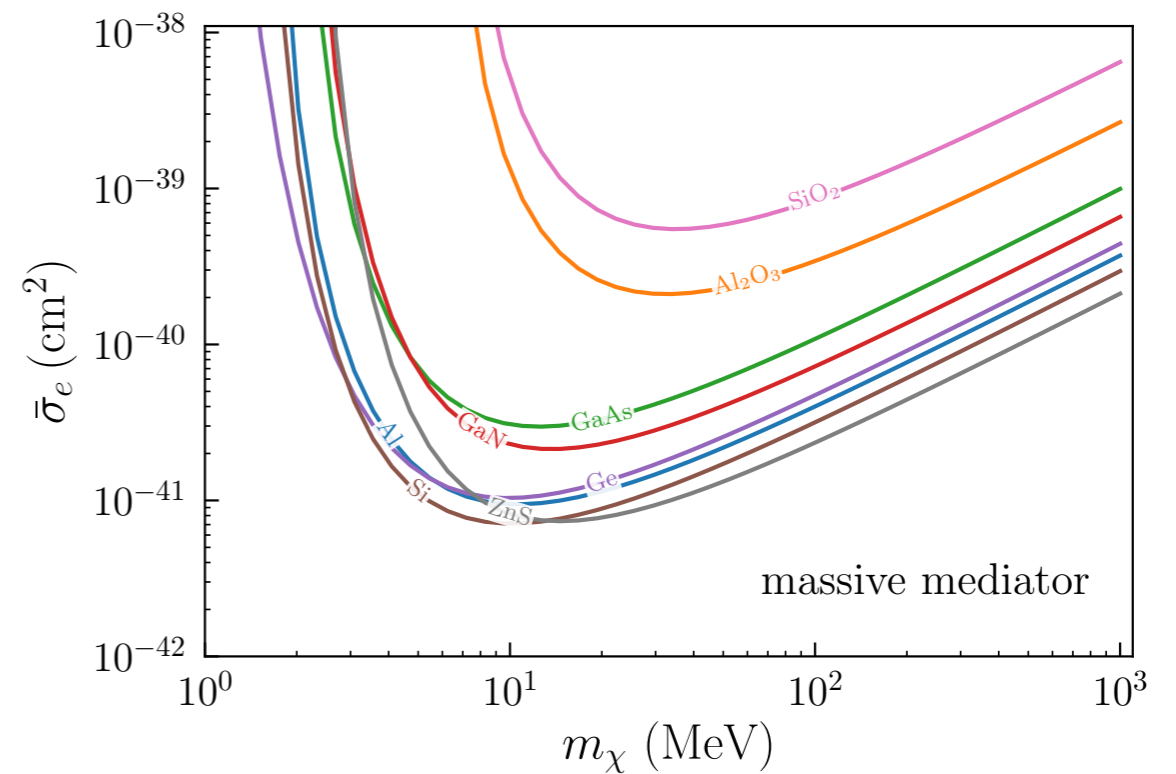
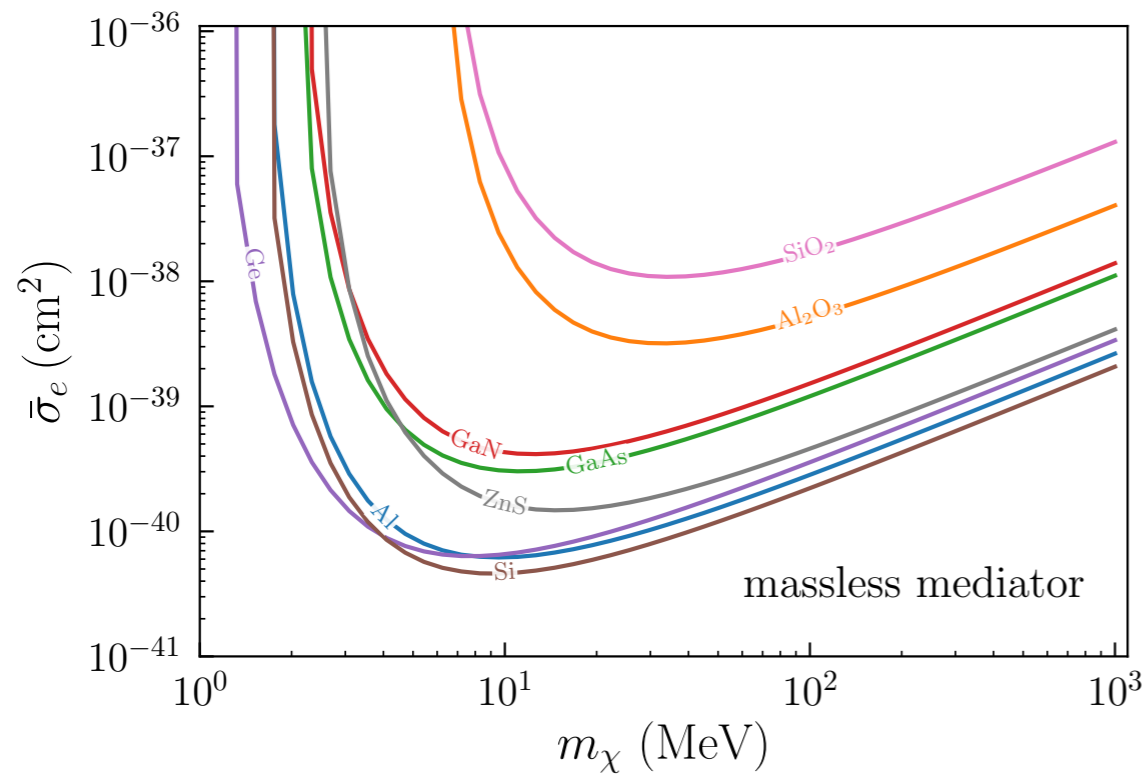
Integrated rate: Screening

Screening has O(1) effect on integrated rate



Integrated rate: Other materials

Using the *Mermin* method we can easily scan over many possible targets:



So far only *GPAW* results for Ge and Si, other materials are work in progress

Outline

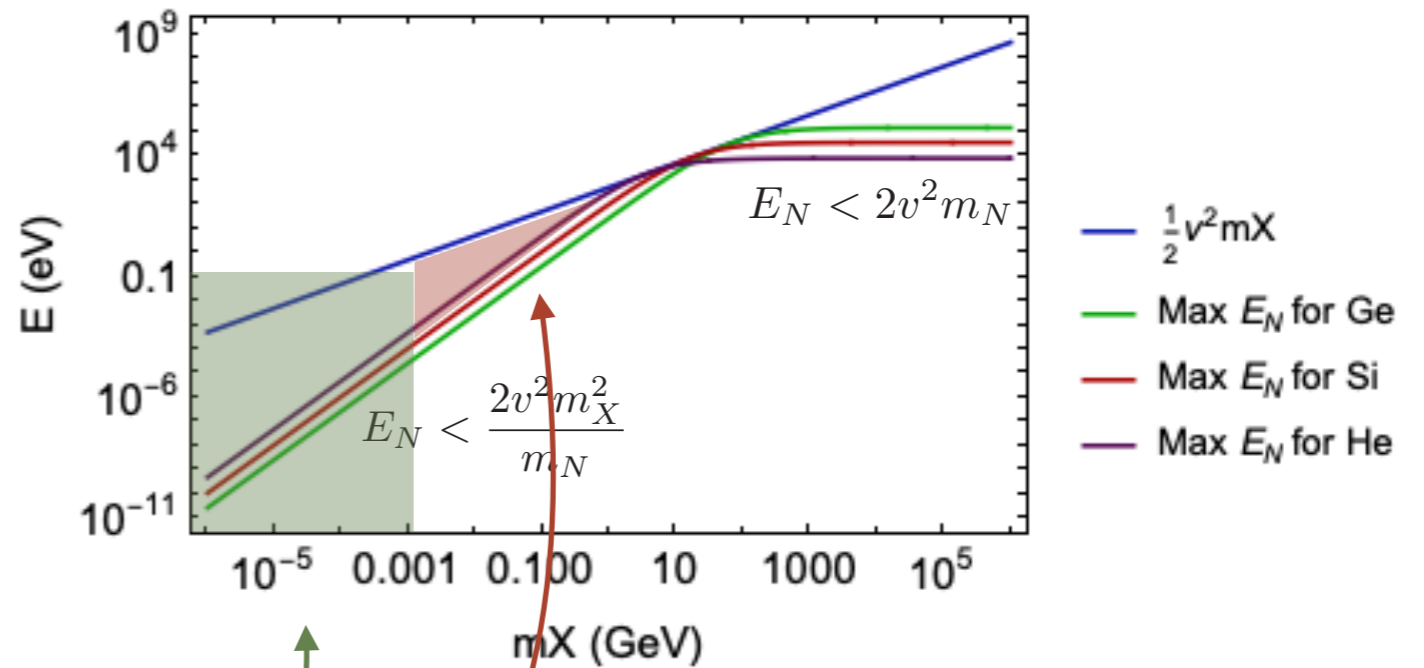
- Dark Matter - e^- recoils in semiconductors
- Migdal effect in semiconductors
- DarkELF package

Elastic nuclear recoil kinematics

Momentum conservation implies

$$E_N < \frac{(2v\mu_{XN})^2}{2m_N}$$

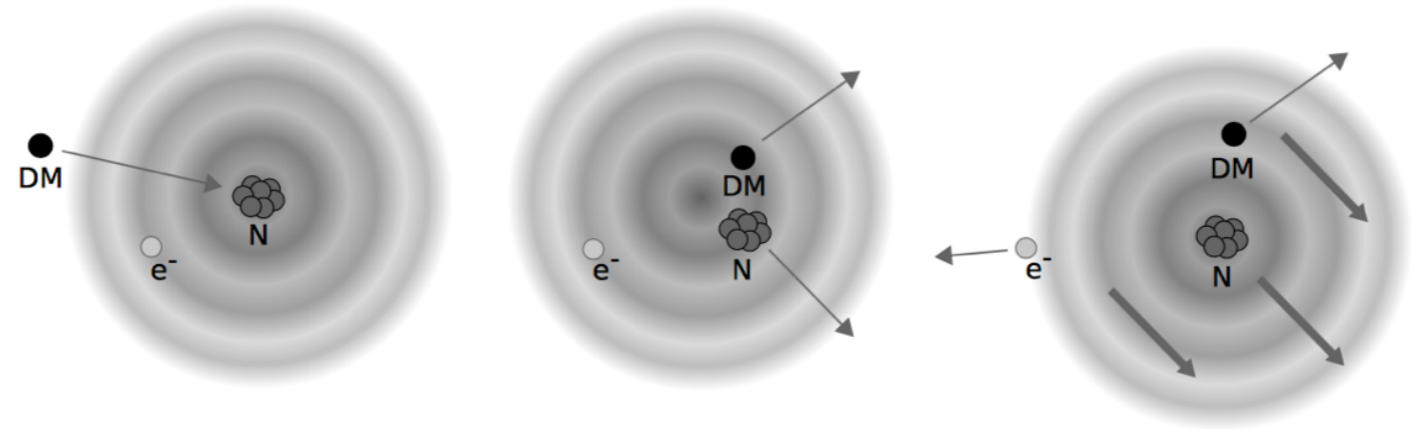
For $m_X \ll m_N$, we are not accessing most of the kinetic energy of the dark matter



- The elastic billiard ball picture breaks (Phonon regime)
- What about *inelastic* recoils? (Migdal effect, Brehmstrahlung)

Migdal effect in atoms

A **hard nuclear recoil** can cause some electrons to be ionized



Studied in detail for atoms (e.g. Xe)

From 1711.09906 (Dolan et al.)

Step 1: boost to the rest frame of recoiling nucleus

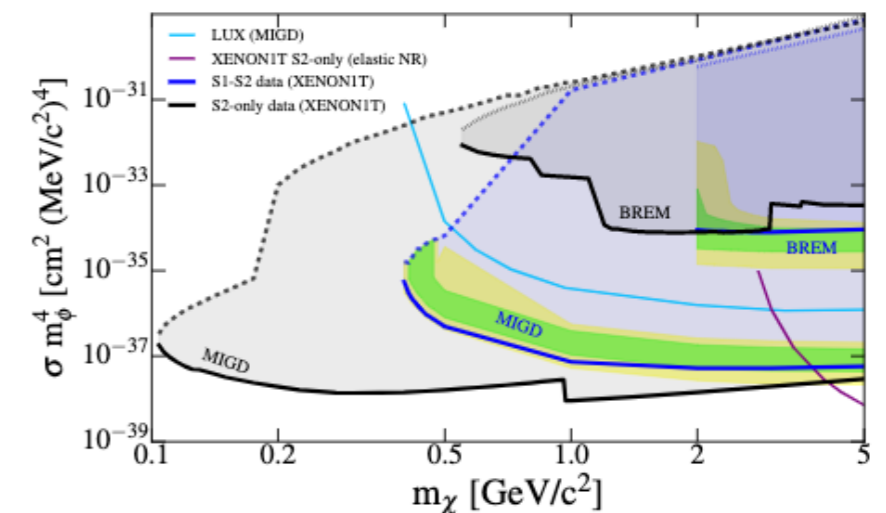
$$|i\rangle \rightarrow e^{im_e \mathbf{v}_N \cdot \sum_{\beta} \mathbf{r}_{\beta}} |i\rangle$$

Step 2: Compute the overlap with the excited wave functions $|f\rangle$

$$\mathcal{M}_{if} = \langle f | e^{im_e \mathbf{v}_N \cdot \sum_{\beta} \mathbf{r}_{\beta}} |i\rangle \approx im_e \langle f | \mathbf{v}_N \cdot \sum_{\beta} \mathbf{r}_{\beta} |i\rangle$$



Transition dipole moment



Alternative calculation

Migdal's trick has a few drawbacks:

- The “brehmstrahlung” analogy is not so clear. E.g. Where is the dependence on the ion charge?
- The boosting feels awkward. Is it really ok in all cases?

We should be able to do a straight-up calculation **in the lab frame, with old fashioned time-dependent perturbation theory!**

$$H(t) = H_0 + H_1(t)$$

$$H_0 = - \sum_{\beta} \frac{Z_N \alpha}{|\mathbf{r}_{\beta}|}$$

$$H_1(t) = - \sum_{\beta} \frac{Z_N \alpha}{|\mathbf{r}_{\beta} - \mathbf{R}_N(t)|} + \sum_{\beta} \frac{Z_N \alpha}{|\mathbf{r}_{\beta}|}$$

With

$$\mathbf{R}_N(t) = \theta(t) \mathbf{v}_N t$$

$$\approx -Z_N \alpha \sum_{\beta} \frac{\hat{\mathbf{r}}_{\beta} \cdot \mathbf{v}_N}{r_{\beta}^2} t \theta(t)$$



Dipole potential

Z_N is the effective charge of the ion; in general it is momentum dependent

Alternative calculation

The transition probability is

$$P_{i \rightarrow f} = \lim_{\eta \rightarrow 0} \left| \frac{1}{\omega} \int_0^\infty dt e^{i(\omega + i\eta)t} \langle f | \frac{dH_1(t)}{dt} | i \rangle \right|^2 = \left| \langle f | \frac{1}{\omega^2} \sum_{\beta} \frac{Z_N \alpha \hat{\mathbf{r}}_{\beta} \cdot \mathbf{v}_N}{\mathbf{r}_{\beta}^2} | i \rangle \right|^2$$

Let's compare the results at the level of the matrix element:

Migdal's trick

$$\mathcal{M}_{if} = im_e \mathbf{v}_N \cdot \langle f | \sum_{\beta} \mathbf{r}_{\beta} | i \rangle$$

Perturbation theory

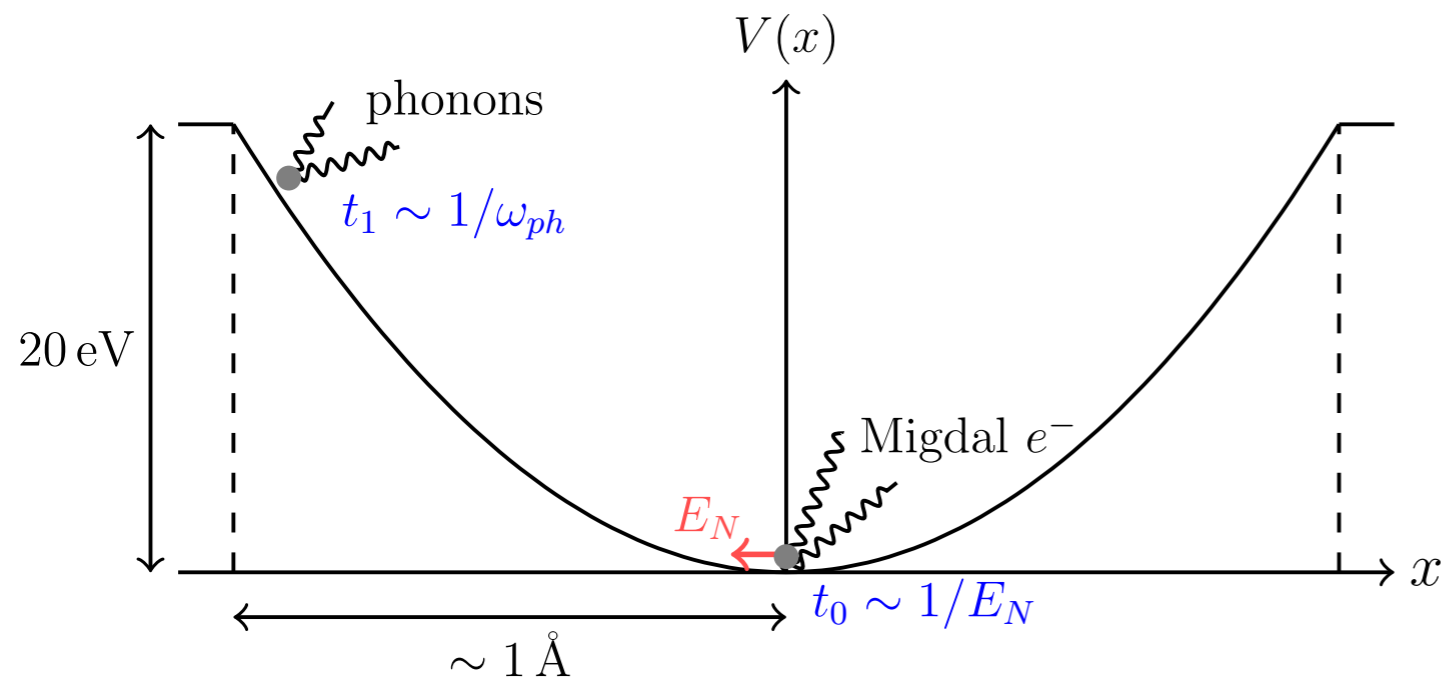
$$\mathcal{M}_{if} = i \langle f | \frac{1}{\omega^2} \sum_{\beta} \frac{Z_N \alpha \hat{\mathbf{r}}_{\beta} \cdot \mathbf{v}_N}{\mathbf{r}_{\beta}^2} | i \rangle$$

Use this for crystals!

One can prove that these are equivalent, but for *isolated* atoms only. (See back-up slides)

For a crystal, we cannot boost the system since the crystal rest frame is a preferred frame!

The impulse approximation



If the DM is heavy enough, most collisions take place at an **energy well** above the **typical phonon energy** ($\sim 30 \text{ meV}$)

If this is the case, the nucleus doesn't feel the crystal potential during the initial hard recoil

We can **treat the outgoing nucleus as plane wave** on the time scale of the DM collision (The *initial state nucleus* is however still treated as bound in the crystal potential)

This is known as the **adiabatic approximation** or the **impulse approximation**

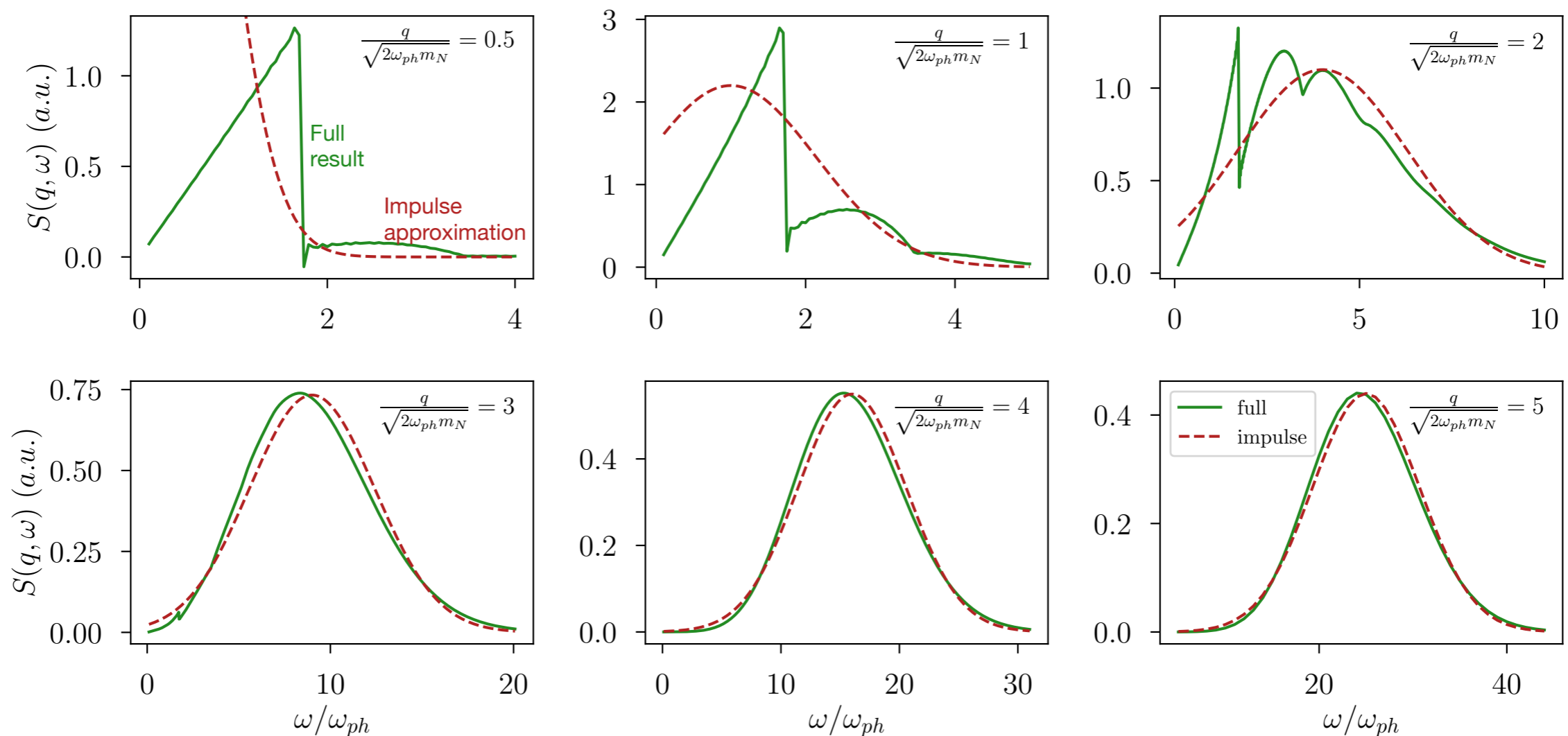
When it is valid we can factorize the long distance physics (phonons) from the short distance physics (Migdal effect).

Crystal form factor

How important is the presence of the lattice for the kinematics of the recoiling nucleus?

Let's analyse a simplified model of a harmonic crystal with a Debye density of states:

Structure function for regular nuclear recoil (no Migdal):

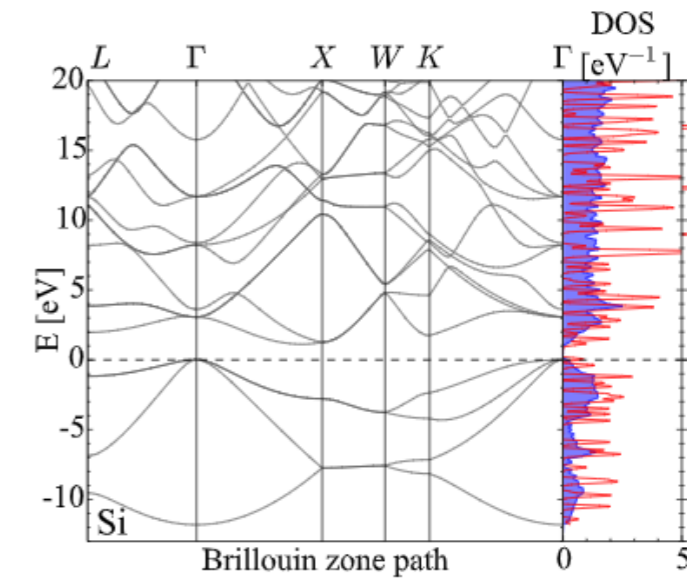


The impulse approximation fails badly for $q^2 \lesssim m_N \omega_{ph}$

Migdal effect in semi-conductors

A **hard nuclear recoil** can cause valence
-> conduction band transition

Confusing to calculate in semi-
conductors, since the electrons don't
belong to any particular atom



From 1509.01598 (Essig et al.)

We cannot boost because the crystal frame is a preferred frame

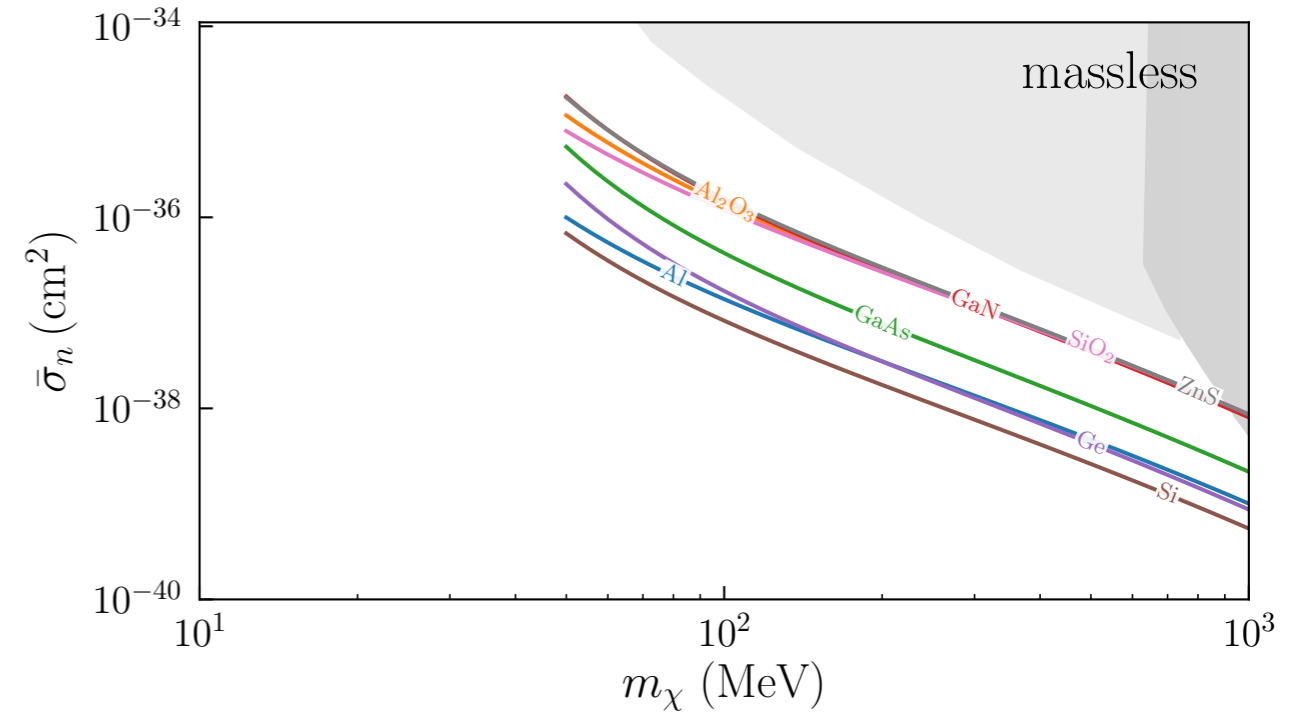
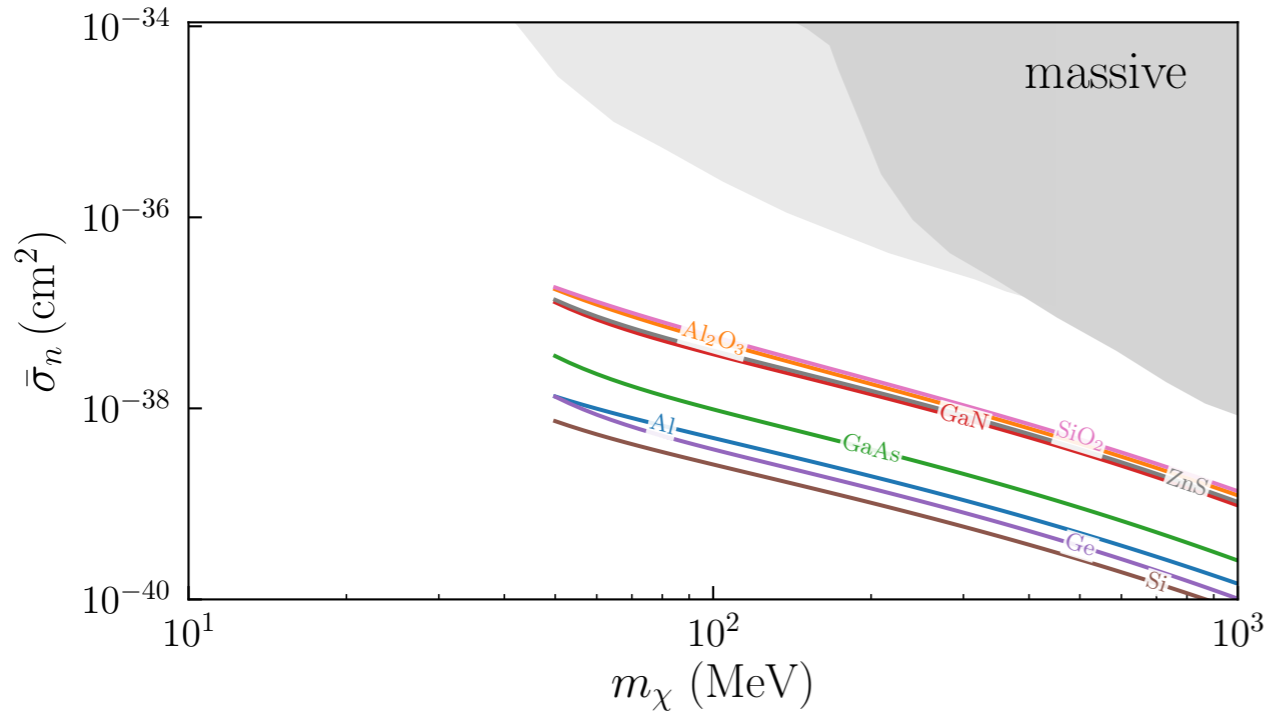
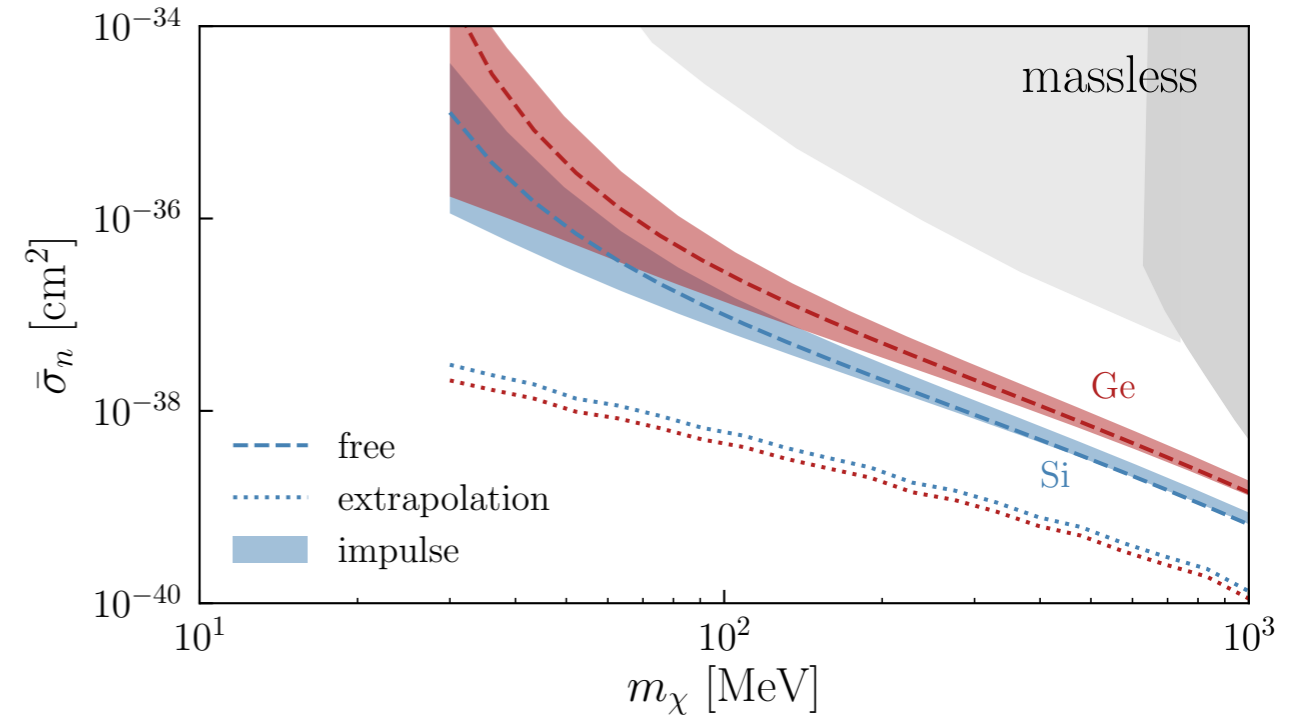
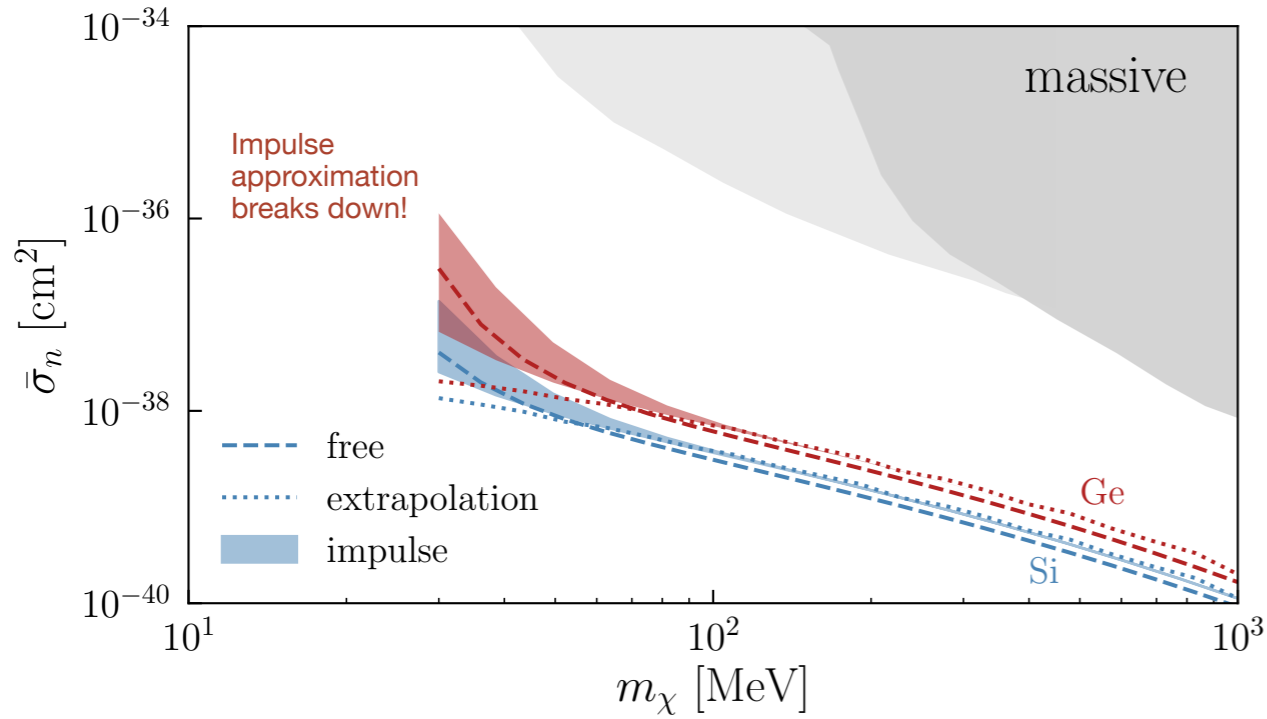
Result:

$$R = \frac{8\pi^2 Z_{\text{ion}}^2 \alpha A^2 \rho_{\chi} \bar{\sigma}_n}{m_N m_{\chi} \mu_{\chi n}^2} \int d^3 v f_{\chi}(v) \int d\omega \int \frac{d^3 \mathbf{q}_N}{(2\pi)^3} \int \frac{d^3 \mathbf{p}_f}{(2\pi)^3} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{1}{k^2} \text{Im} \left[\frac{-1}{\epsilon(\mathbf{k}, \omega)} \right] \left[\frac{1}{\omega - \frac{\mathbf{q}_N \cdot \mathbf{k}}{m_N}} - \frac{1}{\omega} \right]^2$$

DM form factor
Crystal form factor

↑
Nucleus is not a free particle!

Migdal effect results



We believe the electronic response is on solid ground

Nuclear recoil (impulse approximation) is main source of uncertainty

Outline

- Dark Matter - e^- recoils in semiconductors
- Migdal effect in semiconductors
- DarkELF package

main 1 branch 0 tags

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Code

Simon Knapen Merge branch 'main' of github.com:tongylin/DarkELF into main

18a4517 17 days ago 15 commits

darkelf	fixed loading error in Migdal module	17 days ago
data	initial commit	last month
examples	removed checkpoint files	last month
README.md	Update README.md	23 days ago

README.md

DarkELF

DarkELF is a python package capable of calculating interaction rates of light dark matter in dielectric materials, including screening effects. The full response of the material is parametrized in the terms of the energy loss function (ELF) of material, which DarkELF converts into differential scattering rates for both direct dark matter electron scattering and through the Migdal effect. In addition, DarkELF can calculate the rate to produce phonons from sub-MeV dark matter scattering via the dark photon mediator, as well as the absorption rate for dark matter comprised of dark photons. The package currently includes precomputed ELFs for Al, Al₂O₃, GaAs, GaN, Ge, Si, SiO₂, and ZnS, and allows the user to easily add their own ELF extractions for arbitrary materials.

See arXiv [2104.12786](#) for a description of the implementation

Authors

Simon Knapen, Jonathan Kozaczuk and Tongyan Lin

Physics

ELF

Currently DarkELF contains ELF look-up tables obtained with the [GPAW](#) density functional theory code for Si and Ge, as well as data-driven Mermin model for the remaining materials. The Lindhard ELF is also included. DarkELF also comes with a number of measured ELFs in the optical limit for energy depositions below the electronic band gap, which is relevant for phonon processes. Additional materials and ELF computations may be added at a later date. When using a particular ELF computation, please refer to the relevant experimental papers and/or GPAW package. These references can be found in arXiv [2104.12786](#).

About

Calculating dark matter scattering and absorption rates with the energy loss functions (ELF)

Readme


Releases

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Packages

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Contributors 2

 simonknapen86

 tongylin Tongyan Lin

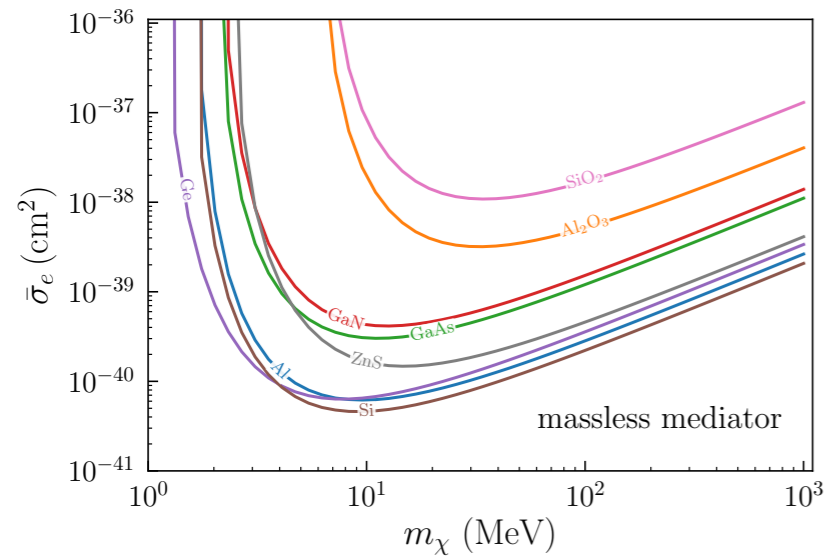
Languages

Python 100.0%

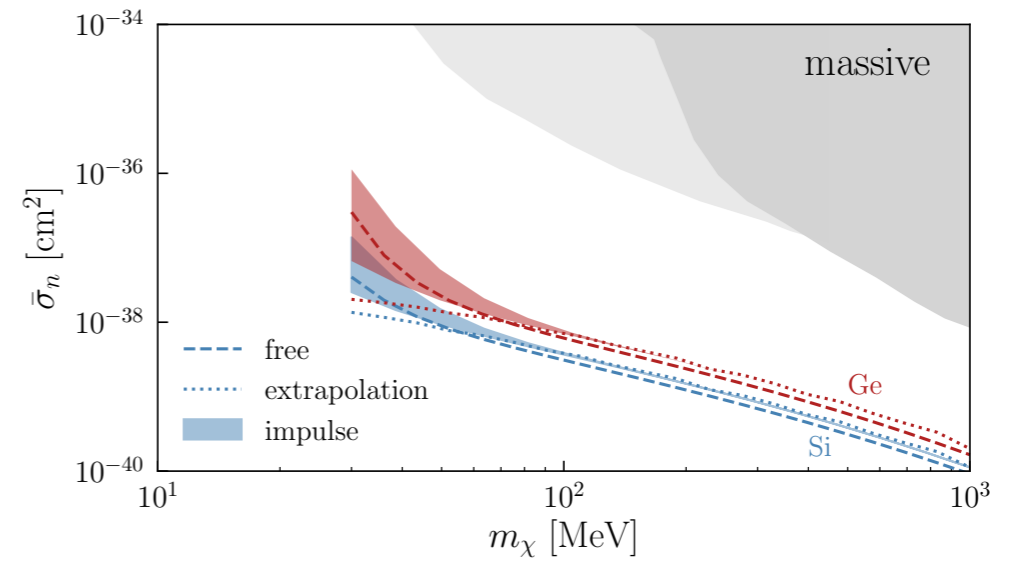
<https://github.com/tongylin/DarkELF>

DarkELF functions

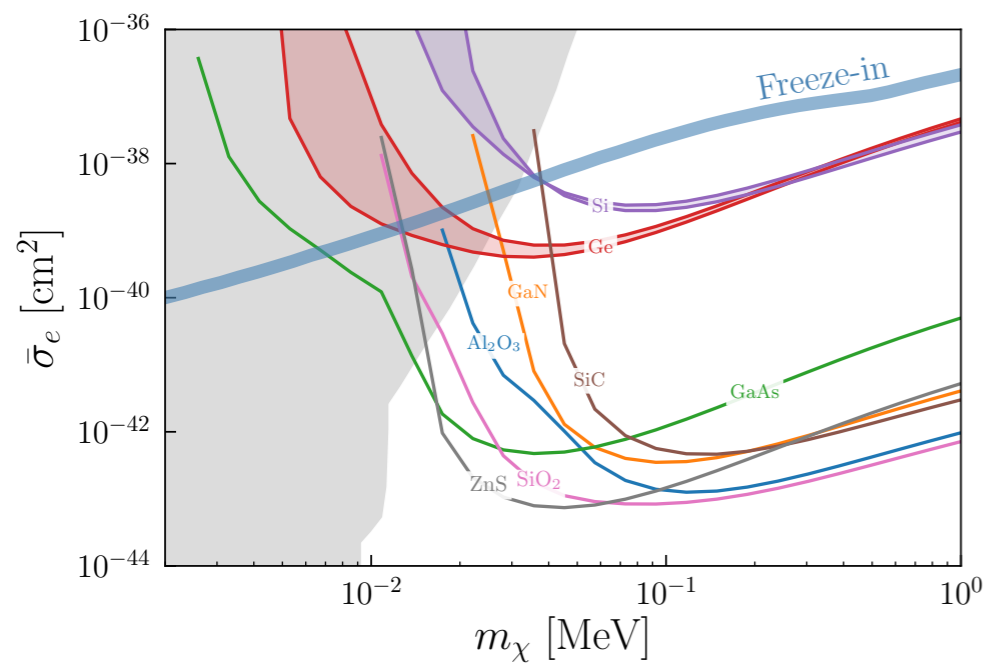
DM - electron scattering



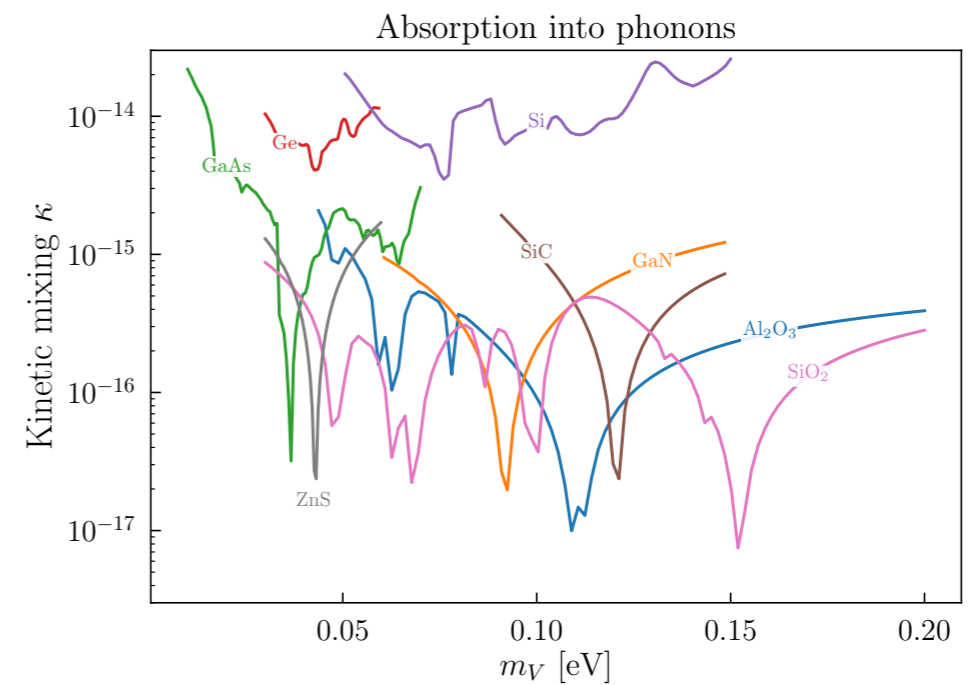
Migdal effect



DM - phonon scattering



Dark photon absorption



Summary

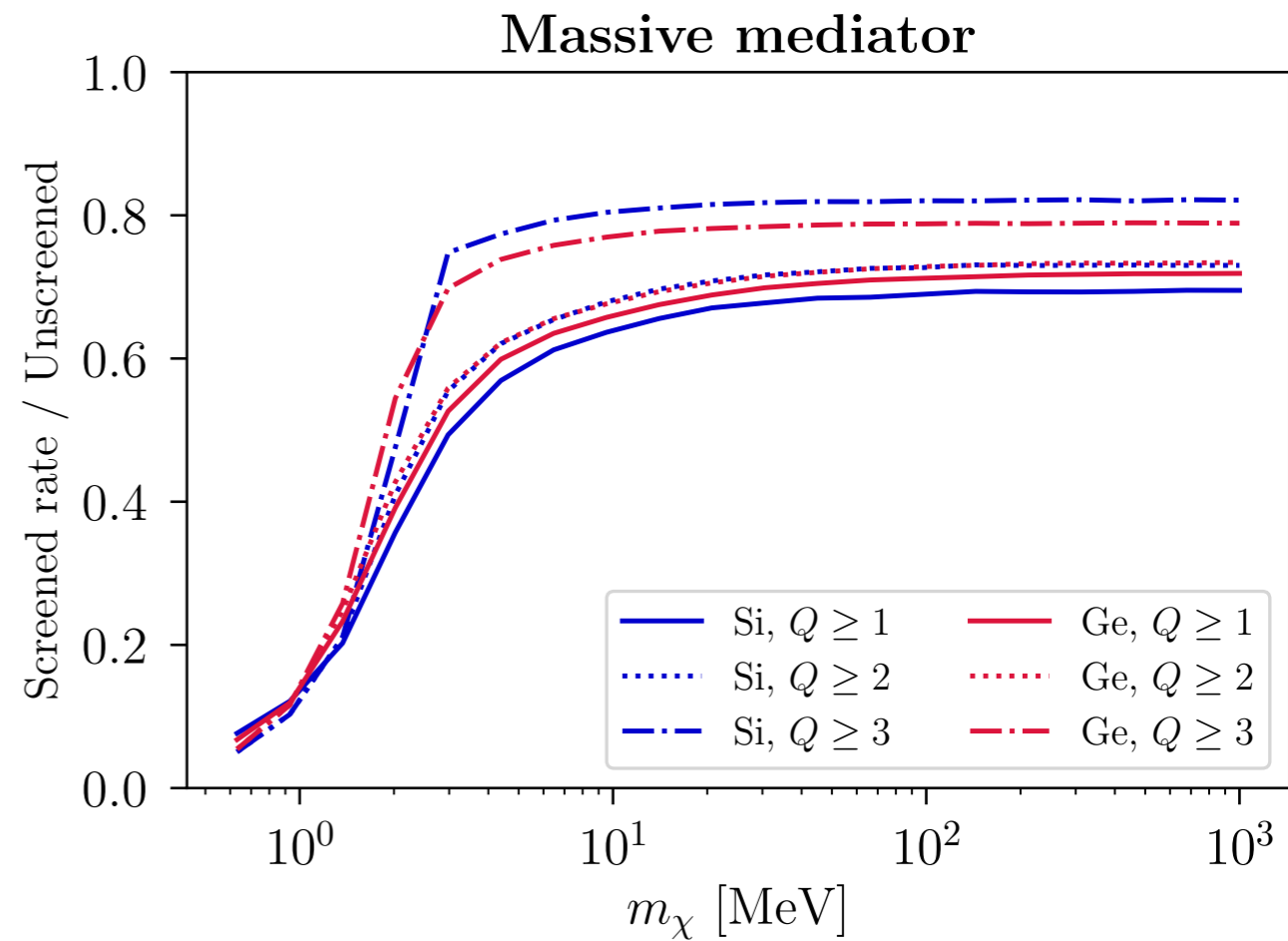
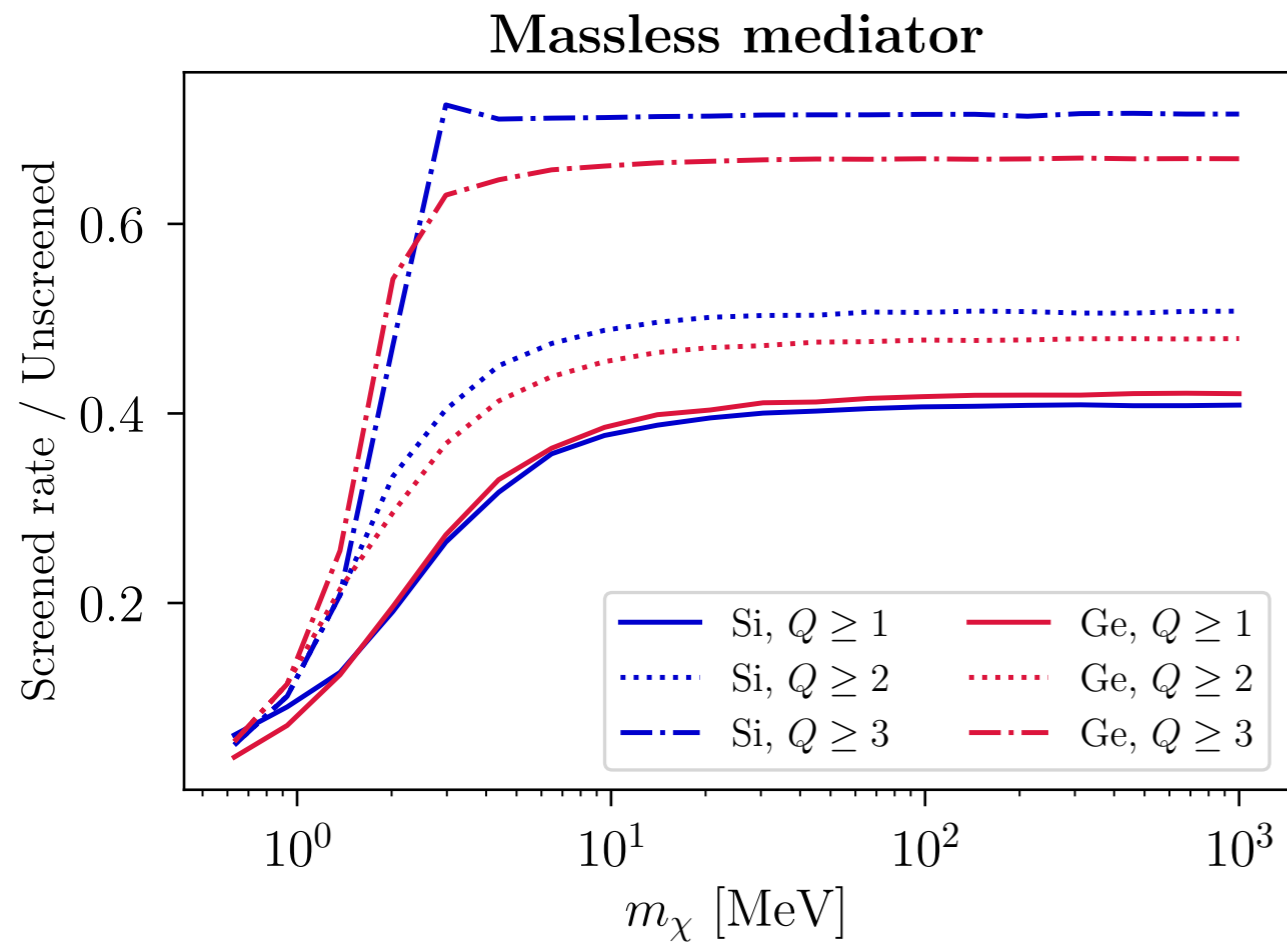
- Electron recoil reach is slightly weaker when screening is included.
- The ELF is a very convenient way to package the material dependent properties in a single function
- Semi-conductor experiments (SENSEI, superCMDS, DAMIC,...) should have very nice sensitivity to low energy nuclear recoils through the Migdal effect.
- darkELF python code can compute inelastic scattering of DM with electrons, nuclei and phonons, as well as absorption processes.

Questions?



Extra slides

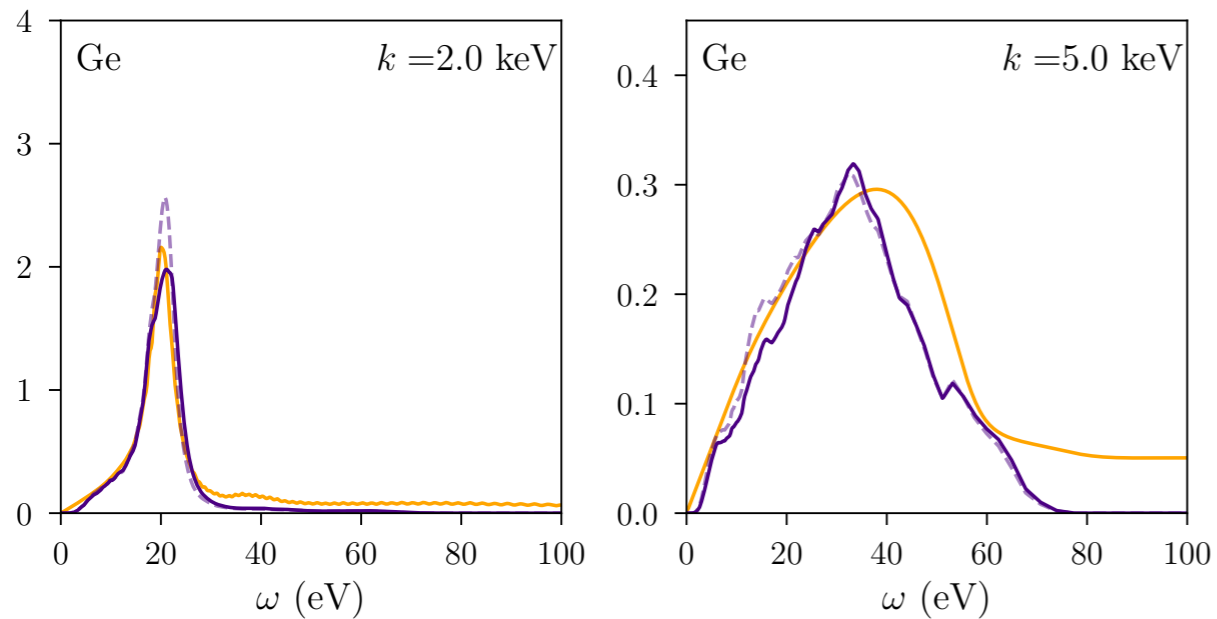
Threshold dependence



The screening is the **strongest for energies near the bandgap**, so the higher the threshold the less important it becomes

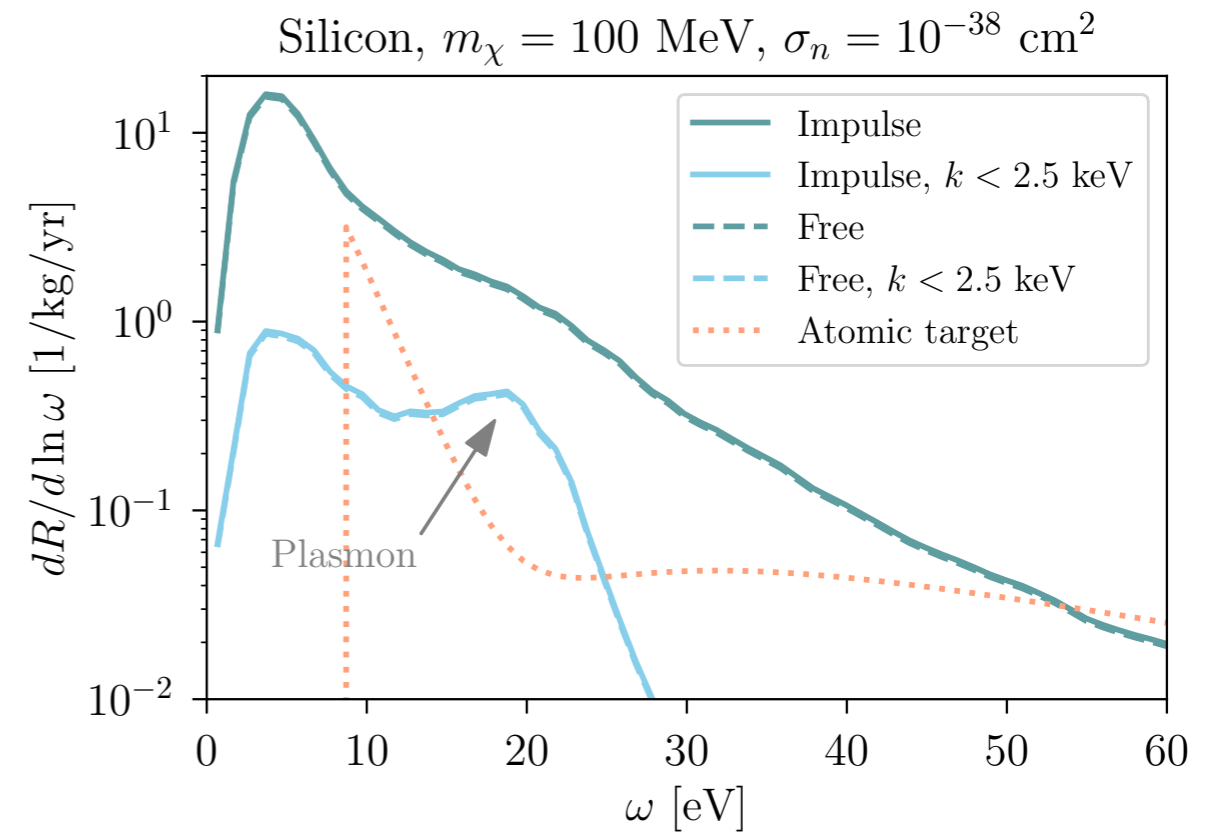
Plasmons

In electron recoils



DM- e^- scattering: $k \gtrsim 4 \text{ keV} \times \omega / (10 \text{ eV})$

In nuclear recoils

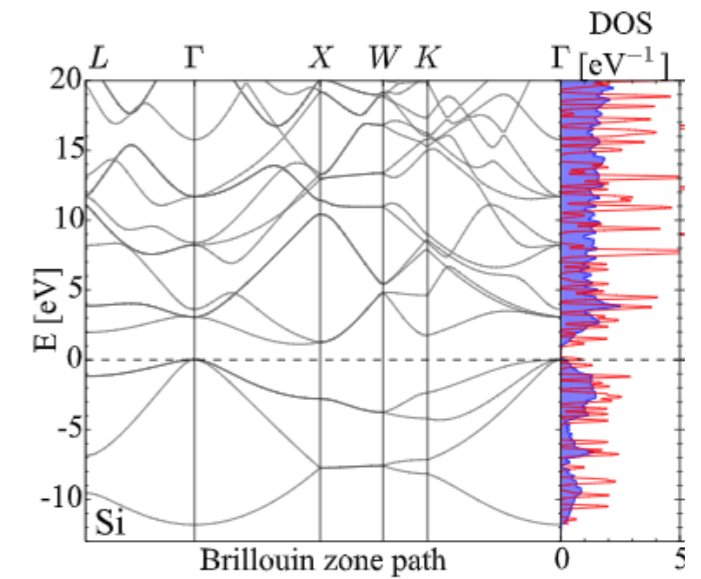


Plasmon production is not relevant in normal materials, for a standard DM velocity profile

Migdal effect in semi-conductors

A **hard nuclear recoil** can cause valence
-> conduction band transition

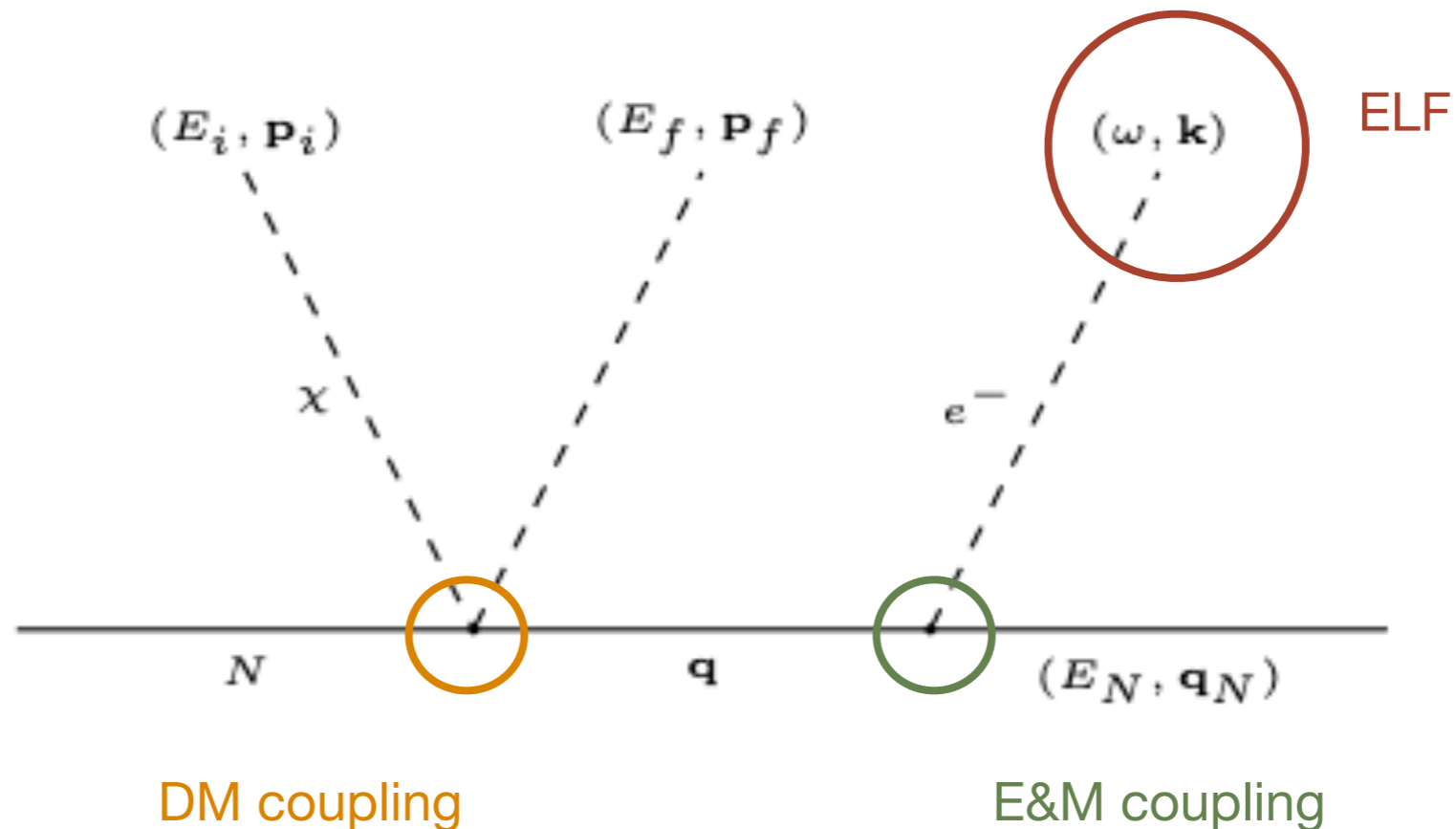
Confusing to calculate in semi-
conductors, since the electrons don't
belong to any particular atom



From 1509.01598 (Essig et al.)

We cannot boost because the crystal frame is a preferred frame

Leading order calculation in E&M



Making sense of this

For the Coulomb Hamiltonian

$$H_0 = \sum_{\beta} \frac{|\mathbf{p}_{\beta}|^2}{2m_e} + V(\mathbf{r}_{\beta}, \mathbf{r}_N)$$

We have a number of operator identities:

$$[\mathbf{r}_{\beta}, H_0] = i \frac{1}{m_e} \mathbf{p}_{\beta}$$

And

$$[p_{\beta}, H_0] = -i \frac{dV}{d\mathbf{r}_{\beta}}$$

Total force exerted on the electron

$$\begin{aligned} \mathcal{M}_{if}^{(Migdal)} &= im_e \mathbf{v}_N \cdot \langle f | \sum_{\beta} \mathbf{r}_{\beta} | i \rangle \\ &= -i \frac{m_e}{\omega} \mathbf{v}_N \cdot \langle f | \sum_{\beta} [\mathbf{r}_{\beta}, H_0] | i \rangle \quad \text{used} \quad \omega = E_f - E_i \\ &= \frac{1}{\omega} \mathbf{v}_N \cdot \langle f | \sum_{\beta} \mathbf{p}_{\beta} | i \rangle \\ &= -\frac{1}{\omega^2} \mathbf{v}_N \cdot \langle f | \sum_{\beta} [\mathbf{p}_{\beta}, H_0] | i \rangle \\ &= i \frac{1}{\omega^2} \mathbf{v}_N \cdot \langle f | \sum_{\beta} \frac{dV}{d\mathbf{r}_{\beta}} | i \rangle \end{aligned}$$

Making sense of this

$$\begin{aligned}
 \mathcal{M}_{if}^{(Migdal)} &= im_e \mathbf{v}_N \cdot \langle f | \sum_{\beta} \mathbf{r}_{\beta} | i \rangle \\
 &= -i \frac{m_e}{\omega} \mathbf{v}_N \cdot \langle f | \sum_{\beta} [\mathbf{r}_{\beta}, H_0] | i \rangle \quad \text{used} \quad \omega = E_f - E_i \\
 &= \frac{1}{\omega} \mathbf{v}_N \cdot \langle f | \sum_{\beta} \mathbf{p}_{\beta} | i \rangle \\
 &= -\frac{1}{\omega^2} \mathbf{v}_N \cdot \langle f | \sum_{\beta} [\mathbf{p}_{\beta}, H_0] | i \rangle \\
 &= i \frac{1}{\omega^2} \mathbf{v}_N \cdot \langle f | \sum_{\beta} \frac{dV}{d\mathbf{r}_{\beta}} | i \rangle \quad \longrightarrow \quad \text{Proportional to total force exerted in the electron}
 \end{aligned}$$

Electron-electron interactions cancel out in the same, only the force from the nucleus remains

$$\begin{aligned}
 &= i \frac{Z_N \alpha}{\omega^2} \mathbf{v}_N \cdot \langle f | \sum_{\beta} \frac{\hat{\mathbf{r}}_{\beta}}{|\mathbf{r}_{\beta} - \mathbf{r}_N|^2} | i \rangle \\
 &= i \frac{Z_N \alpha}{\omega^2} \mathbf{v}_N \cdot \langle f | \sum_{\beta} \frac{\hat{\mathbf{r}}_{\beta}}{|\mathbf{r}_{\beta}|^2} | i \rangle \quad \text{taking} \quad \mathbf{r}_{\beta} \gg \mathbf{r}_N \\
 &= \mathcal{M}_{if}^{(pert)}
 \end{aligned}$$

