

# Inelastic nuclear recoils

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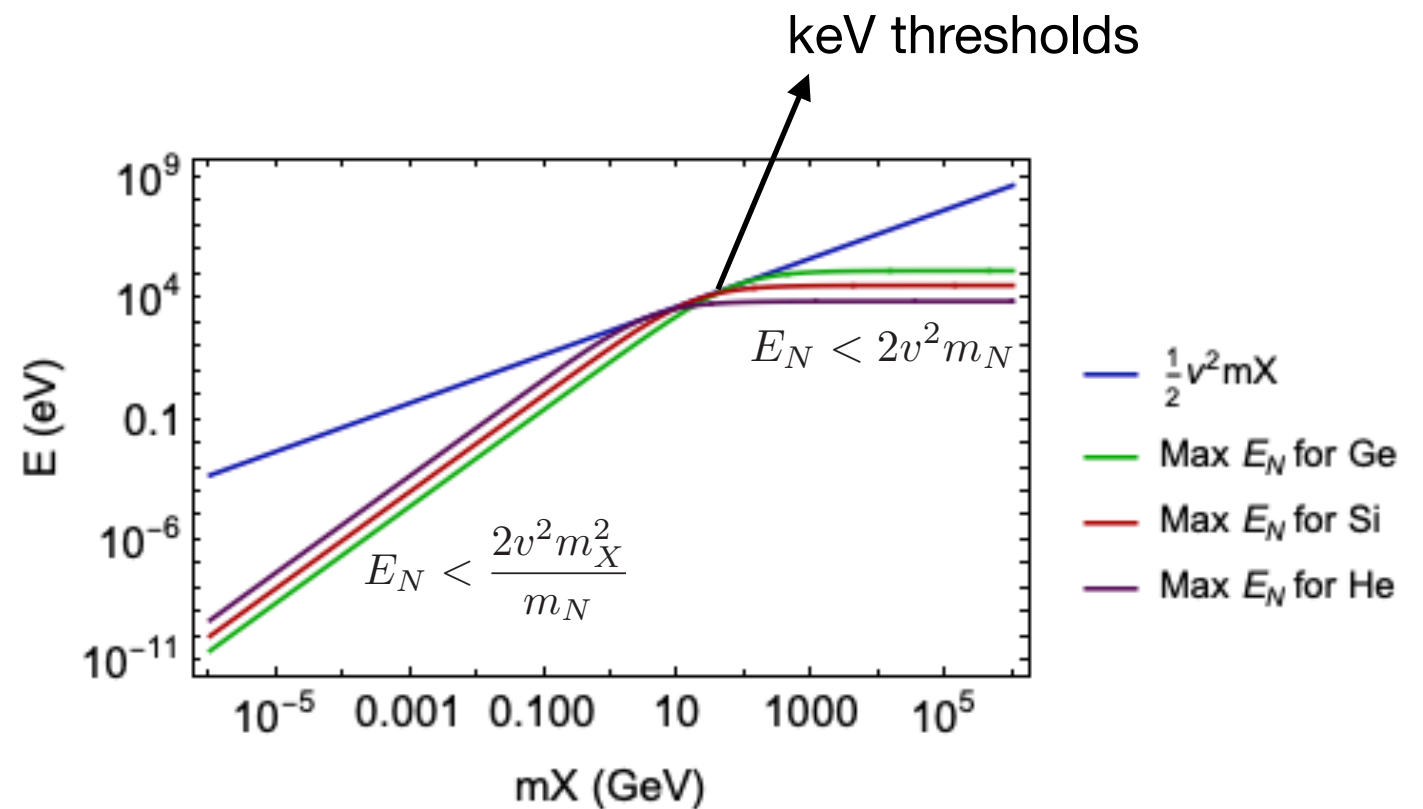
<http://dingercatadventures.blogspot.com/2012/08/>

# Elastic nuclear recoil kinematics

Momentum conservation implies that for elastic nuclear recoils we have

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

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

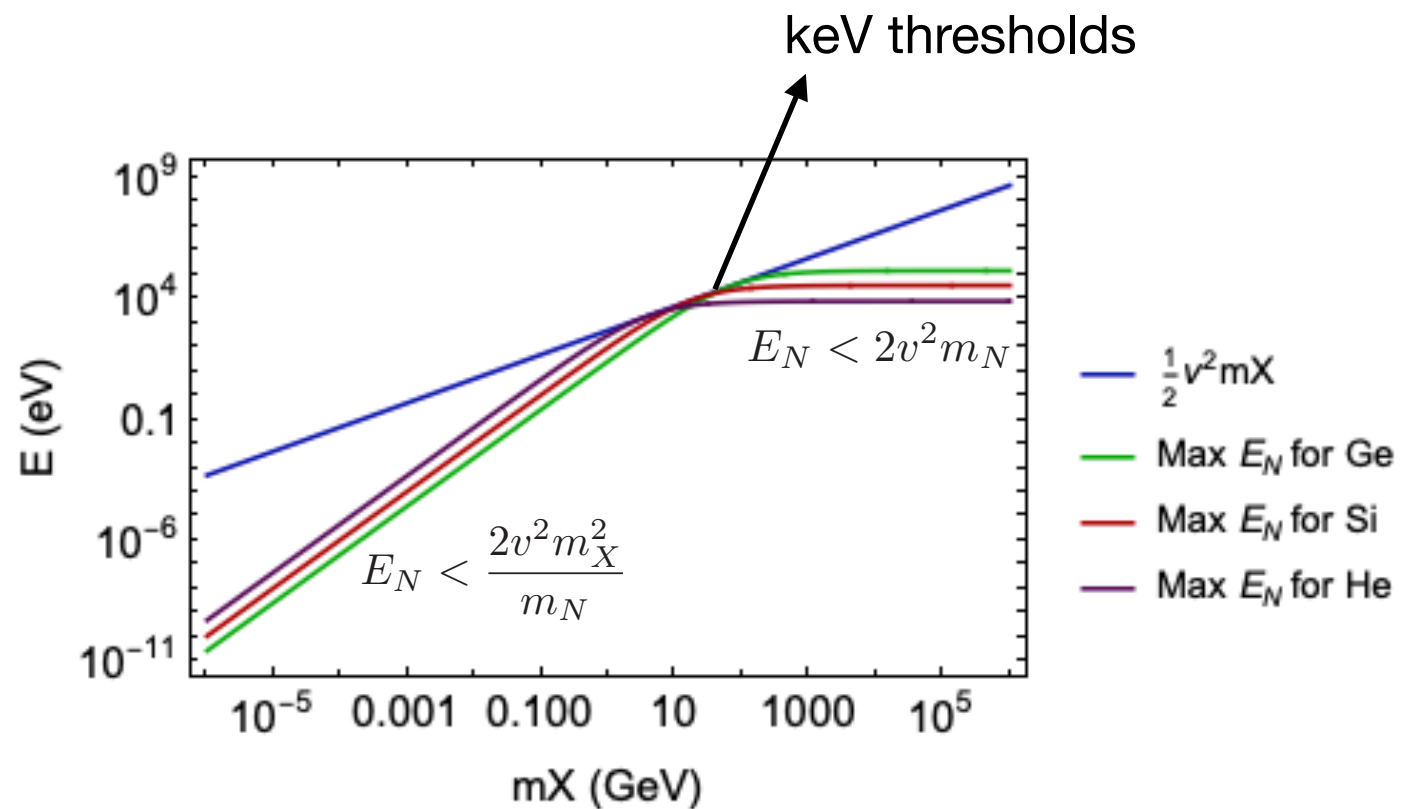


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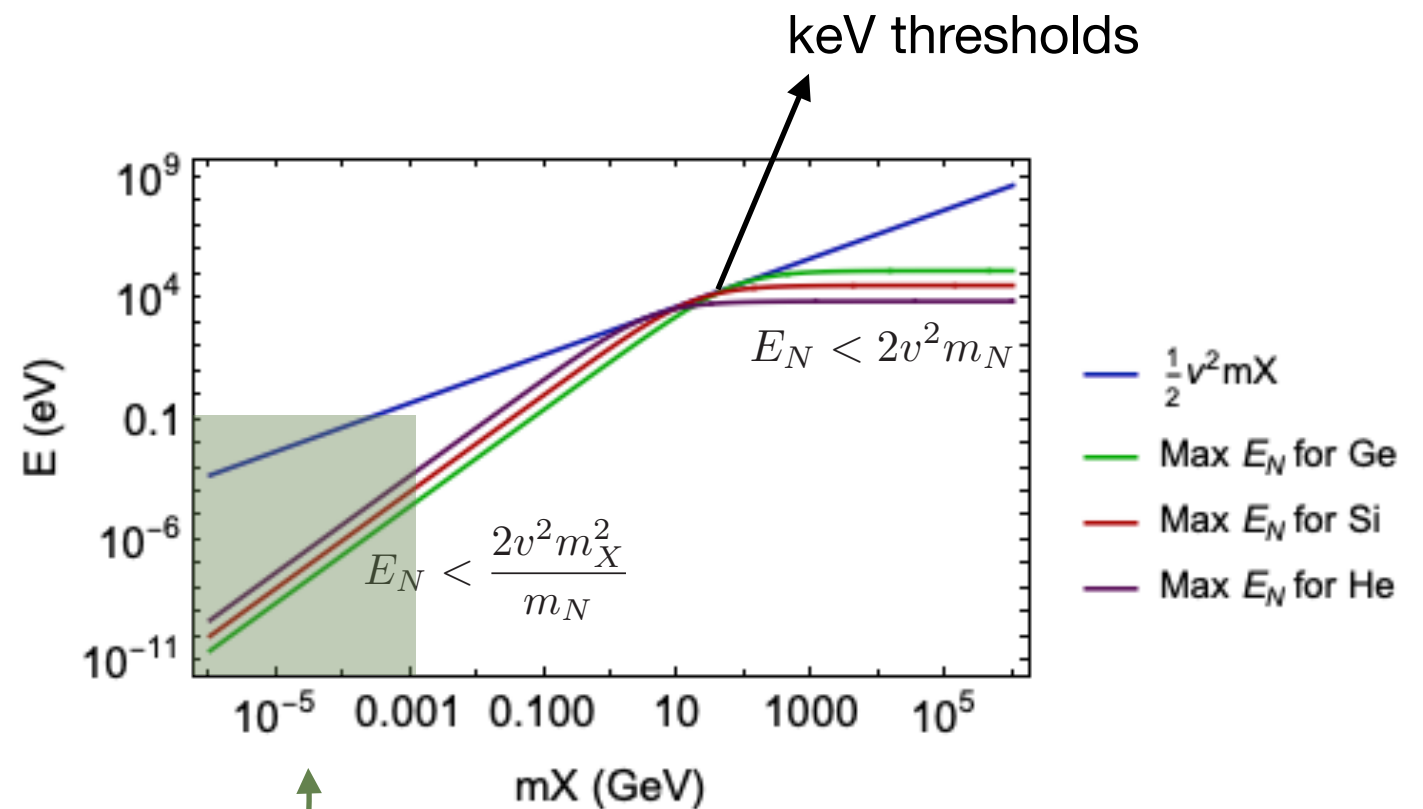
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(Tomorrow's lecture)
2. What about *inelastic* recoils?  
(Today's lecture)

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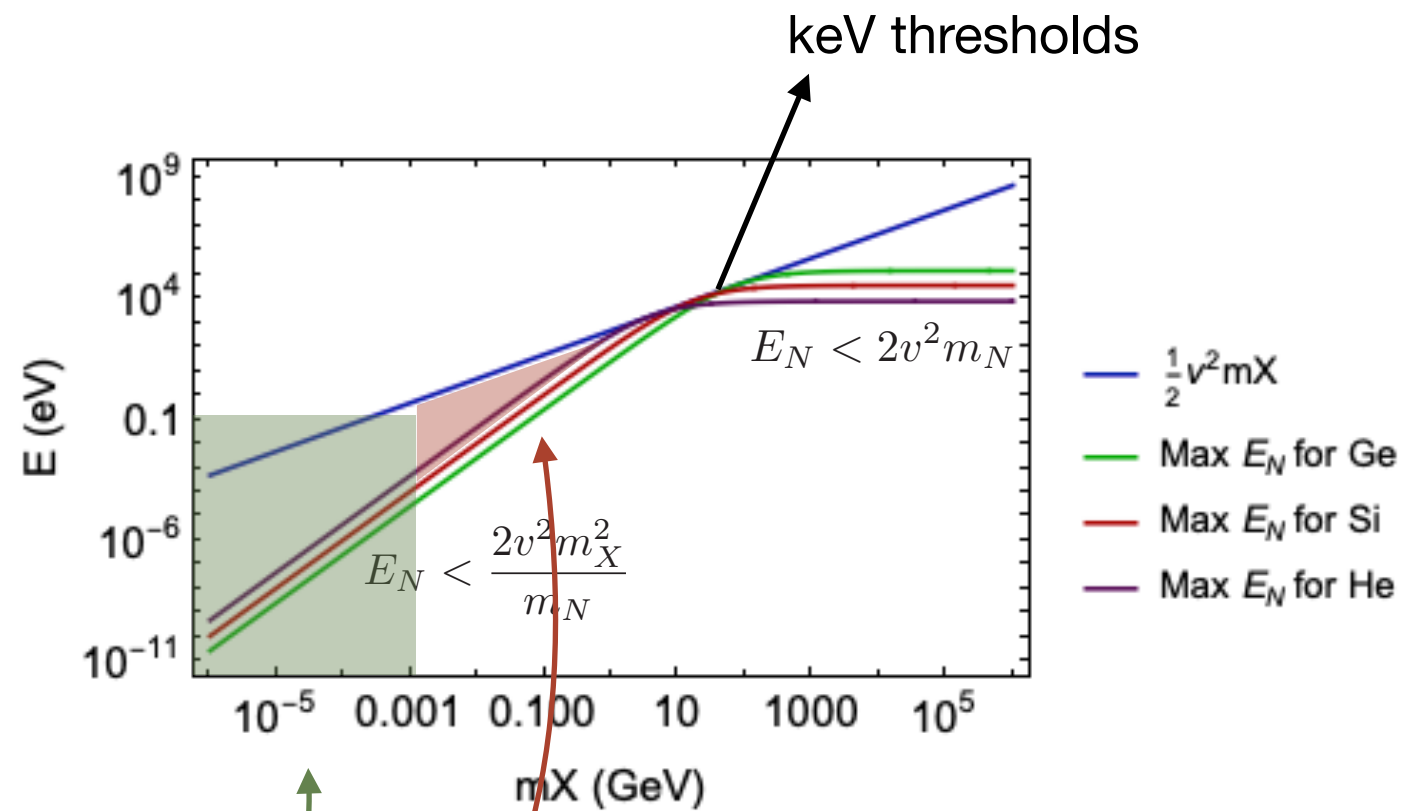


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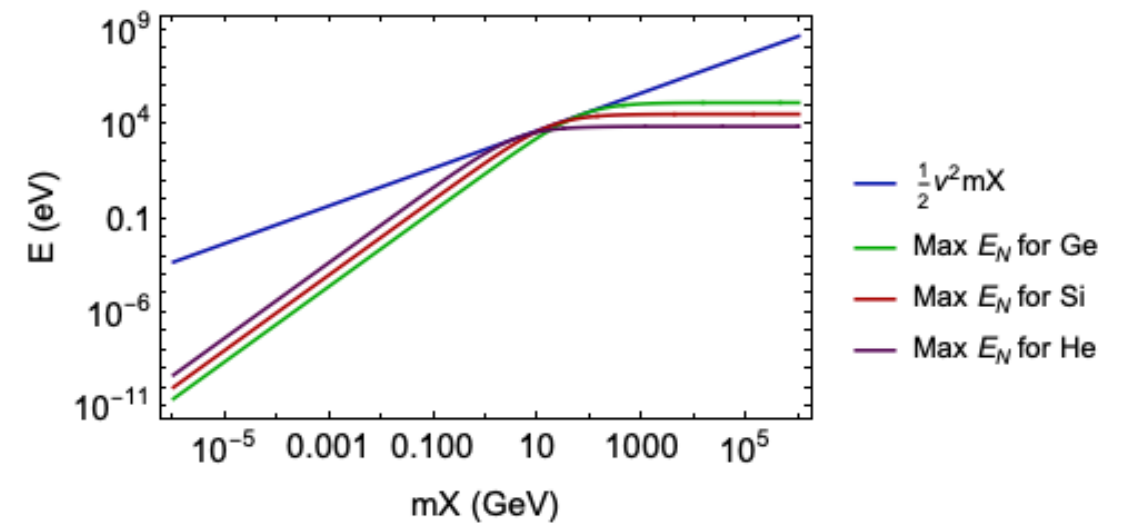
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# Inelastic nuclear recoils

Kinetic energy is much too low to excite nuclear excitations

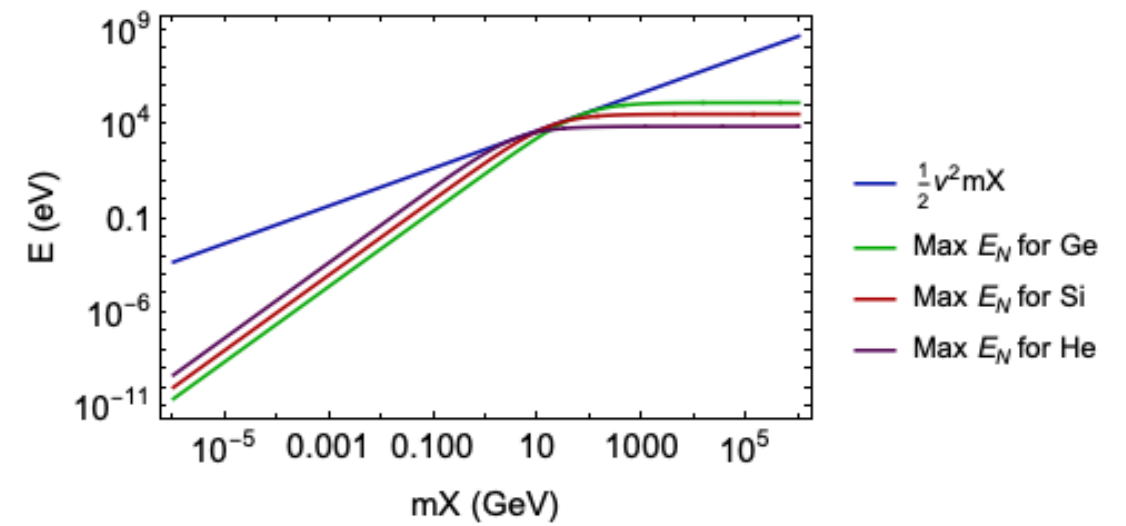
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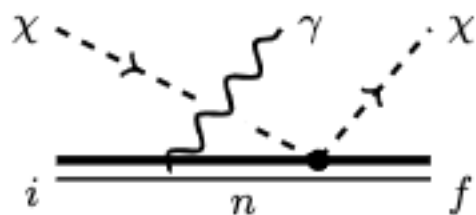
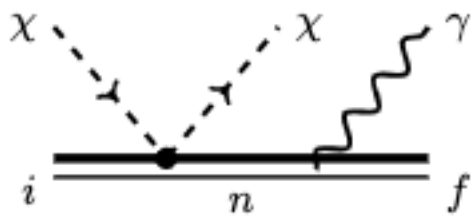
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Photons:

Brehmstrahlung

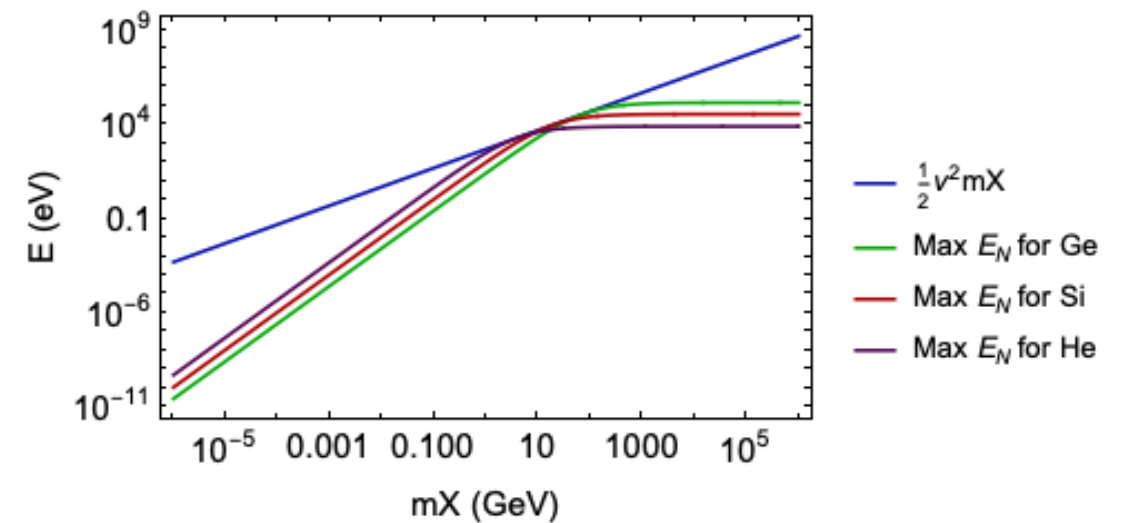
C. Kouvaris, J. Pradler: arXiv 1607.01789



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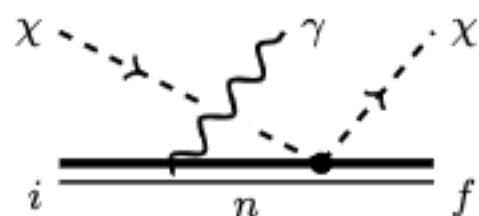
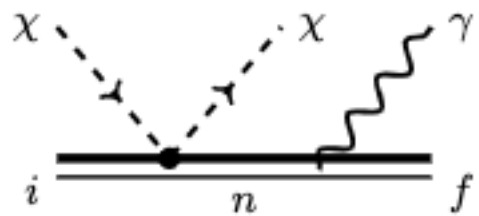
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Photons:

Brehmstrahlung

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Electrons (Migdal effect):

In atoms (Xe, Ar, He, etc)

A. Migdal (1939)

R. Bernabei et. al.: arXiv 0706.1421

M. Ibe, W. Nakano, Y. Shoji and K. Suzuki: arXiv 1707.07258

...

In crystals (Si, Ge, GaAs, etc)

SK, J. Kozaczuk, T. Lin: arXiv 2011.09496

Z.-L. Liang, C. Mo, F. Zheng and P. Zhang: arXiv 2011.13352

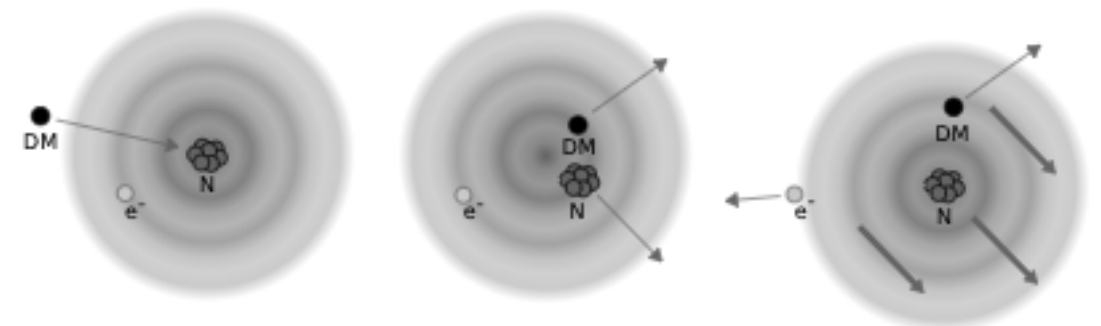
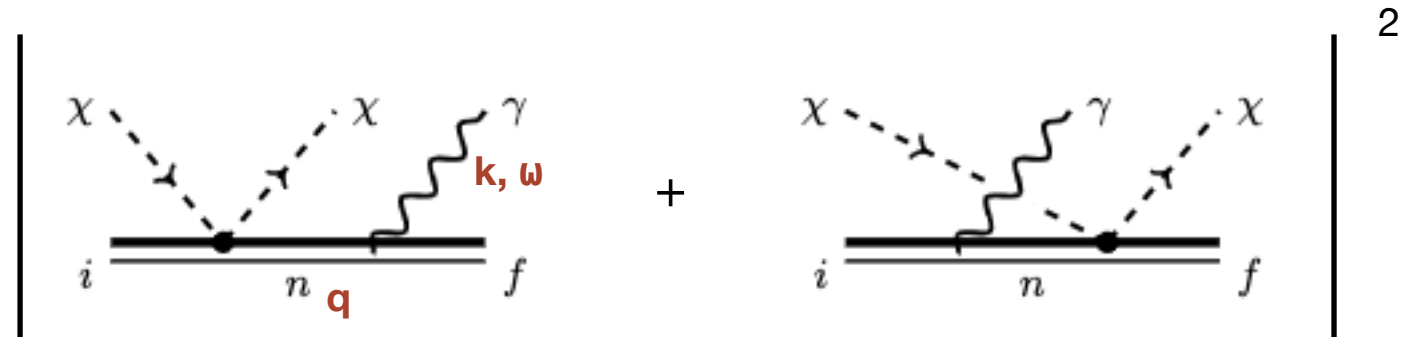


Fig from arXiv 1711.09906

# Brehmstrahlung

## Main features:

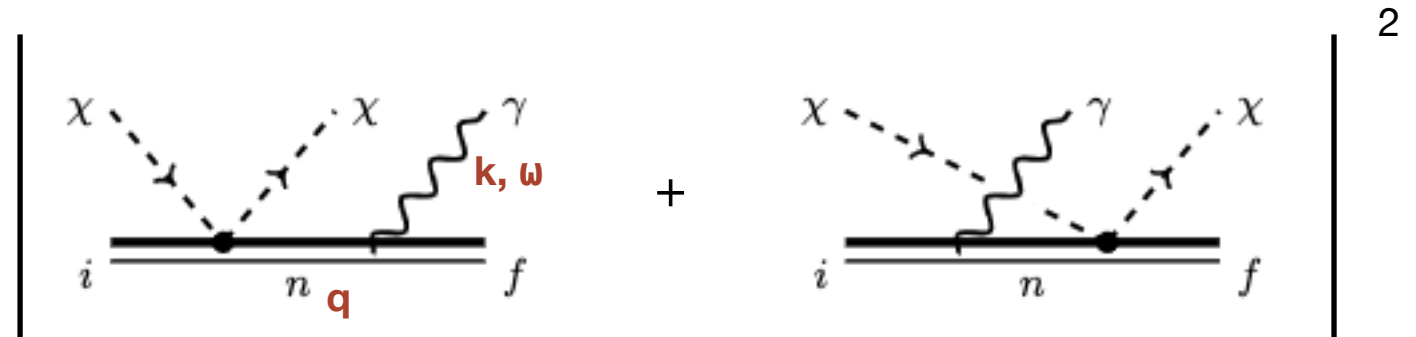
- Leading order in  $\alpha$
- Destructive interference
- Three body phase space



# Brehmstrahlung

## Main features:

- Leading order in  $\alpha$
- Destructive interference
- Three body phase space



## Soft limit:

If  $k \ll q$ , we can treat the photon emission as a small correction on top of an elastic nuclear recoil

Holds if

$$\omega \ll qv = \sqrt{m_N E_R} v \approx 10 \text{ keV} \times \sqrt{\frac{A}{130}} \times \sqrt{\frac{E_R}{1 \text{ keV}}}$$

No problem, detectors like XENON, CMDS etc can easily see  $\sim \text{keV}$  photons, as they leave a strong *ionization* signal

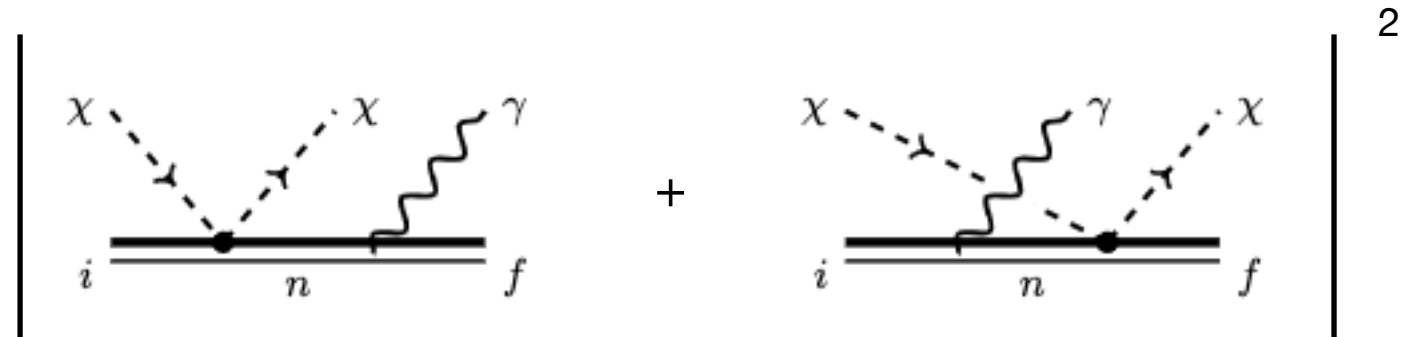
# Brehmstrahlung

Free ion approximation:

$$\left. \frac{d^2\sigma}{dE_R d\omega} \right|_{\text{naive}} = \frac{4Z^2\alpha}{3\pi} \frac{1}{\omega} \frac{E_R}{m_N} \times \frac{d\sigma}{dE_R} \Theta(\omega_{\text{max}} - \omega).$$

Not very good, because electrons provide **screening**

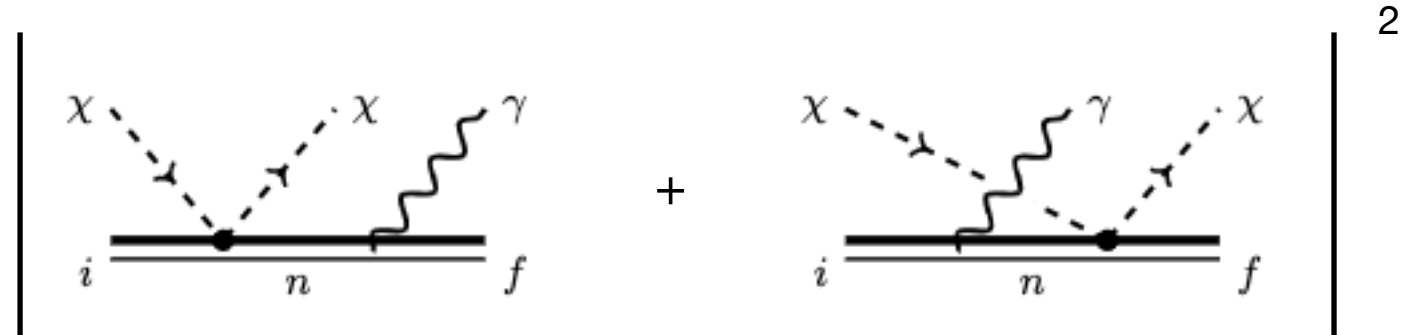
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Instead

Frequency-dependent effective charge

$$\frac{d^2\sigma}{d\omega dE_R} = \frac{4\alpha}{3\pi\omega} \frac{E_R}{m_N} |Z(\omega)|^2 \times \frac{d\sigma}{dE_R} \theta\left(\frac{m_X v^2}{2} - \omega\right)$$

The effective charge is related to the polarizability of the atom

$$Z(\omega) = -\frac{\alpha(\omega)}{\alpha} m_e \omega^2$$

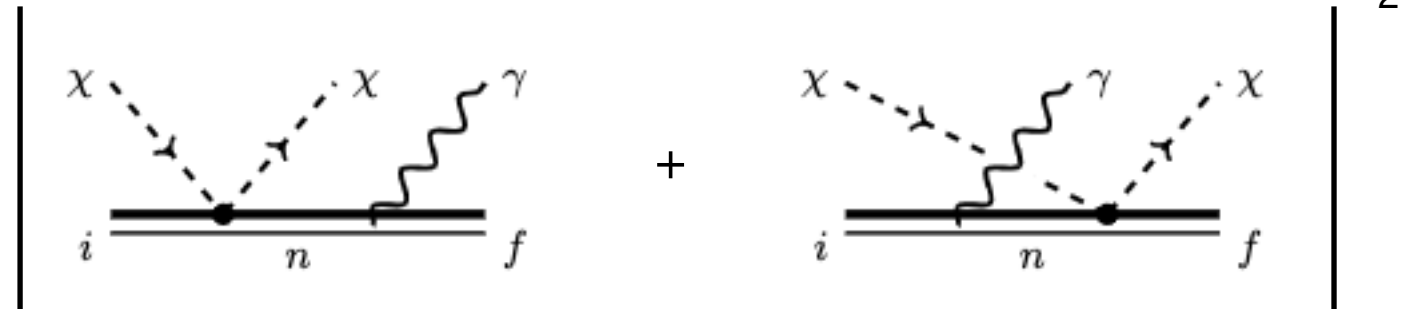
In the high energy limit this reduces to the free-ion ion result  $Z(\omega) \rightarrow Z$  for  $\omega \rightarrow \infty$



# Brehmstrahlung

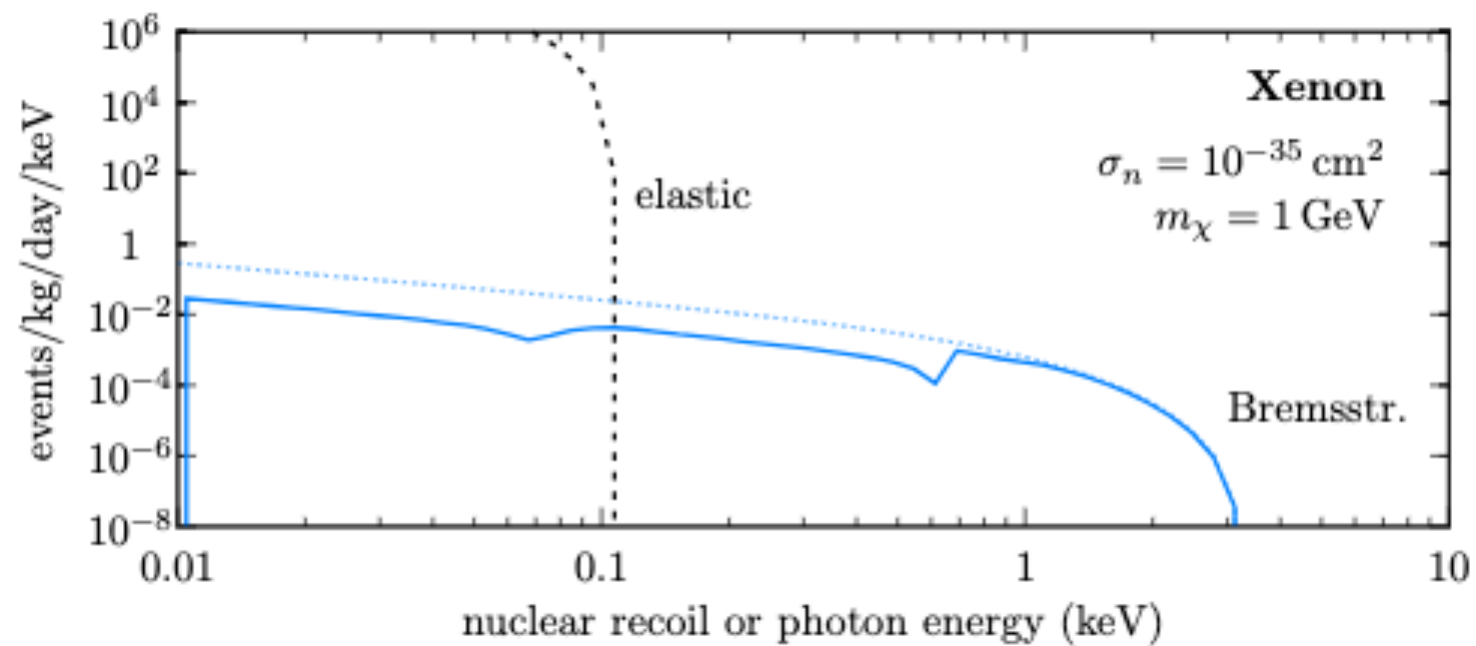
Full result

$$\frac{d^2\sigma}{d\omega dE_R} = \frac{4\alpha}{3\pi\omega} \frac{E_R}{m_N} |Z(\omega)|^2 \times \frac{d\sigma}{dE_R} \theta\left(\frac{m_X v^2}{2} - \omega\right)$$



Extract  $Z(\omega)$  from measured data

Result



# The Migdal effect

Usual explanation:

Nucleus is **suddenly kicked** and rushes away. Not all the electron wave functions have time to respond and one or more electron is left behind

↓  
Ionization

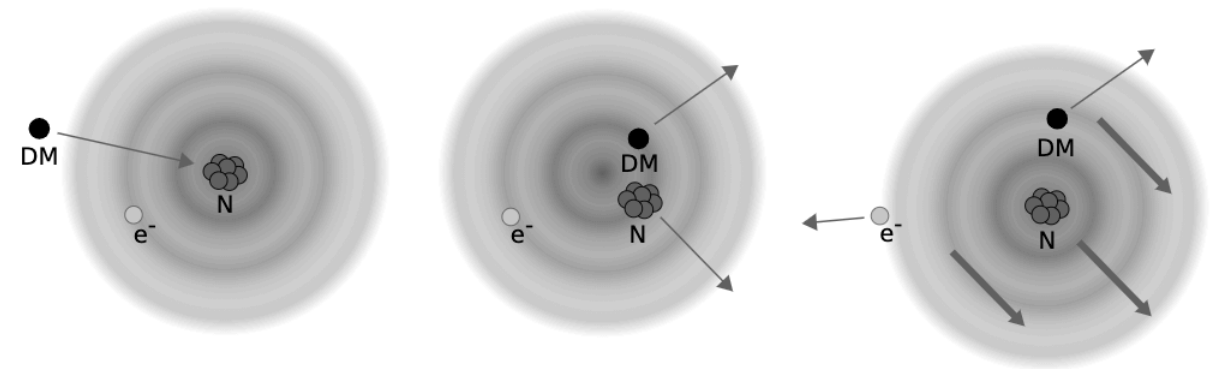


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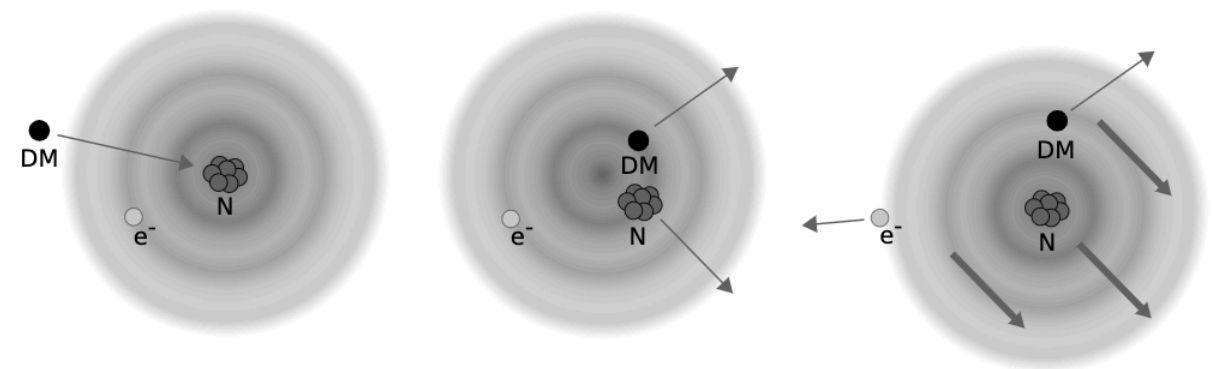
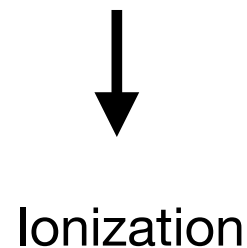
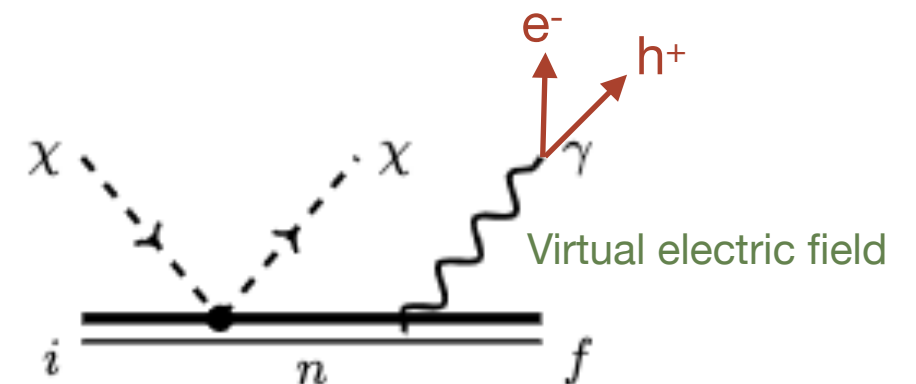


Figure from arXiv 1711.09906

## More microscopic explanation:

The **change in the Coulomb field** felt by the electrons causes energy transfer from the DM to the electrons, and causes the ionization

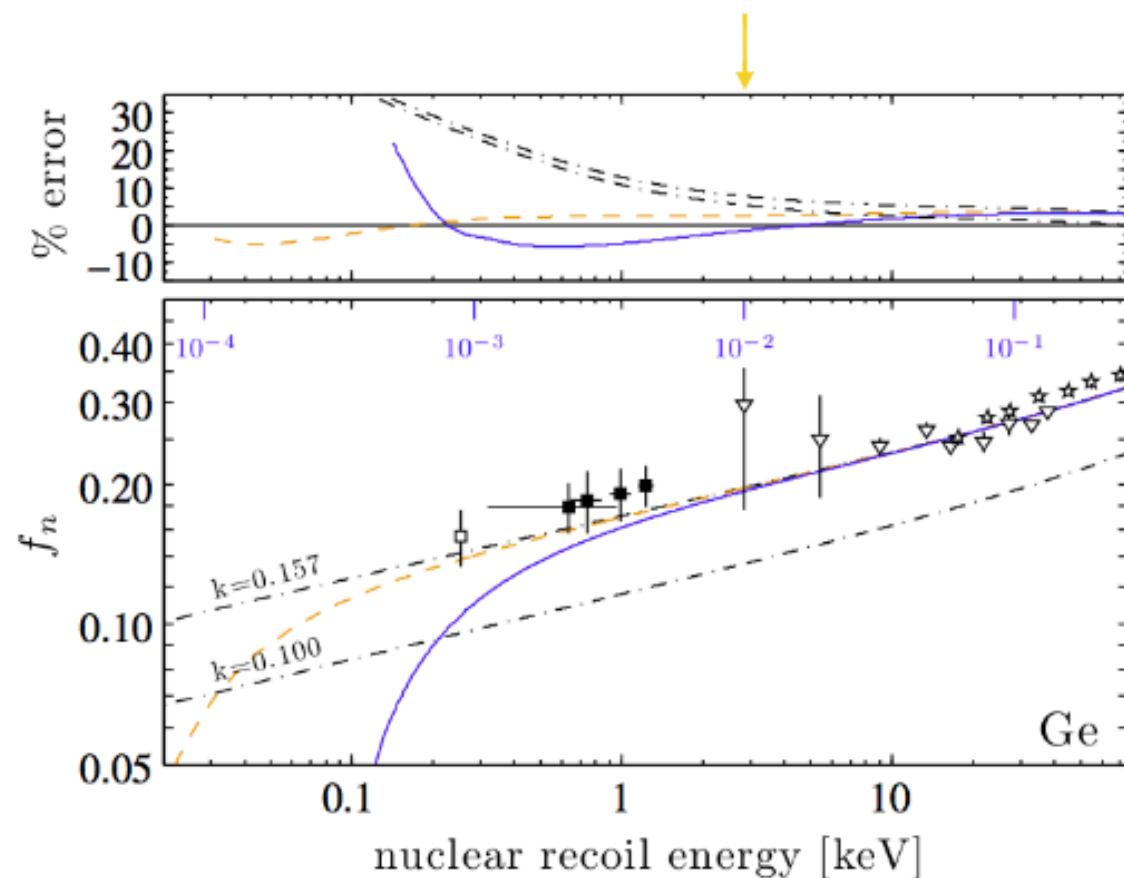
The Migdal effect is very analogous to the brehmstrahlung process, but now energy is dissipated into  $e^- h^+$  pairs instead of a photon



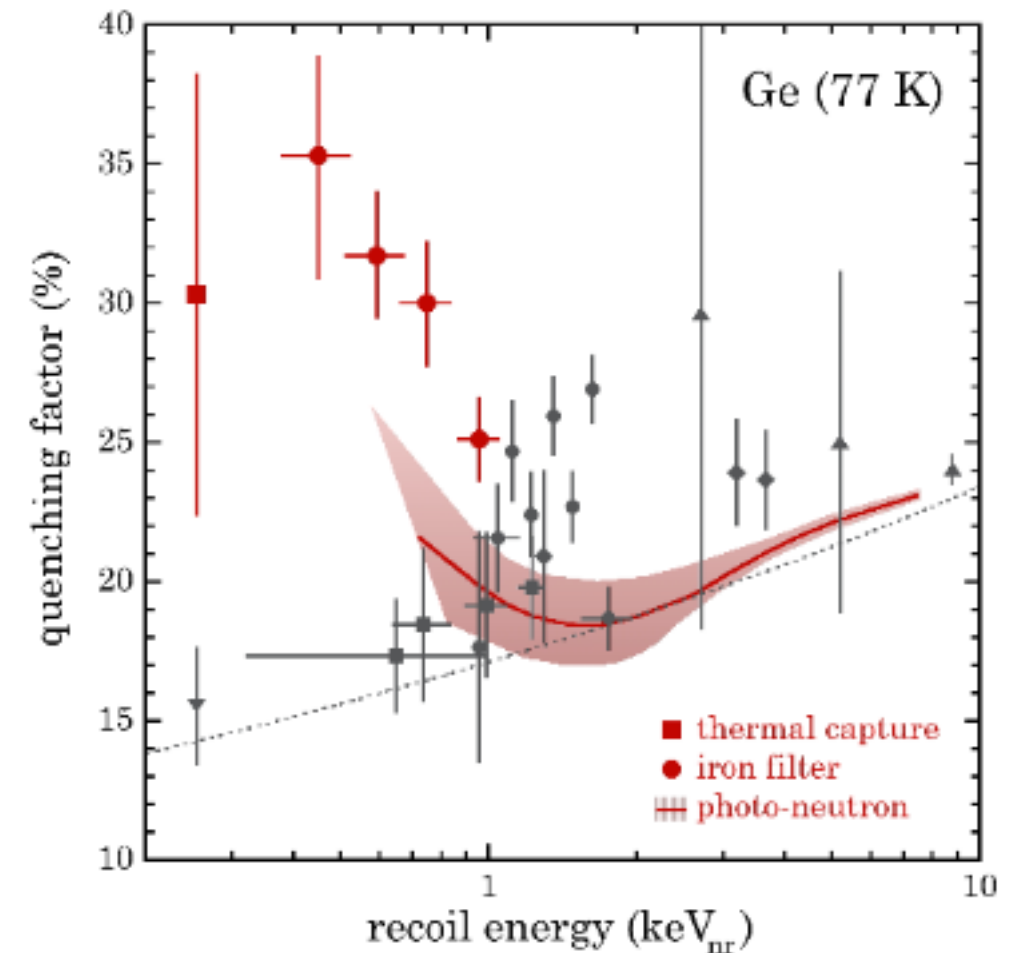
# What the Migdal effect is not

The Migdal effect describes ionization/electronic excitations during the **initial hard DM-nucleus collision**

The recoiling nucleus **produces secondary ionization e-** when encountering *other* nuclei in the crystal. This is described by the *quenching factor*:



This is important, but unrelated to the Migdal effect



# Notation

$|i\rangle, |f\rangle$

Initial and final state of the atom or crystal

$E_i, E_f$

Energy of the initial and final state

$E_N, v_N$

Energy and velocity of the recoiling nucleus

$\mathbf{r}_N, \mathbf{r}_\alpha$

Position operator corresponding to nucleus and electron labeled with  $\alpha$

$\omega, \mathbf{k}$

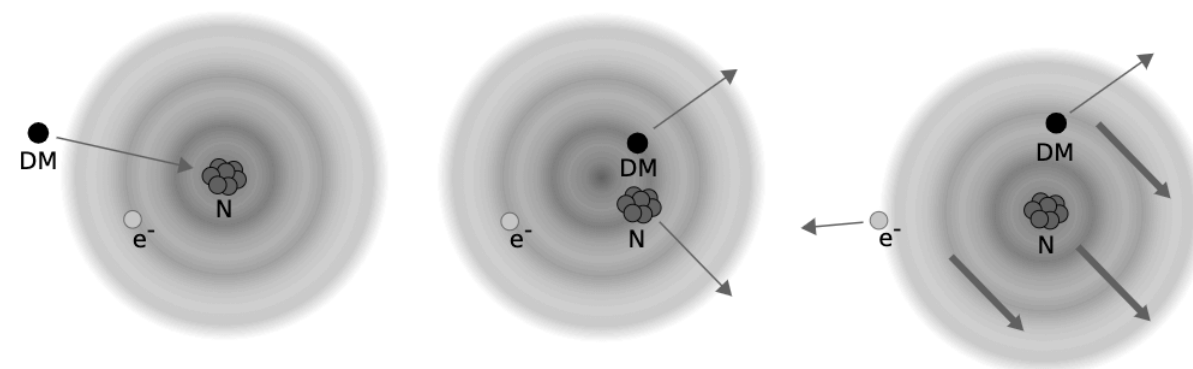
Energy and momentum deposited to the electrons

# Calculation with Migdal's trick

This is how the calculation goes using the original method by Migdal:

If  $E_N \gg \omega$ , the electron cloud cannot adjust itself to on the time scale of the DM-nucleus impact

This means that the excited electron wave functions **in the rest frame of the recoiling nucleus**, are simply **the ground state wave function, boosted to the frame of the recoiling nucleus**.



Migdal's trick

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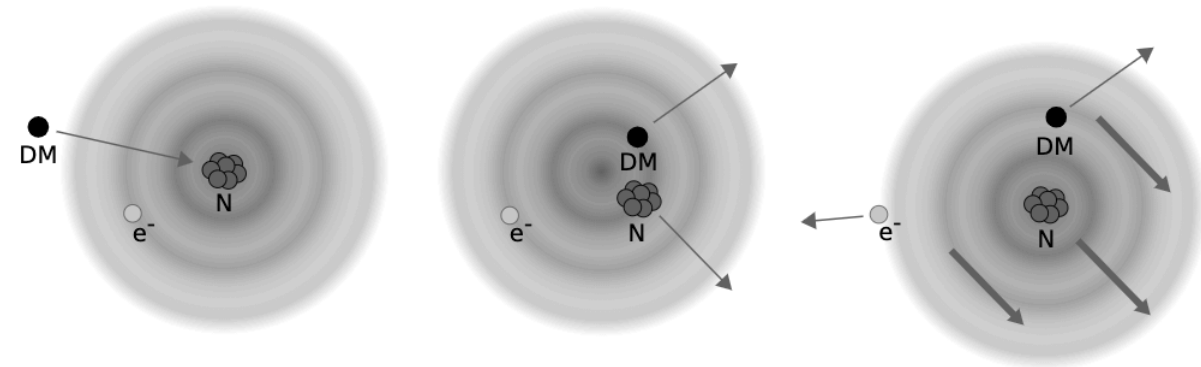
In equations, boosting the wave function with a velocity  $v_N$  is equivalent to multiplying it with a phase factor:

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

The transition matrix element to a particular final state  $f$  is therefore just

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

Transition dipole moment



Migdal's trick

# Numerical evaluation

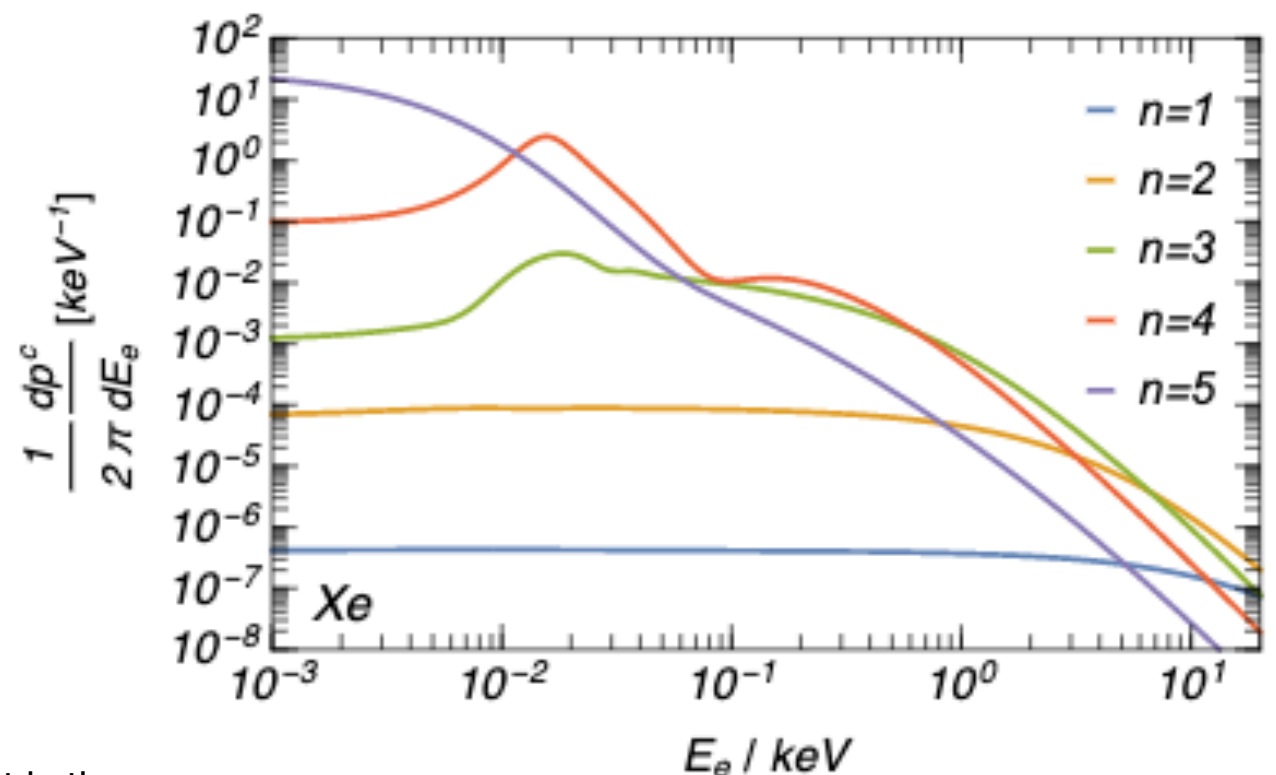
Ibe, Nakano, Shoji & Suzuki (1707.07258) used the numerical package “Flexible Atomic Code” (FAC) to compute the wave functions for a large collection of atoms

This is fairly painful, but once you have them, you can compute the transition probabilities\*

$$\frac{dP_{i \rightarrow f}}{d\omega} = m_e^2 \left| \mathbf{v}_N \cdot \langle f | \sum_{\beta} \mathbf{r}_{\beta} | i \rangle \right|^2 \delta(E_i - E_f + \omega)$$

Thankfully they provide tabulated ionization probabilities, so one can easily reconstruct their results

Example:



\* My normalization here is a bit different from theirs, but the physical object is the same



# Alternative calculation

Migdal's calculation is cute, but has a few drawbacks:

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

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

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

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

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

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

With

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

Dipole potential

$Z_N$  is the charge of the ion; for the moment we tread this as fixed, lumping the inner-shell electrons together with the nucleus.

# Alternative calculation

The transition probability is

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

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

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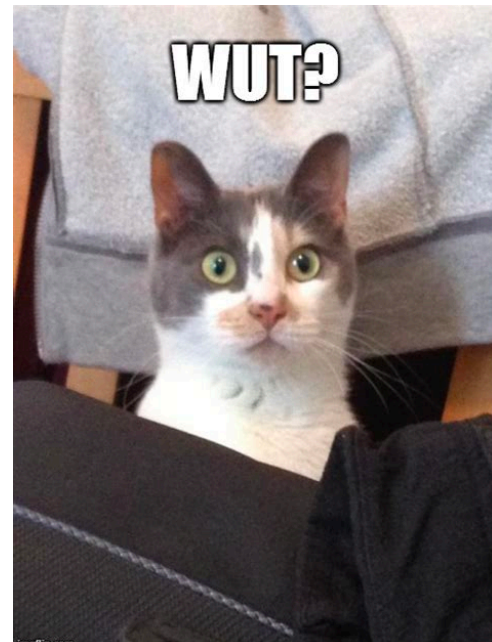
Migdal's trick

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

Perturbation theory

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

Which one is right???



# 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:

$$[\mathbf{r}_{\beta}, H_0] = i \frac{1}{m_e} \mathbf{p}_{\beta} \quad \text{And} \quad [p_{\beta}, H_0] = -i \frac{dV}{d\mathbf{r}_{\beta}}$$

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Total force exerted on the electron

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

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 &= i \frac{1}{\omega^2} \mathbf{v}_N \cdot \langle f | \sum_{\beta} \frac{dV}{d\mathbf{r}_{\beta}} | i \rangle \longrightarrow \text{Proportional to total force exerted in the electron}
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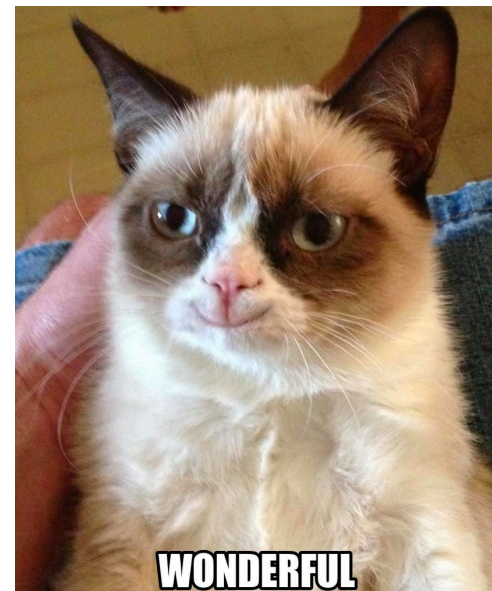


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 \end{aligned}$$

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

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



# A closer look...

Just removing some intermediate steps here, same derivation...

$$\begin{aligned}
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This step assumes that only the recoiling nucleus exerts a force on the electrons!

The Migdal trick and the perturbative calculation are equivalent, *but only for atomic targets!*

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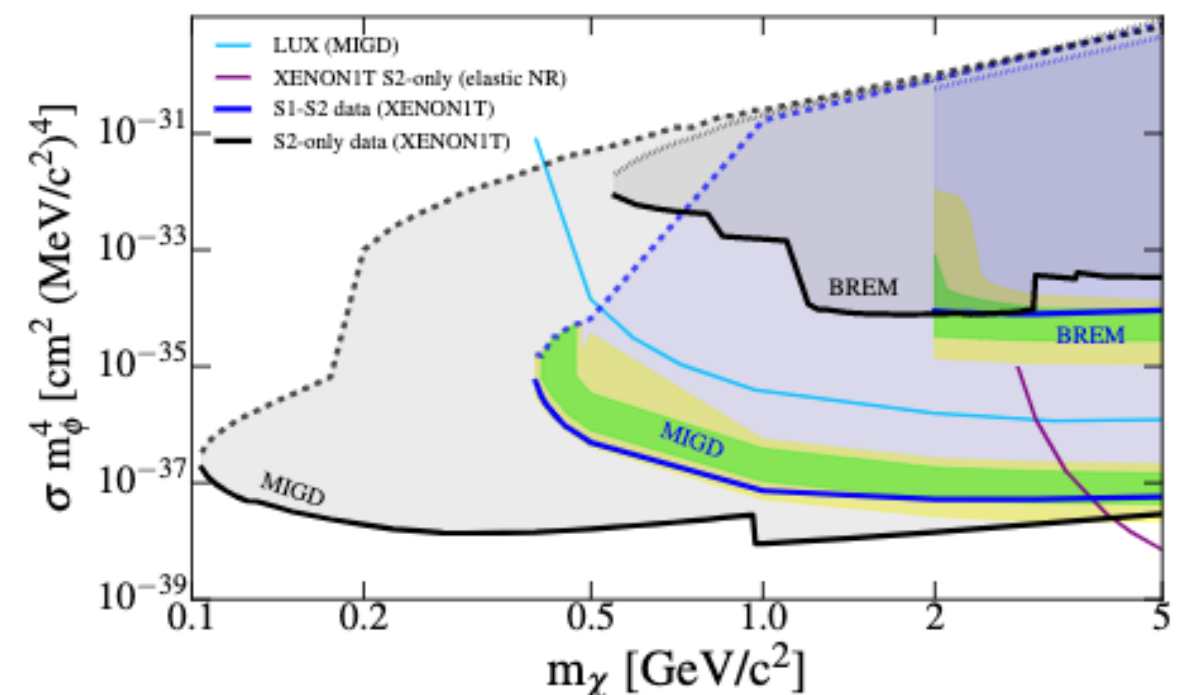
The Migdal trick and the perturbative calculation are equivalent, *but only for atomic targets!*

In hindsight, the reason is rather obvious: **The boosting trick doesn't work for a crystal**, because we'd be boosting all the spectator ions as well! Those contribution would need to be subtracted off in Migdal's calculation, which are exactly the terms that are missing above.

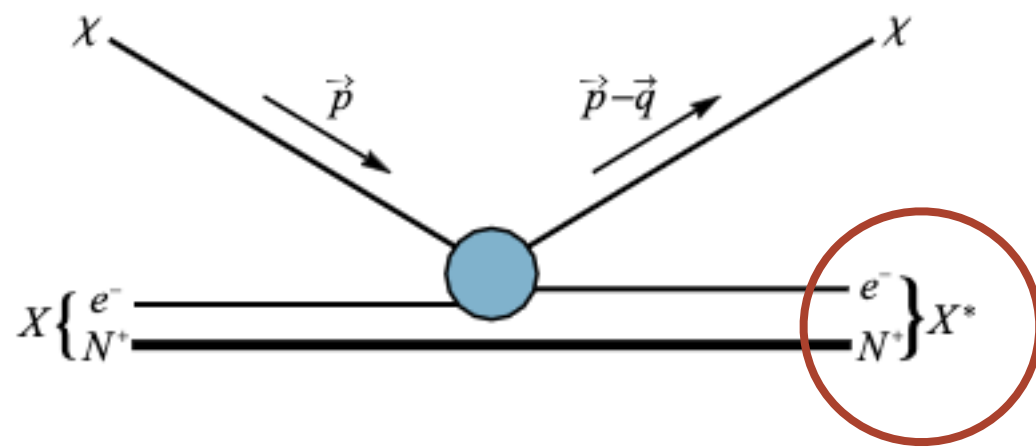
# Intermediate conclusions

- The Migdal effect is very **analogous to brehmstrahlung**, with the difference that the photon is virtual and excites one or more electrons
- We've shown this by showing that the **Migdal trick is equivalent to a perturbative computation...**
- ... but **only for isolated atoms!**
- The numerical Ibe et al results are super useful but can only be relied for atomic targets, such as Xe, Ar, He etc

*Now let us look at crystals...*



# Crystals are complicated



$e^-$  are not free

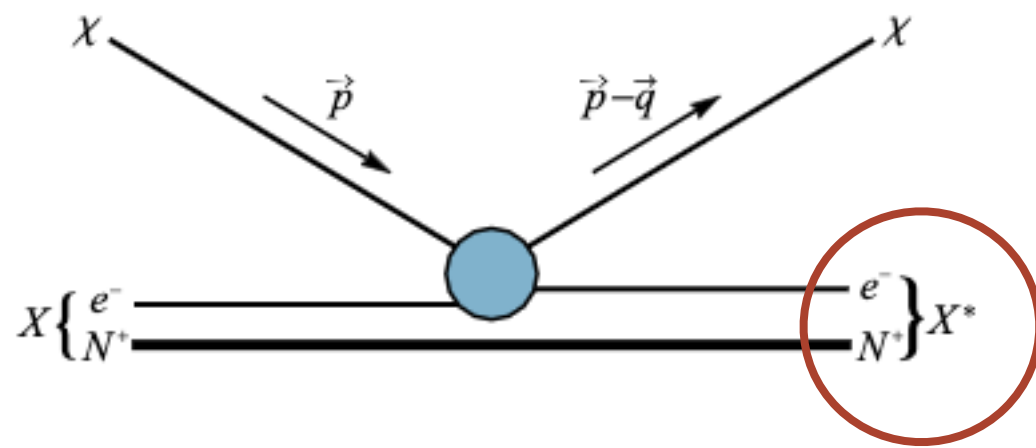
$e^-$  are not at rest

$e^-$  are not localized

$e^-$  are not alone

→ screening

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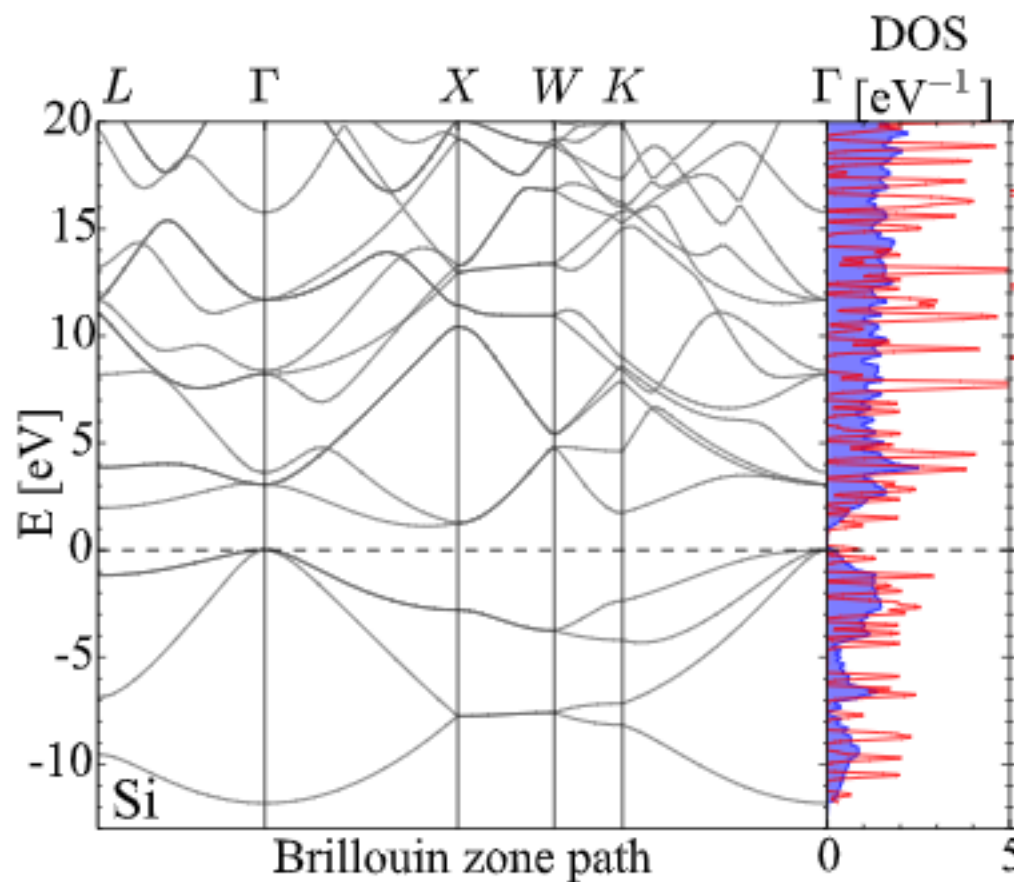
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$e^-$  are not localized

$e^-$  are not alone

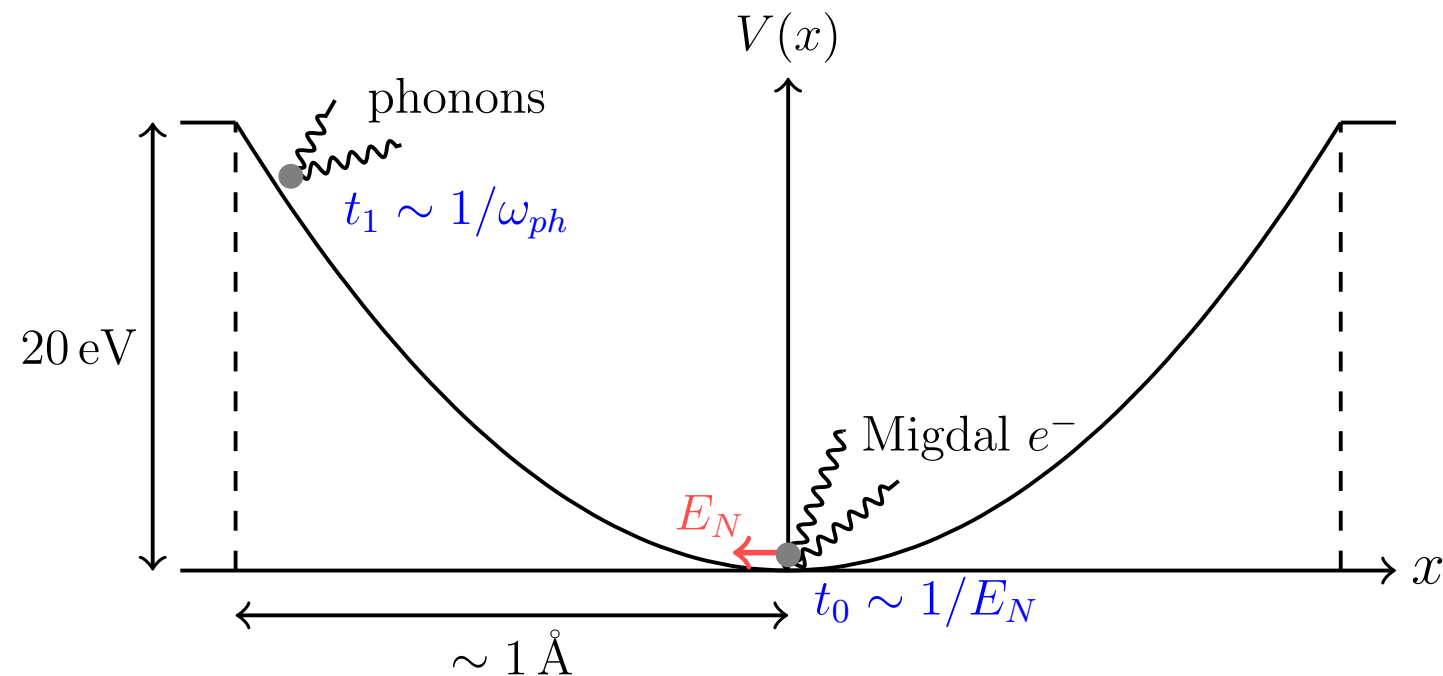
→ screening



Bloch wave functions

Obtain with density functional theory (DFT)

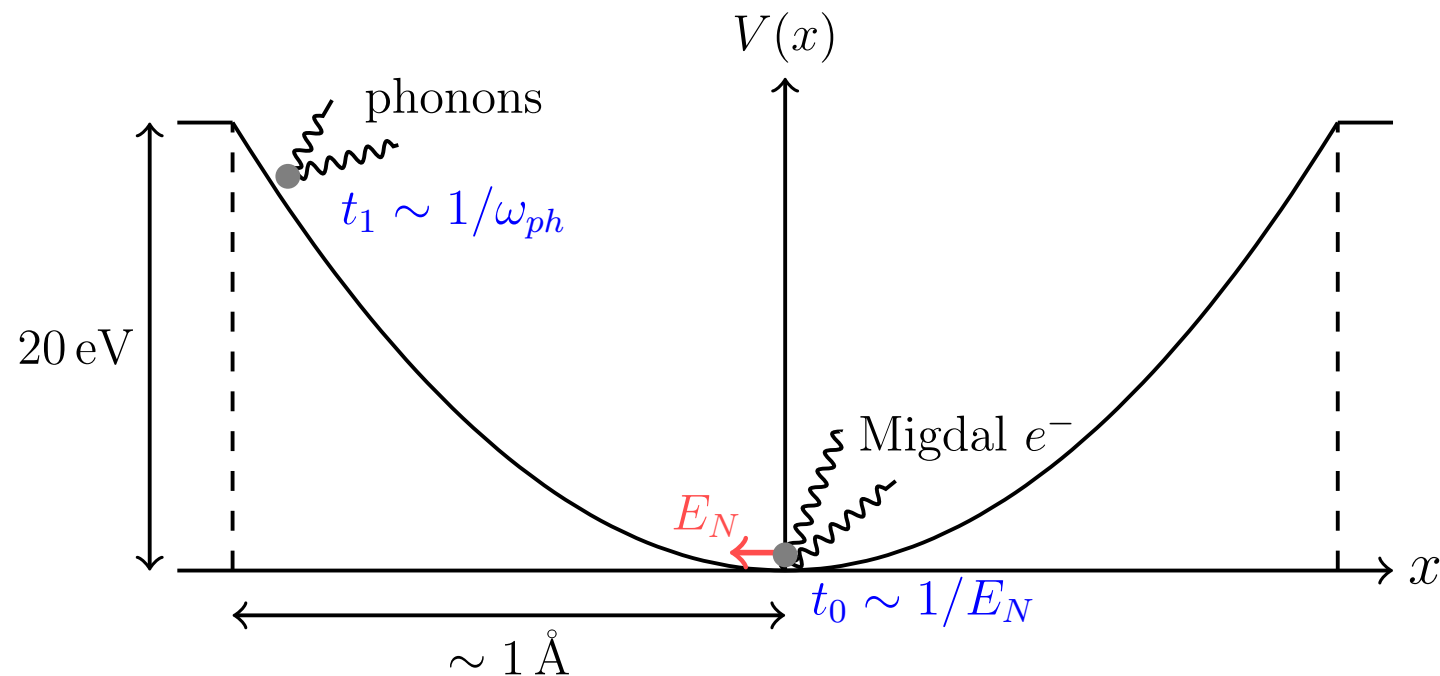
# The impulse approximation in a crystal



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

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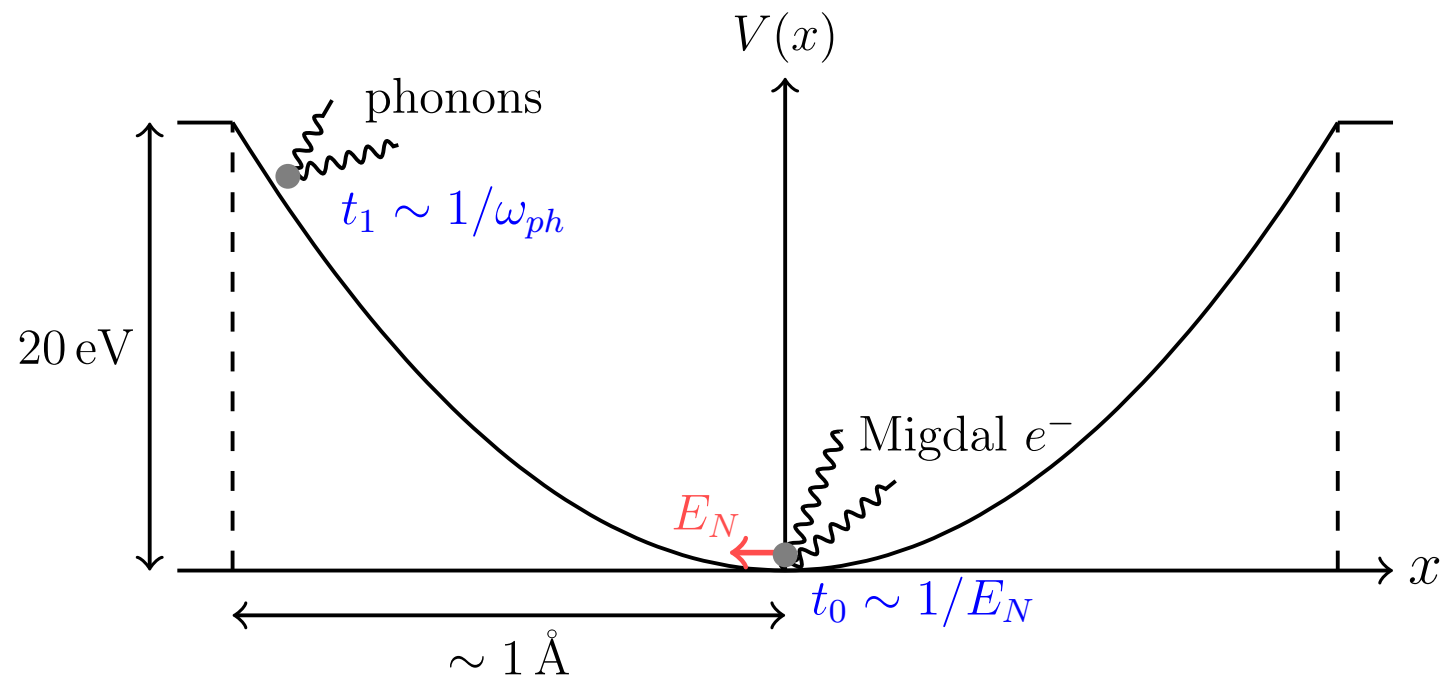
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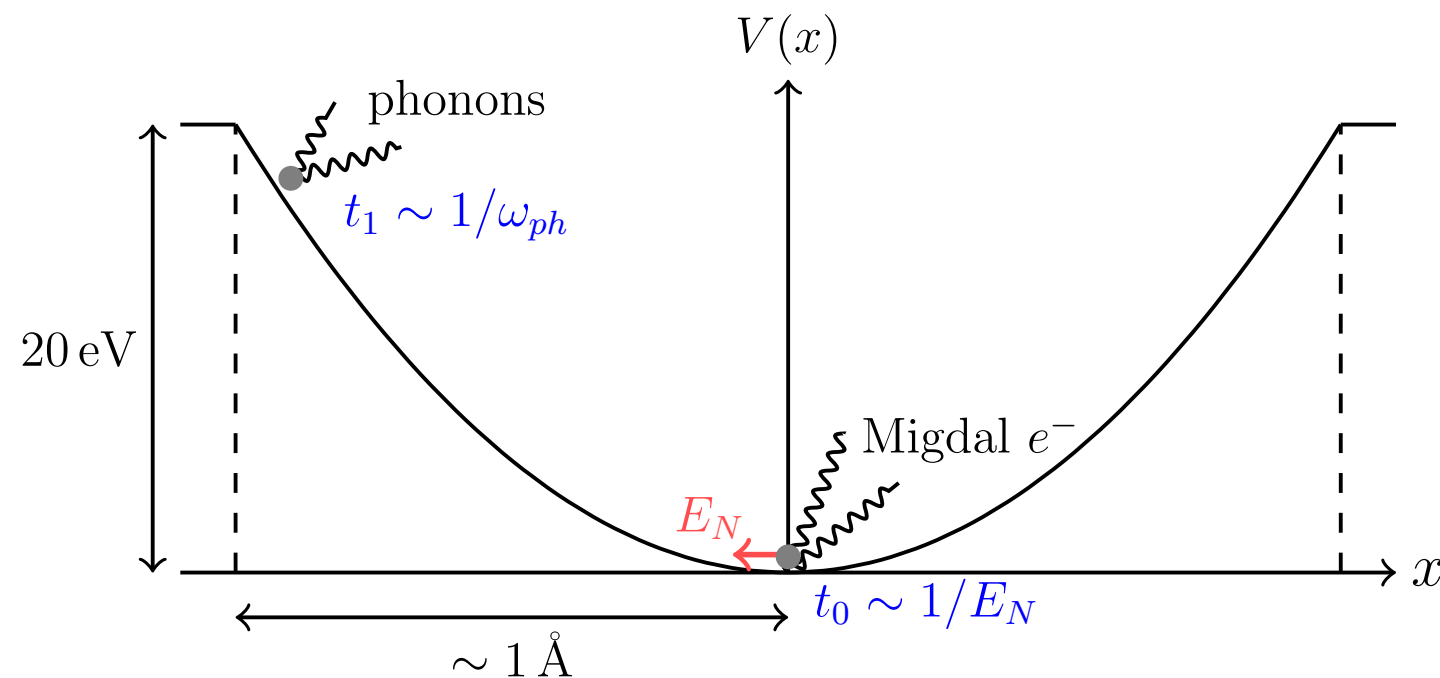
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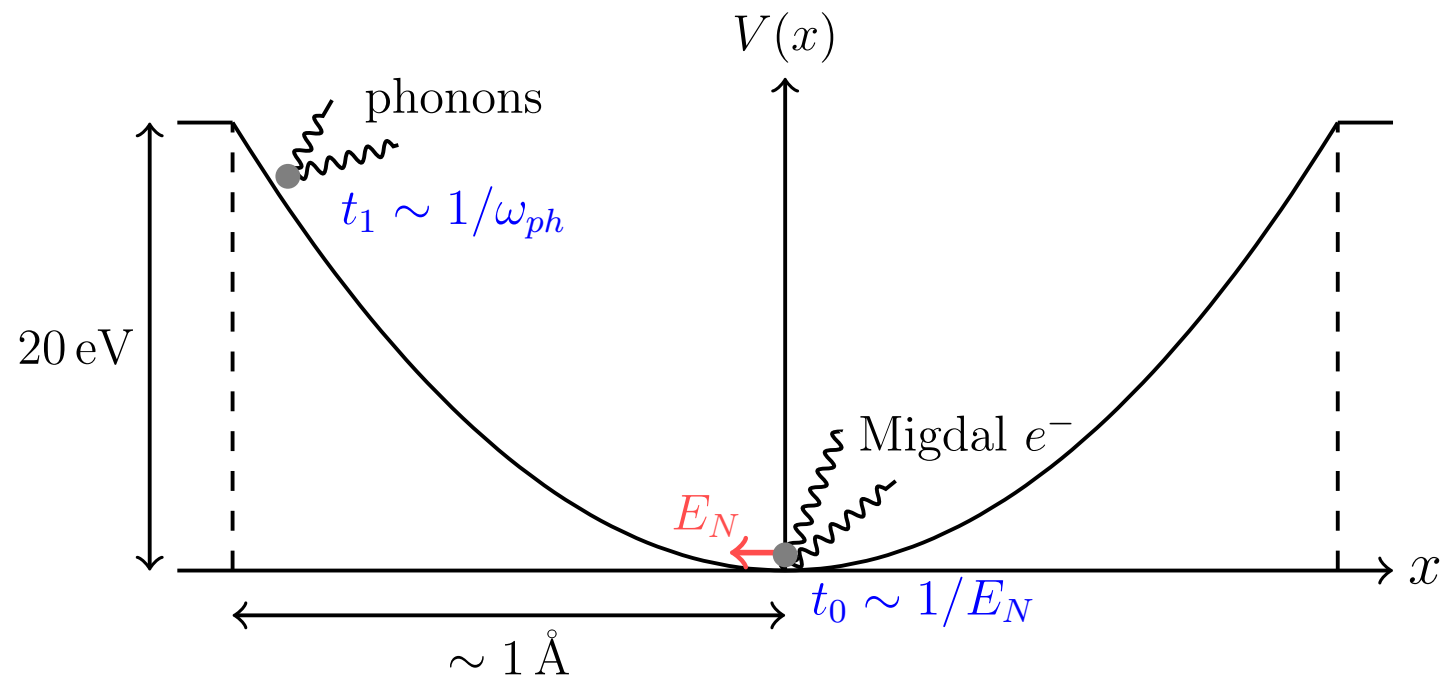
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When it is valid we can factorize the long distance physics (phonons) from the short distance physics (Migdal effect).

# Soft nuclear recoils



Nuclei are not free

Nuclei are roughly at rest

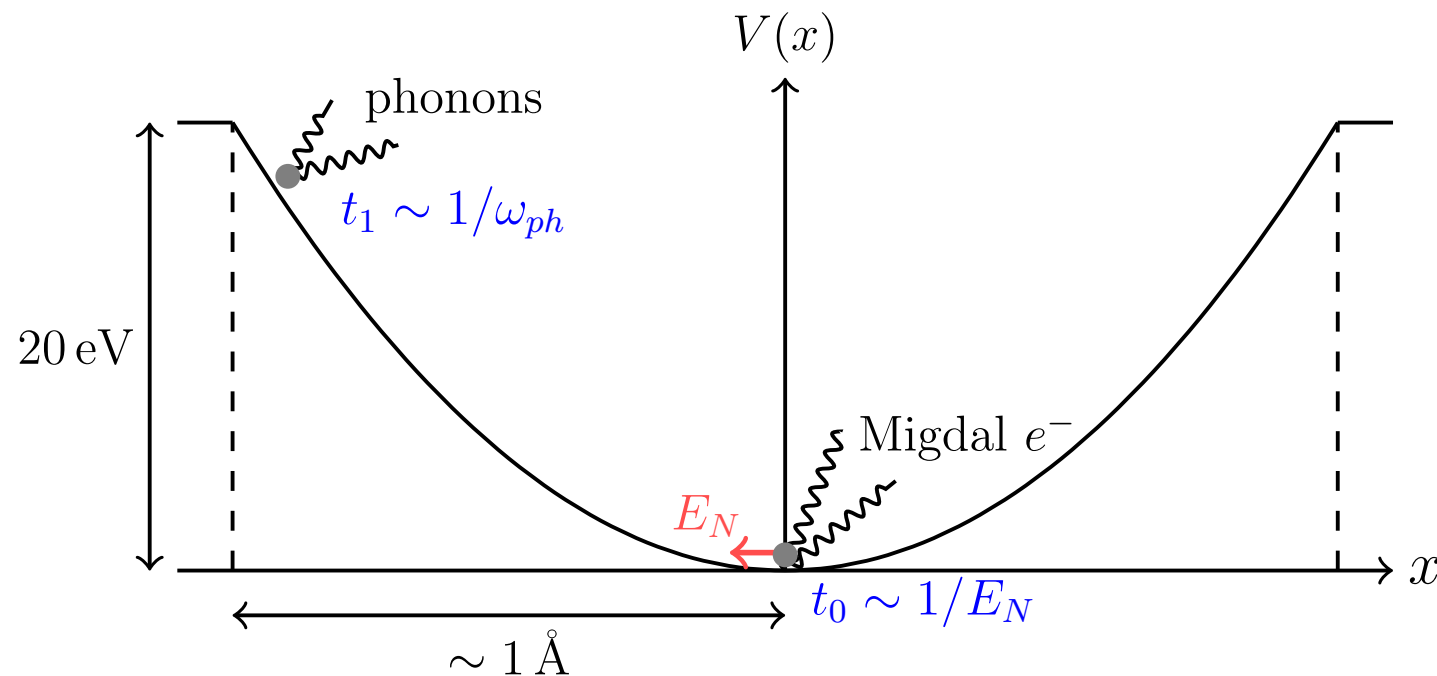
Nuclei are pretty localized

Lets first look at soft nuclear recoils **without Migdal effect** (bit of a preview for tomorrow)

A short-ranged interaction is described by a delta-function potential:

$$\mathcal{V}(\mathbf{r}) = V_0 \delta(\mathbf{r}_N - \mathbf{r}) \rightarrow \tilde{V}(\mathbf{q}) = \tilde{V}_0 e^{i\mathbf{q} \cdot \mathbf{r}_N}$$

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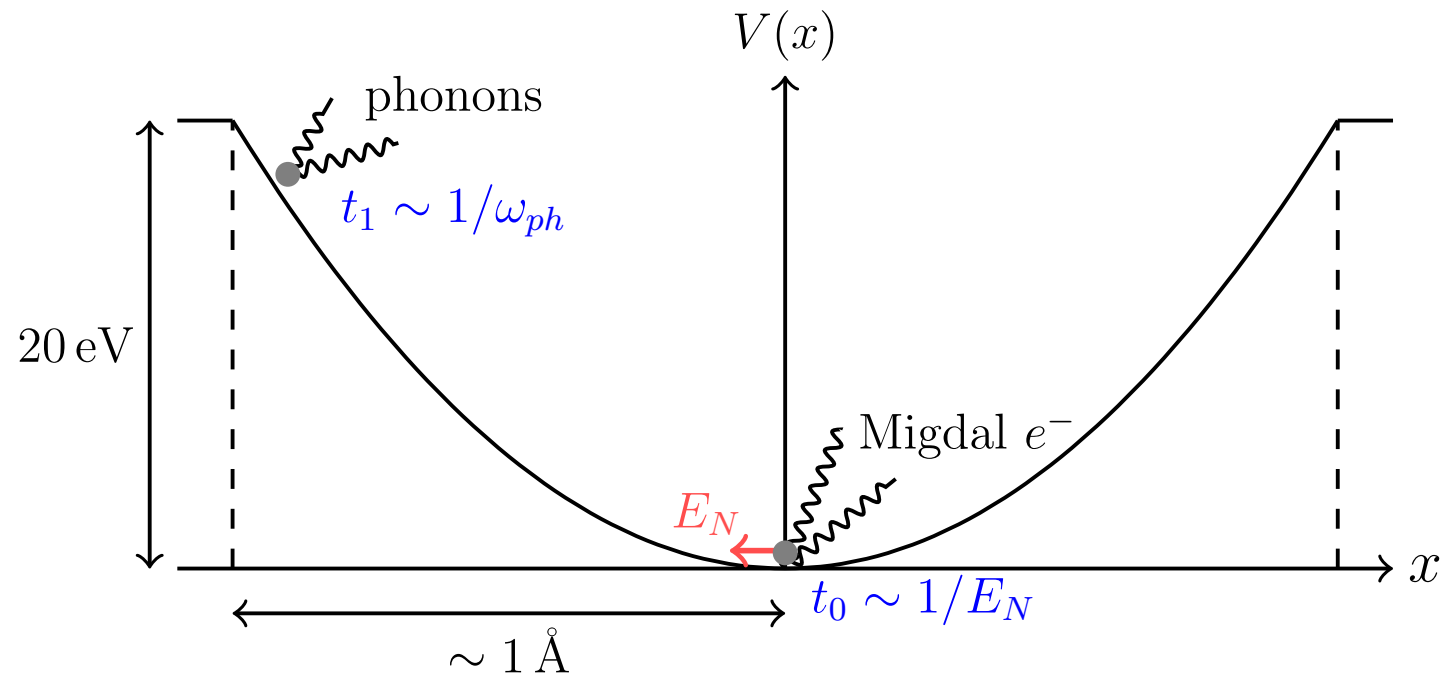
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The scattering process is described by the “**dynamical structure factor**” or “**response function**”

$$S(\mathbf{q}, \omega) \equiv \sum_{\lambda_f} \left| \langle \lambda_f | e^{-i\mathbf{q} \cdot \mathbf{r}_N} | \lambda_i \rangle \right|^2 \delta(E_{\lambda_f} - E_{\lambda_i} - \omega)$$

Initial and final states of the nucleus, sitting in its potential well

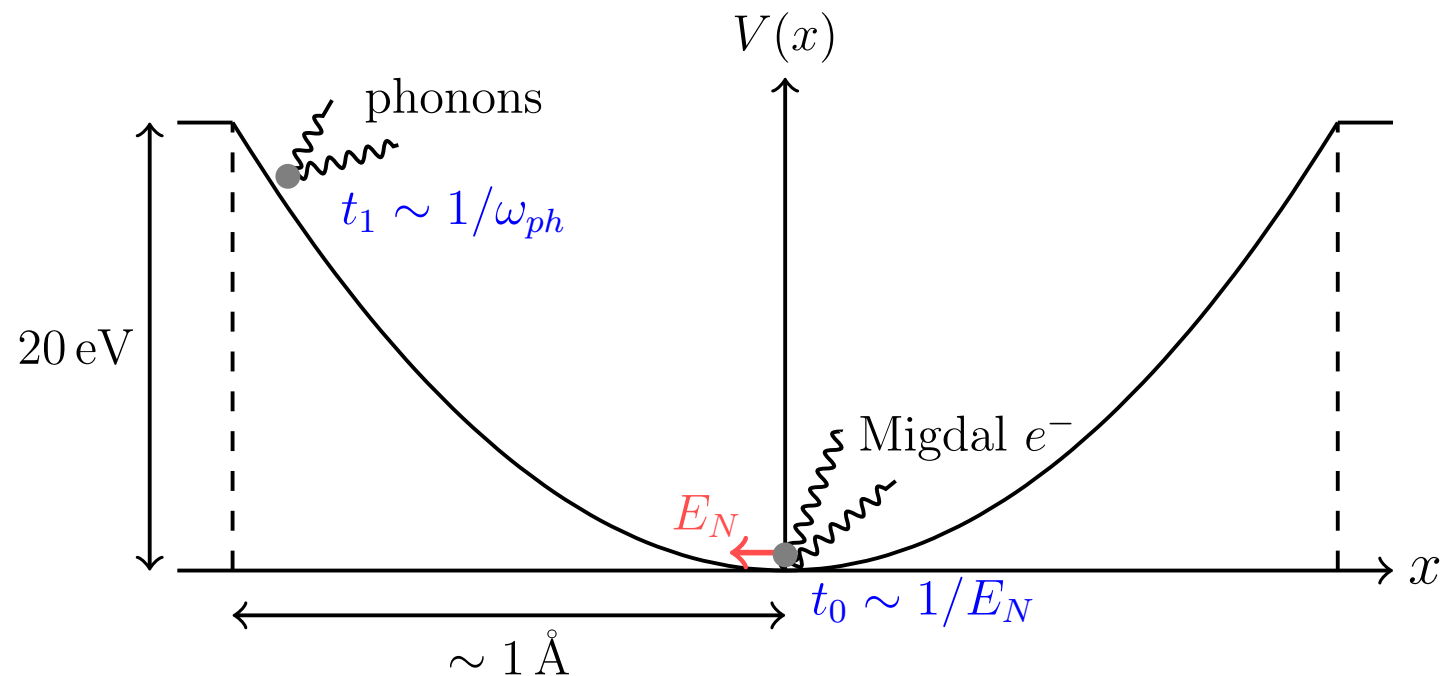
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(This step is a page of algebra)

# Soft nuclear recoils

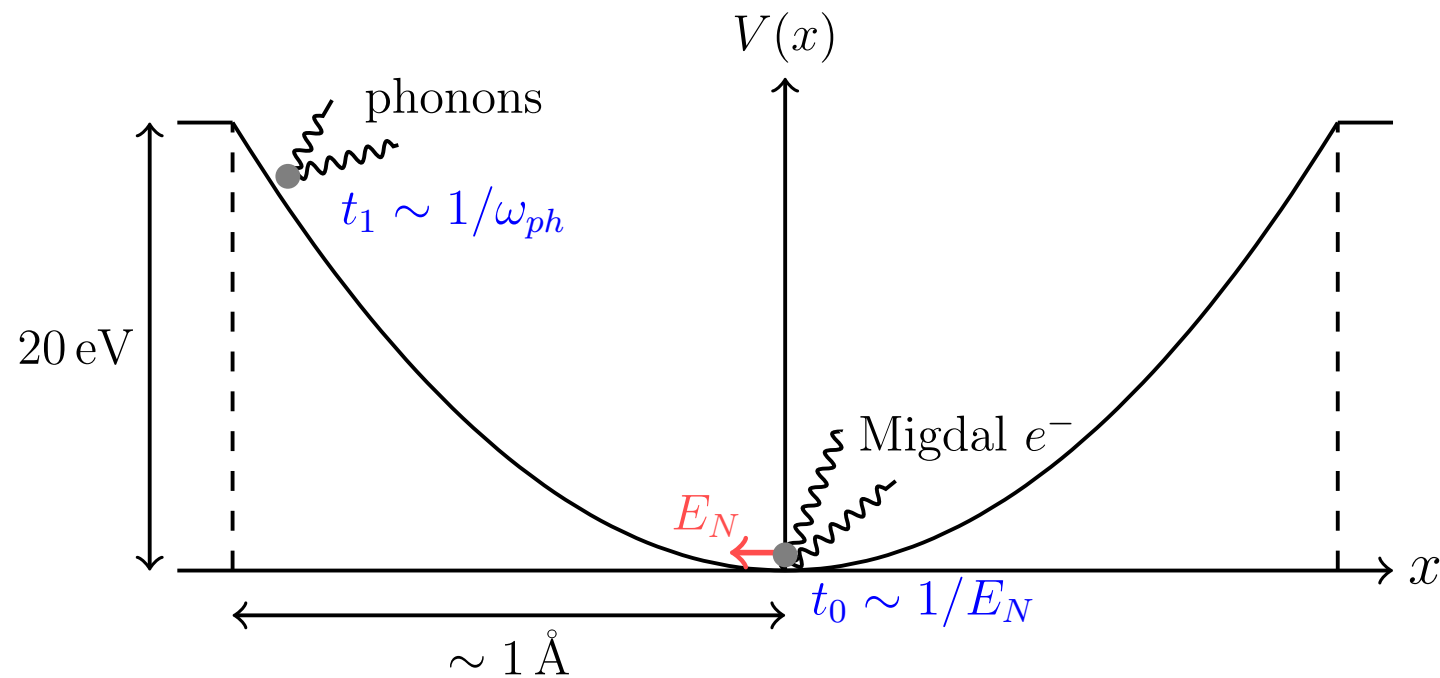


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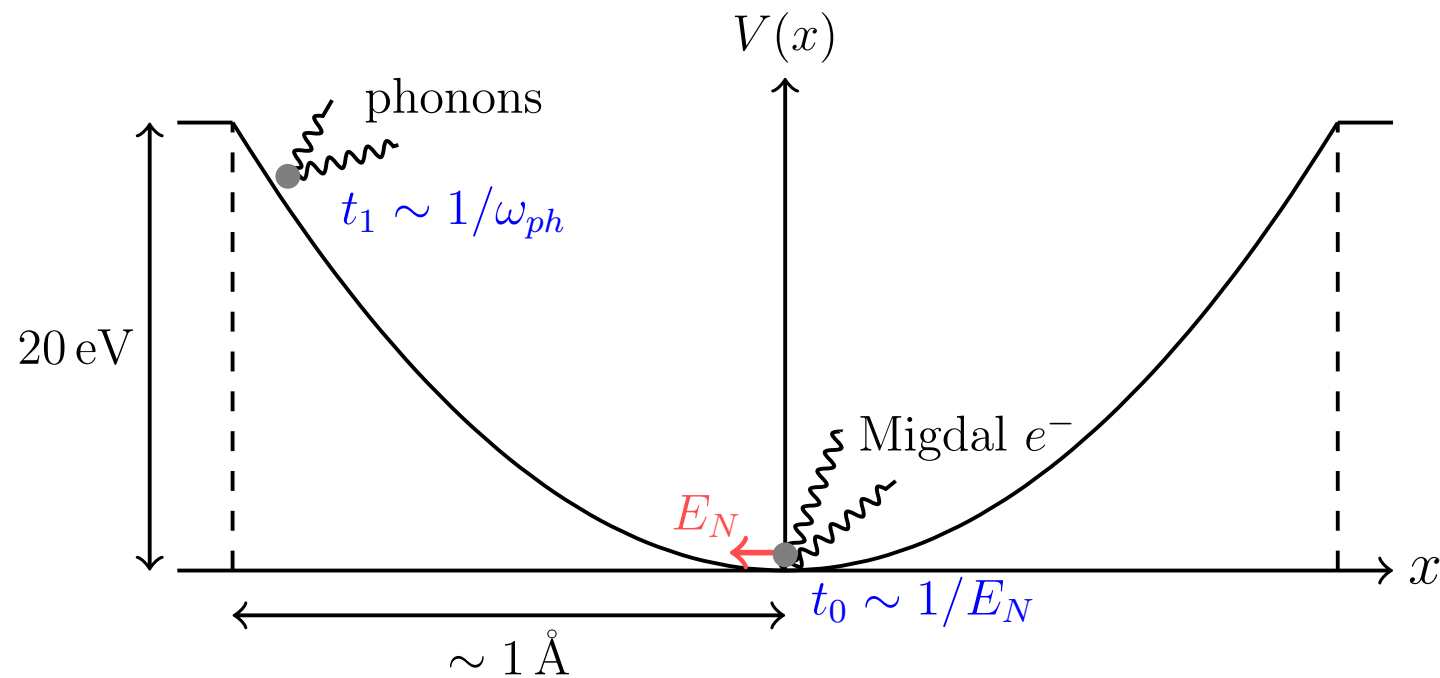
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In a harmonic potential

$$\langle \mathbf{q} \cdot \mathbf{r}_N(0) \mathbf{q} \cdot \mathbf{r}_N(t) \rangle = \frac{q^2}{2m_N} \int d\omega' \frac{D(\omega')}{\omega'} \left[ \cos(\omega' t) \coth\left(\frac{\omega'}{2T}\right) + i \sin(\omega' t) \right]$$

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Density of states



# Soft nuclear recoils

In the impulse approximation, the response function is gaussian

$$S^{IA}(\mathbf{q}, \omega) = \frac{1}{\sqrt{2\pi}\Delta^2} e^{-\frac{\left(\omega - \frac{q^2}{2m_N}\right)^2}{2\Delta^2}} \quad \text{with} \quad \Delta^2 \equiv \frac{q^2 \bar{\omega}}{2m_N} \quad \text{Typical phonon frequency}$$

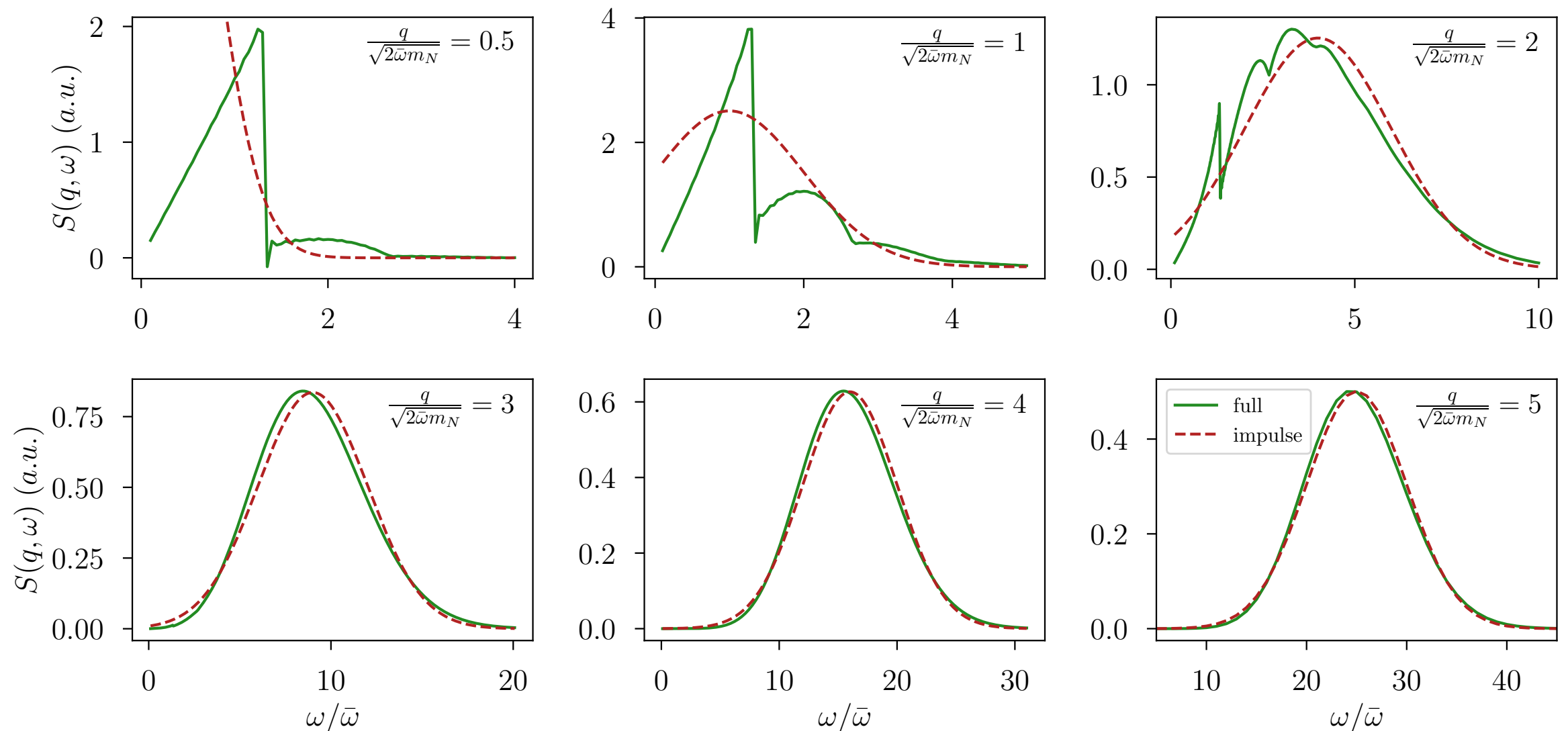
Asymptotes to a  $\delta$ -function for  $q^2/2m_N \gg \bar{\omega}$  (Free limit)

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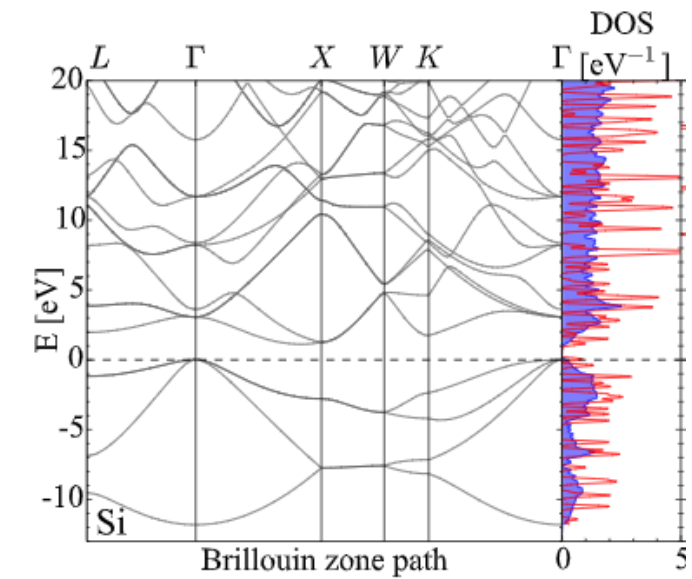


We can use the impulse approximation as long as  $\frac{q^2}{2m_N \bar{\omega}} \gtrsim 4$

# Back to electrons

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



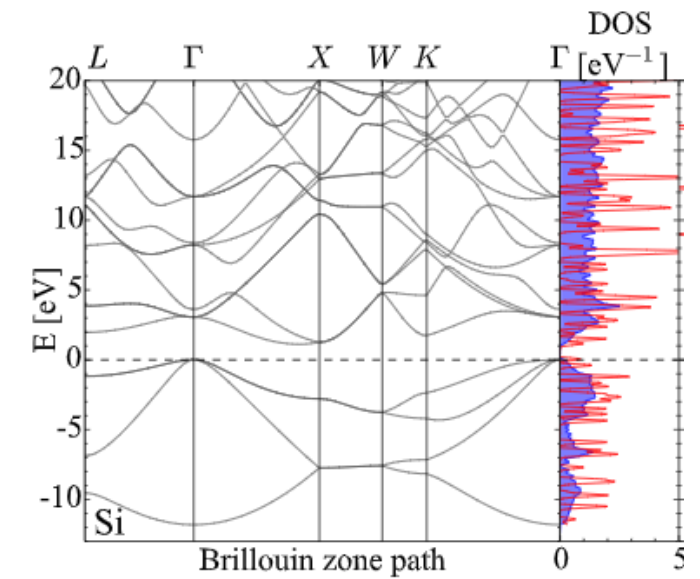
From 1509.01598 (Essig et al.)

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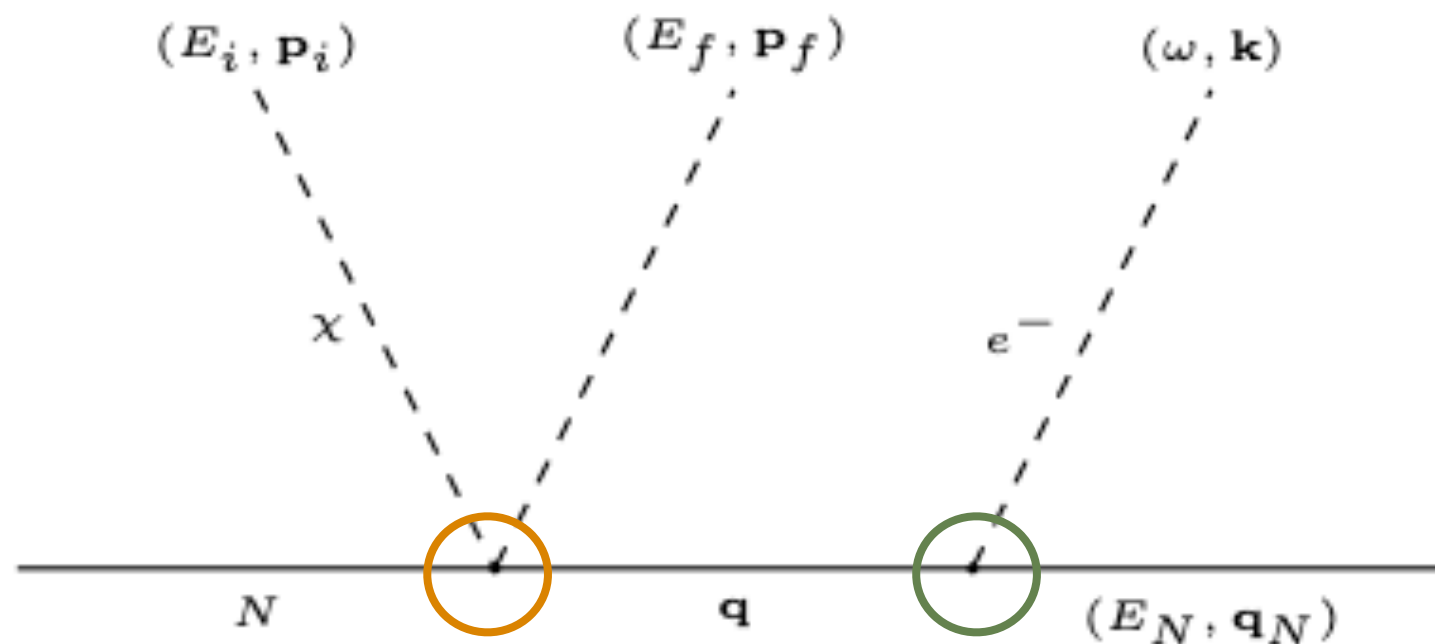
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Leading order calculation in E&M force



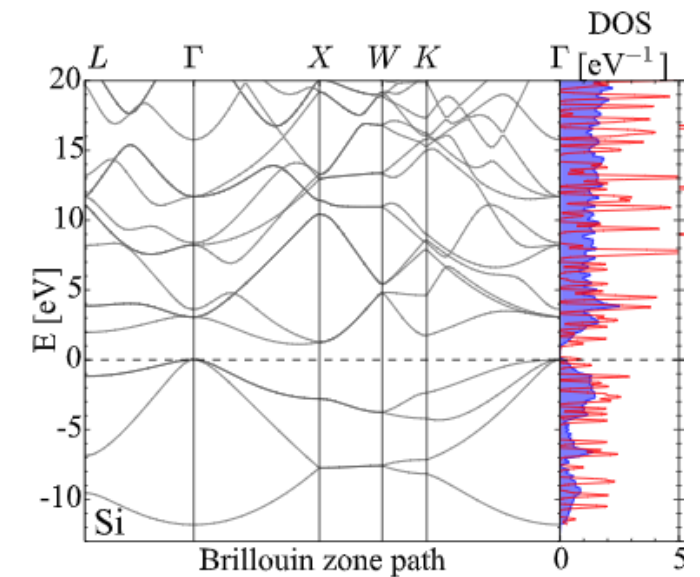
DM coupling

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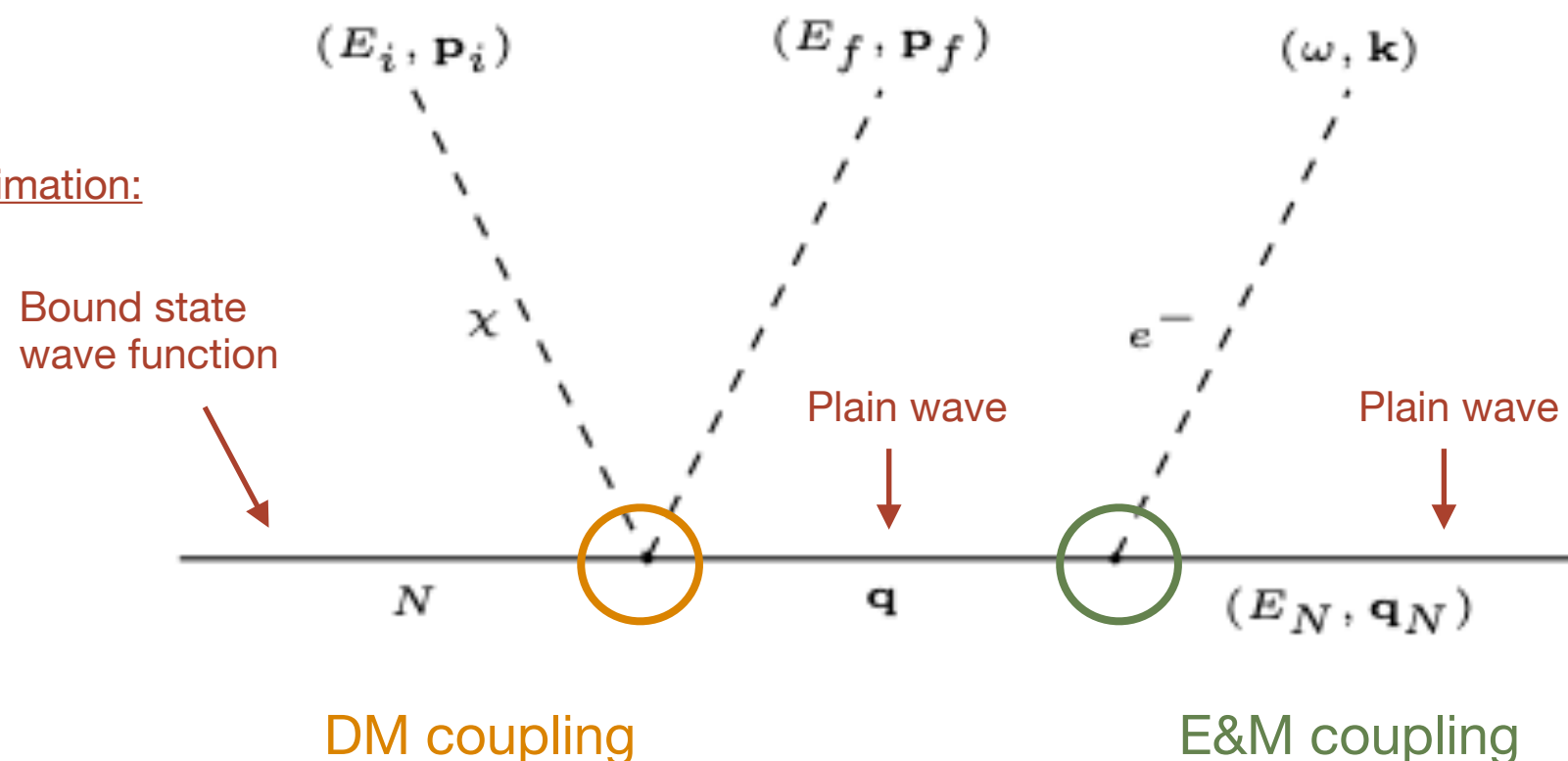


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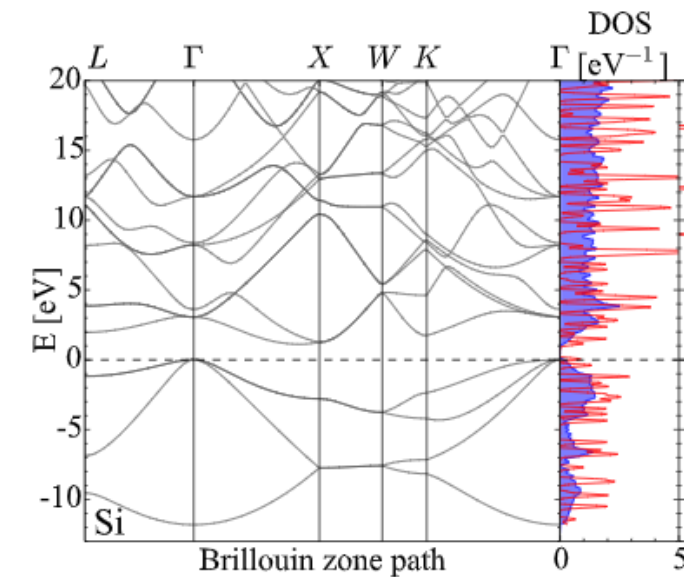
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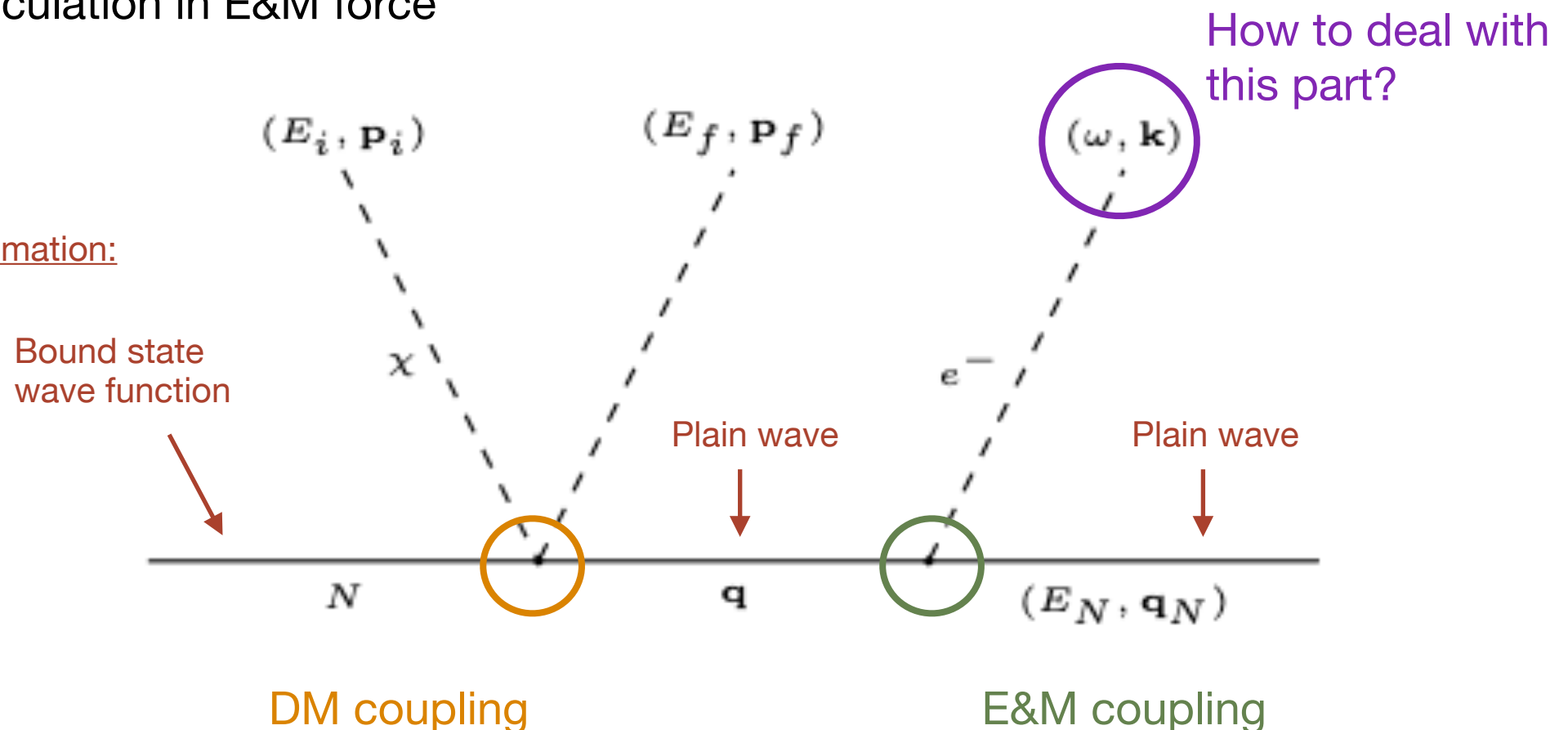


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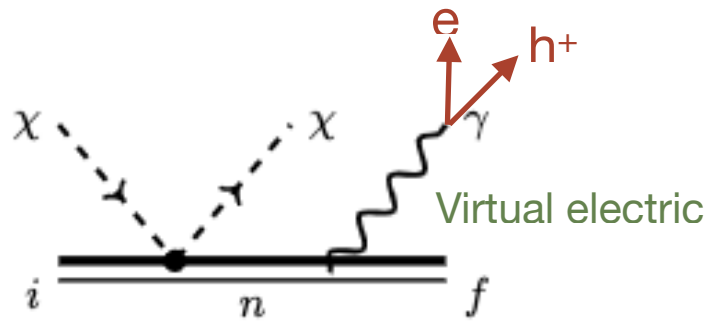
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# The energy loss function (ELF)

Recall that we are looking for a virtual photon splitting into an electron-hole pair

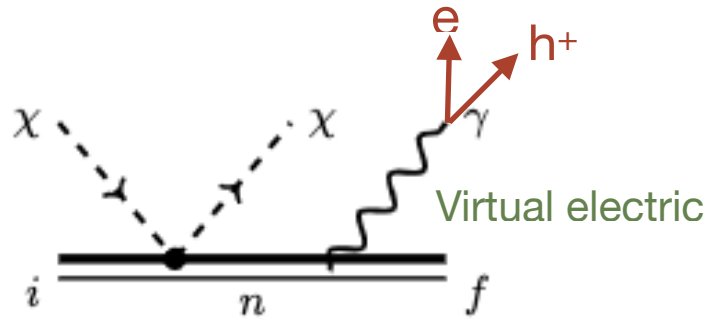


Coulomb potential in a dielectric:

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

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In QFT language:

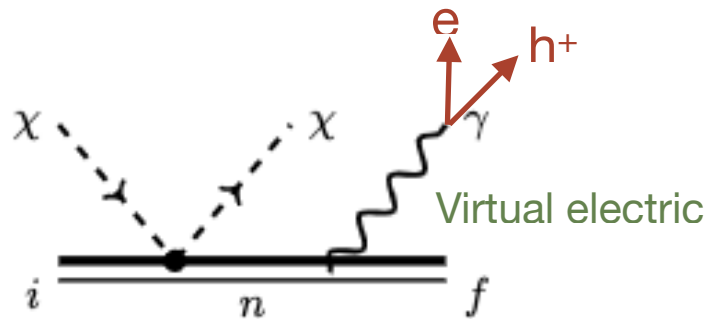
A Feynman diagram showing two wavy lines connected by a shaded circular vertex. The diagram is followed by the expression  $\sim \frac{1}{\epsilon(\mathbf{k}, \omega)} \frac{1}{k^2}$  and the text "(Non-relativistic limit)".

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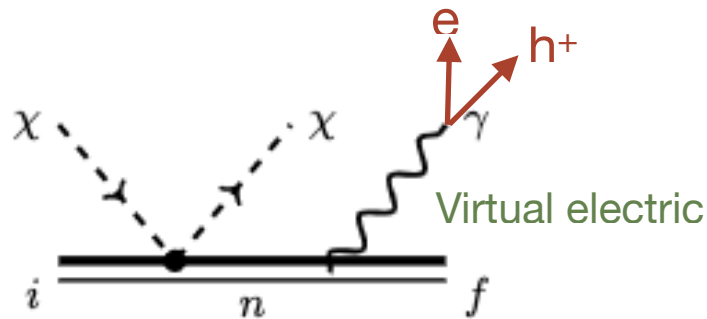
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In QFT language:

A Feynman diagram showing a virtual photon exchange between two particles, represented by wavy lines connected by a shaded circle. The diagram is followed by the expression  $\sim \frac{1}{\epsilon(\mathbf{k}, \omega)} \frac{1}{k^2}$  and the text "(Non-relativistic limit)".

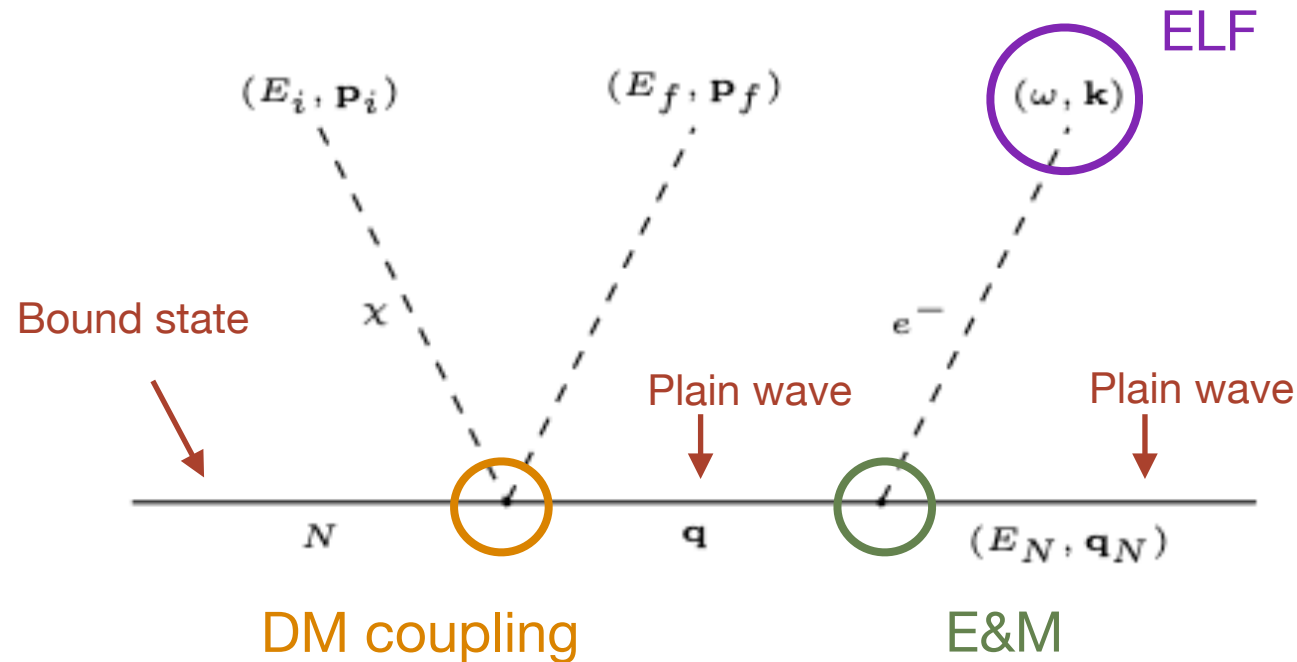
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"Energy Loss Function" (ELF)

# Result

With impulse approximation:



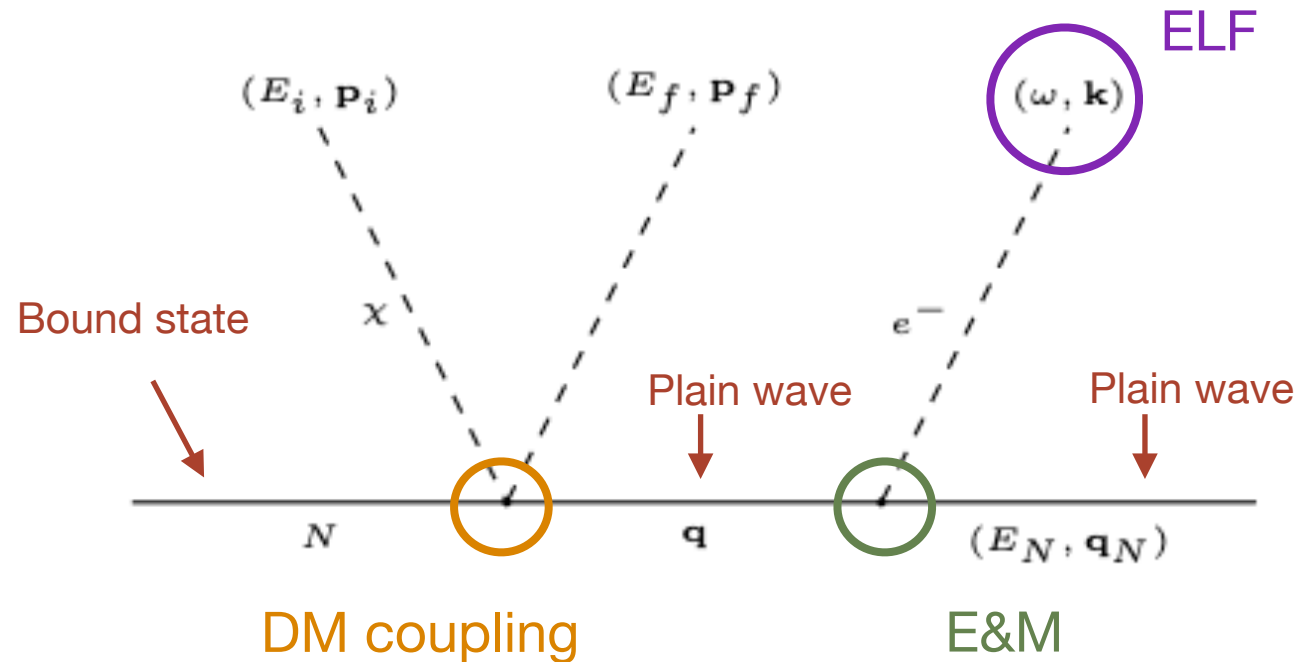
Explicit calculation is a little tedious since we need Bloch functions etc, like you learned from Tien-Tien. The derivation is straightforward, but the formulas tend to be fairly long etc

Result:

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

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$$\times |F_{DM}(\mathbf{p}_i - \mathbf{p}_f)|^2 |F(\mathbf{p}_i - \mathbf{p}_f - \mathbf{q}_N - \mathbf{k})|^2 \delta(E_i - E_f - E_N - \omega).$$

DM form factor
Crystal form factor

# In the soft limit

Analogous to the brehmstrahlung case. Valid for  $k \ll v m_X$ :

$$\frac{d\sigma_{\text{ion}}}{dE_N d\omega} \approx \frac{d\sigma_{\text{el}}}{dE_N} \frac{dP}{d\omega}$$

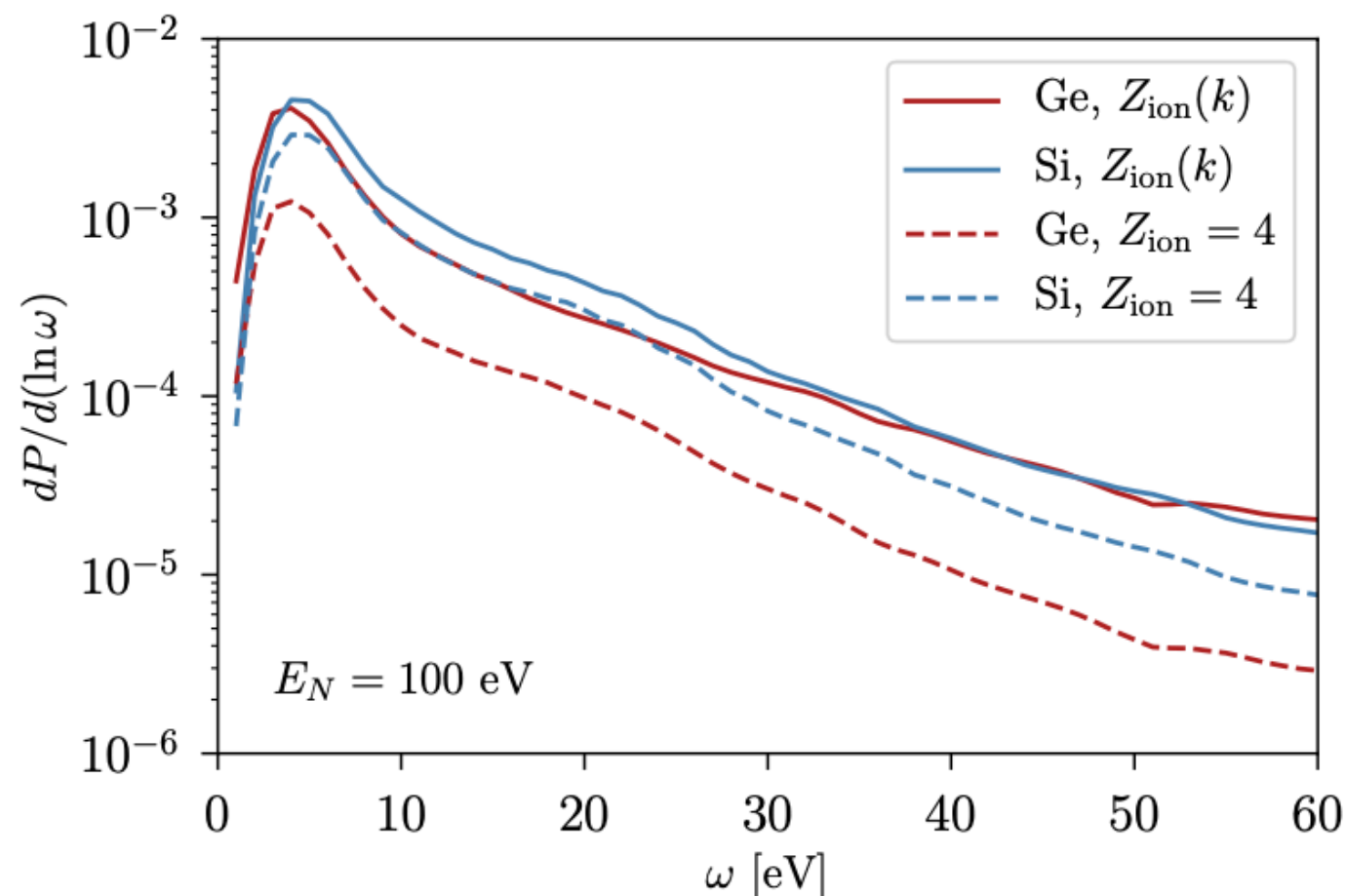
$$\frac{dP}{d\omega} = 4\alpha \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{Z_{\text{ion}}^2(k)}{k^2} \frac{|\mathbf{v}_N \cdot \mathbf{k}|^2}{\omega^4} \text{Im} \left[ \frac{-1}{\epsilon(\mathbf{k}, \omega)} \right].$$

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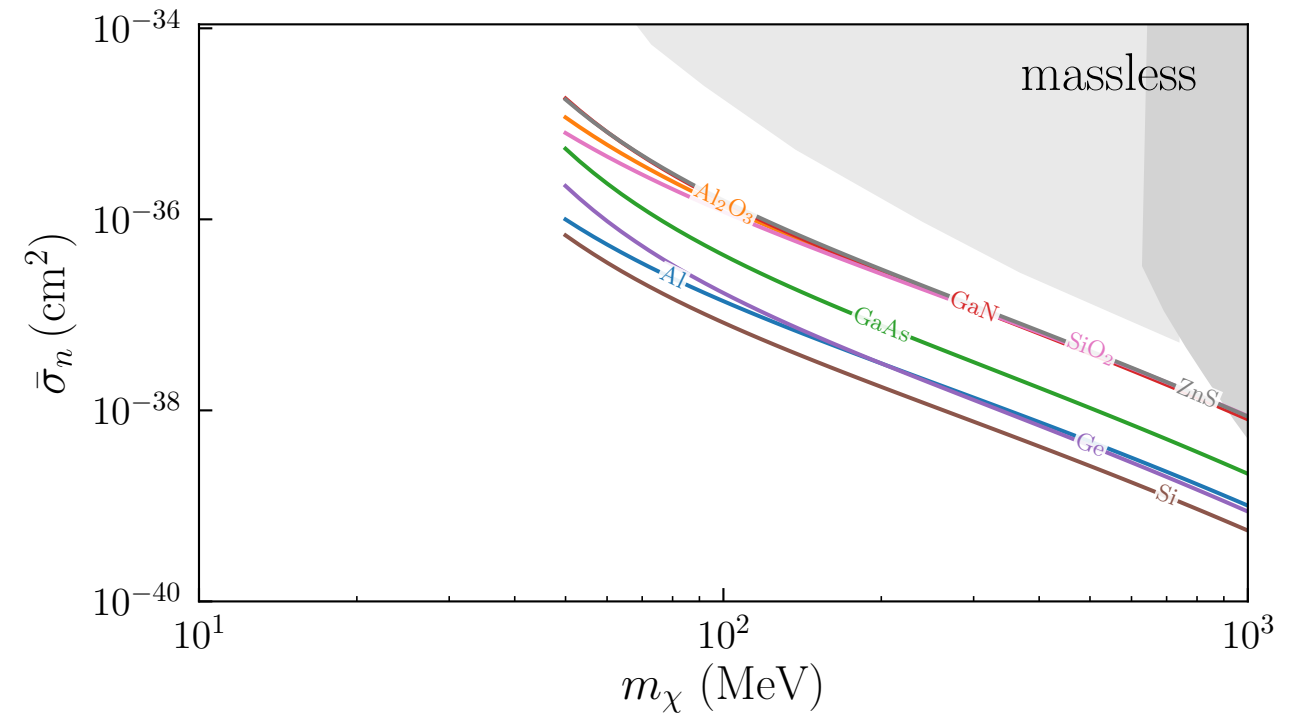
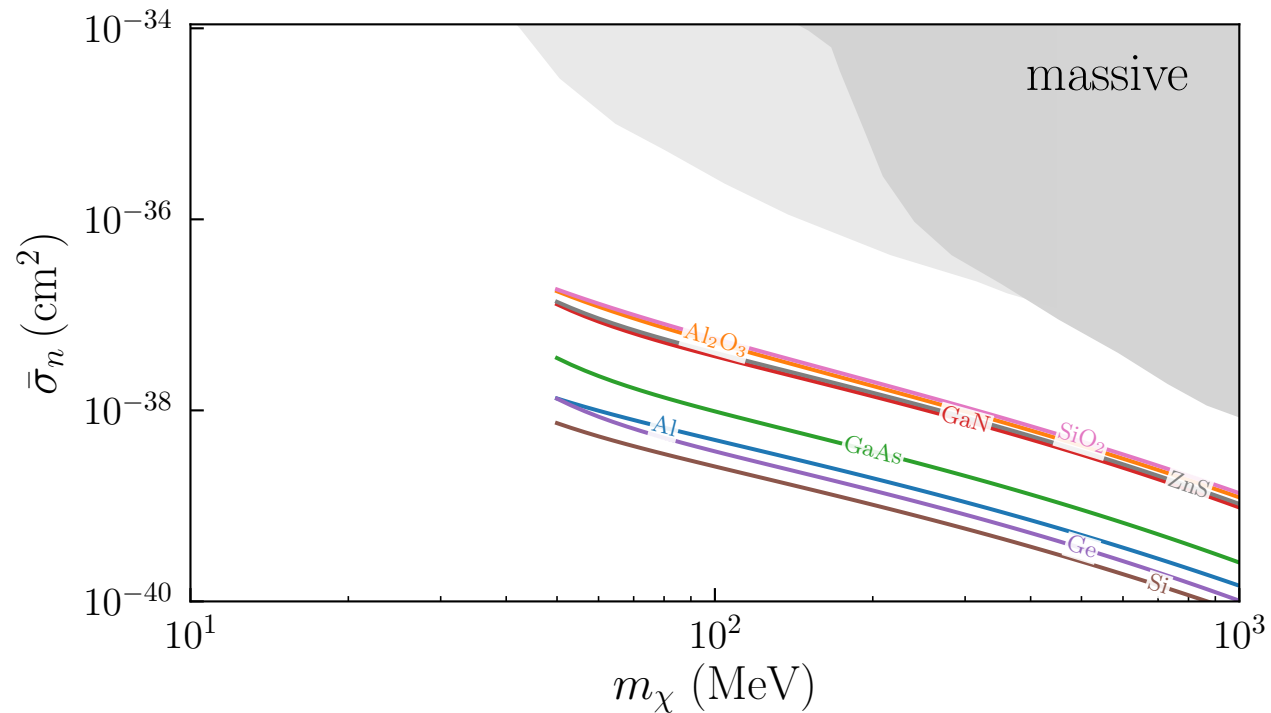
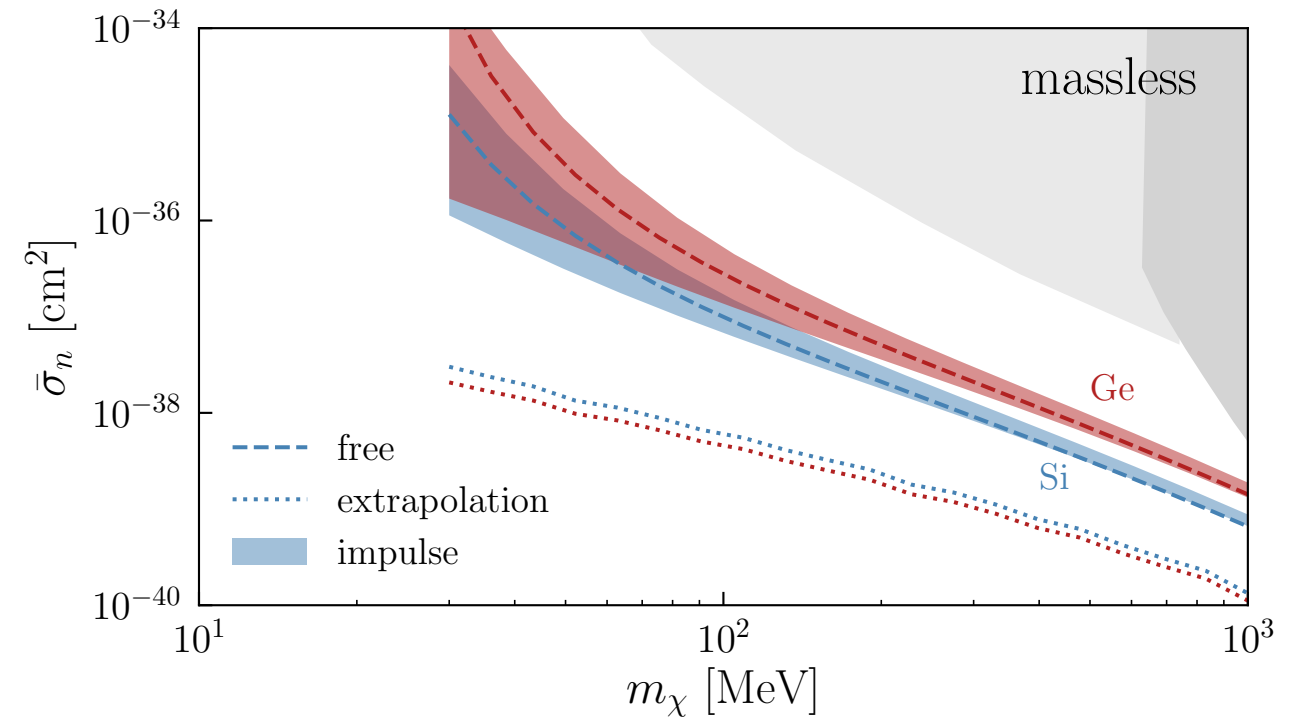
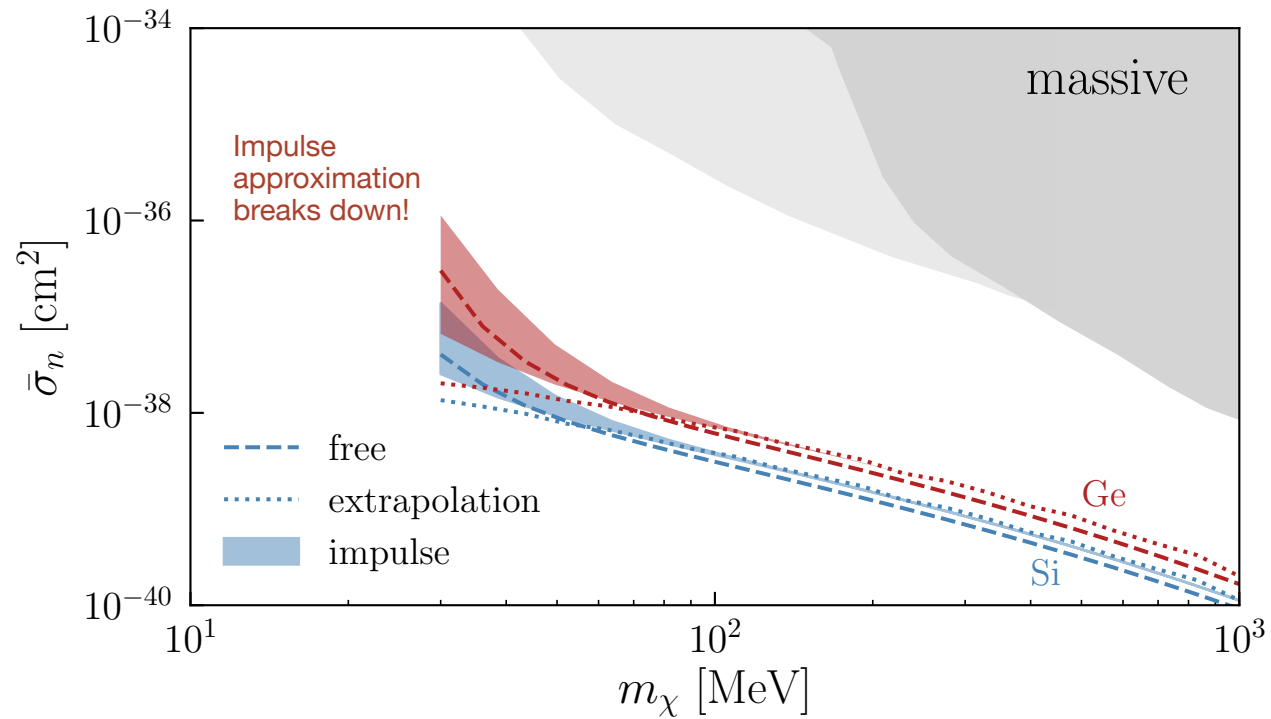
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As for brehmstrahlung the momentum dependence of the effective charge is quite important.


Because the probability is weighted towards fairly high  $k$ , screening isn't as effective

# Migdal effect results



We believe the electronic response is on solid ground

Nuclear recoil (impulse approximation) is main source of uncertainty

 main ▾

 1 branch


 0 tags

Go to file

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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 ELF's 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 ELF's 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

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### Releases

No releases published  
[Create a new release](#)

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### Packages


No packages published  
[Publish your first package](#)

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### Contributors

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 simonknapen86

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### Languages

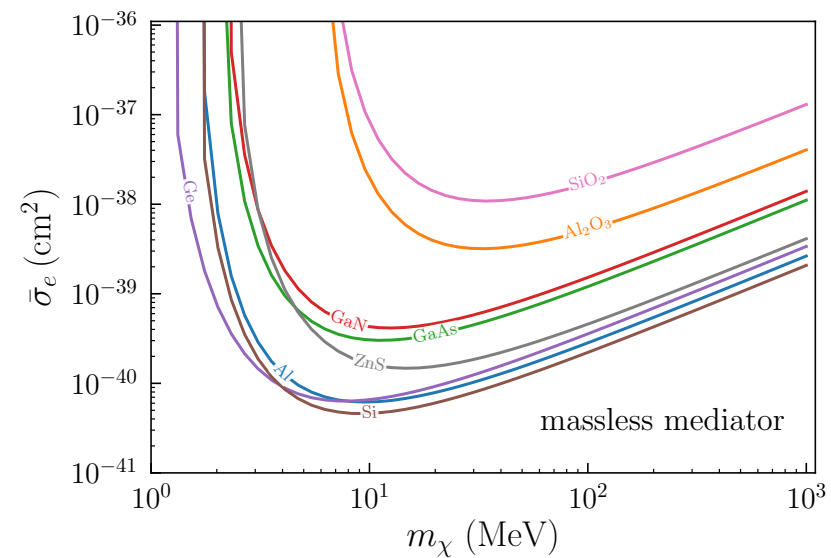
Python 100.0%

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

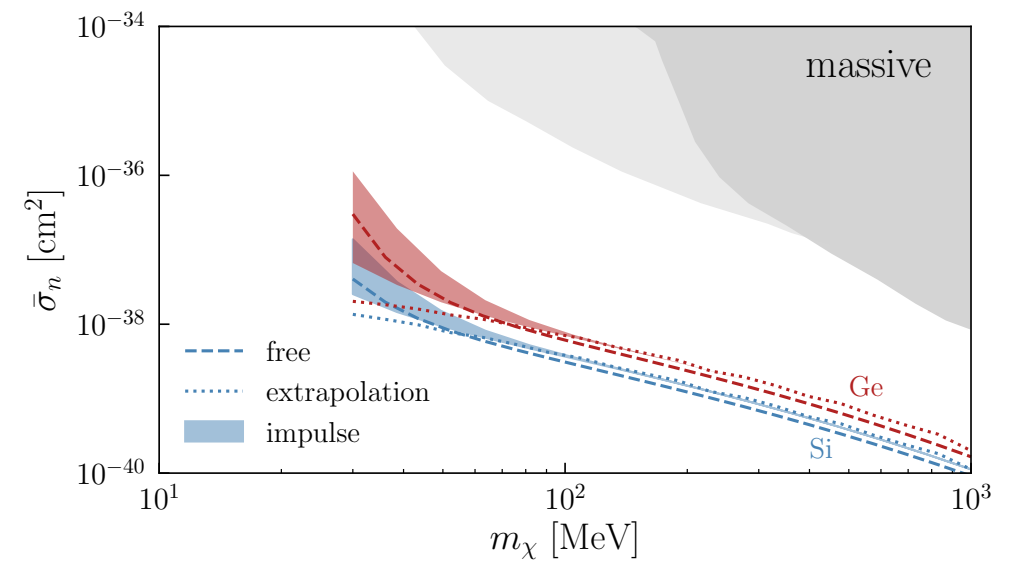


# DarkELF functions

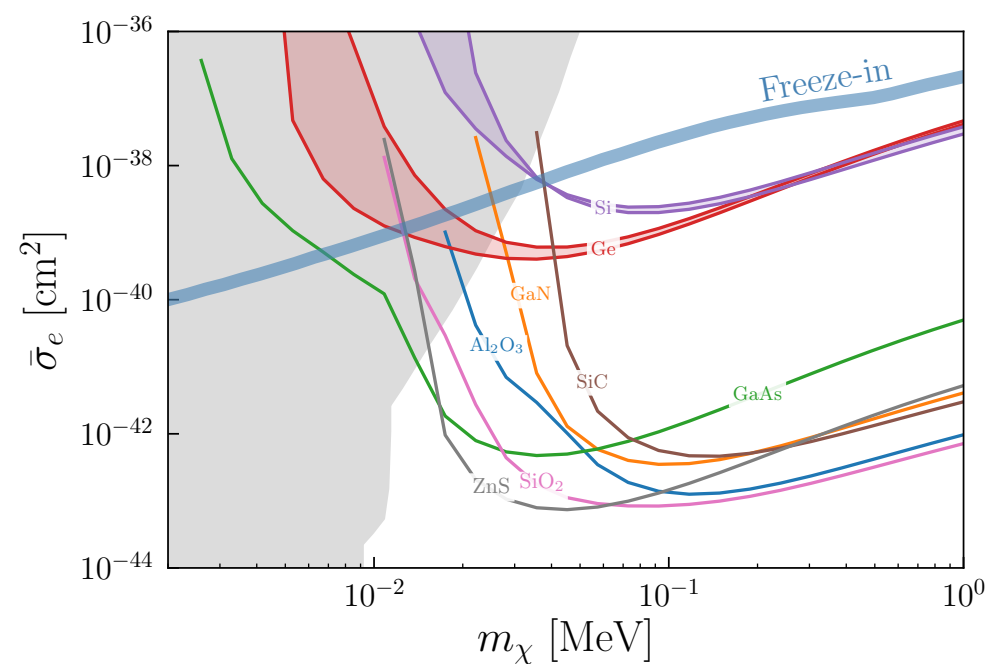
## DM - electron scattering



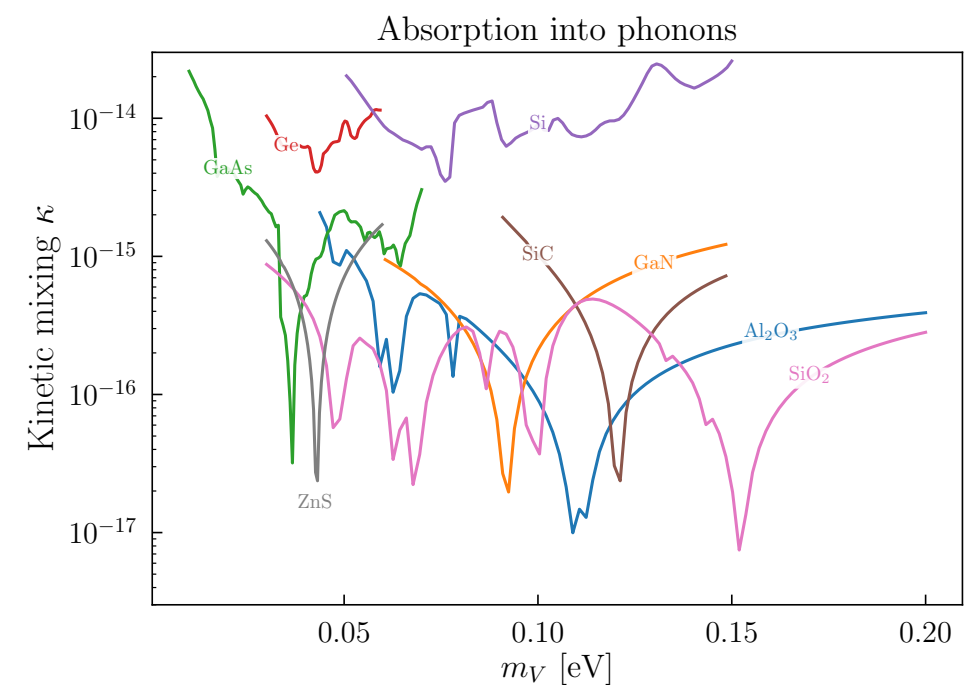
## Migdal effect



## DM - phonon scattering



## Dark photon absorption



# For tomorrow's discussion session

If you don't have them already, please install:

- python3 with numpy & scipy
- Jupyter

In my experience this is most straightforward by installing a full scientific python environment such as Anaconda

<https://www.anaconda.com/>

Once you have this, download and unpack the **darkELF** package.

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

No compilation is needed. Try to run one of the example notebooks.

# Summary

- Inelastic processes such as brehmstrahlung and the Migdal effect give experiments access to **DM candidates whose elastic recoils are below threshold**
- This comes a **price in scattering rate...**
- ...and a bit of pain/fun for the theorists
- The **Migdal trick works for atomic targets**, for crystals a direct calculation is needed
- **For low DM mass, the impulse approximation breaks** for both for noble liquids and crystals. In the regime the correct answer is not yet known.

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Questions?

