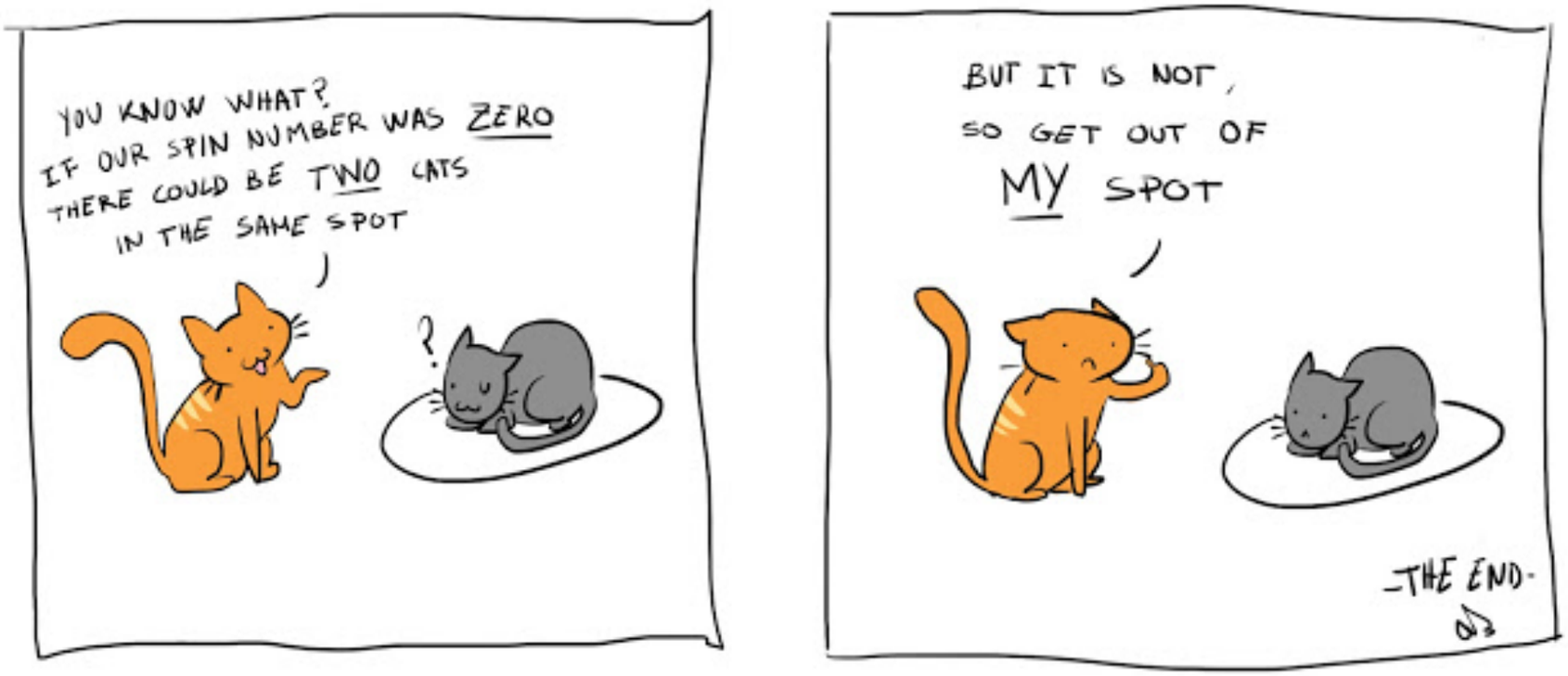
The Migdal effect in semi-conductors

Simon Knapen

Lawrence Berkeley National Laboratory



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

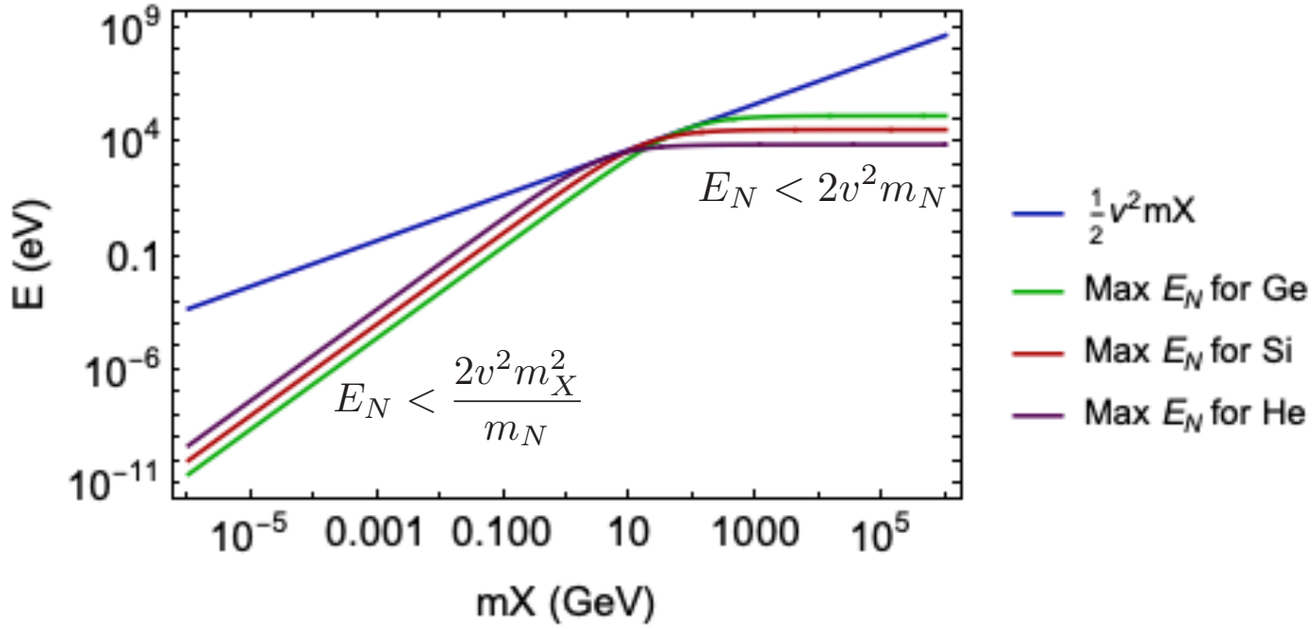
SK, J. Kozaczuk, T. Lin: arXiv 2104.12786, 2101.08275, 2011.09496
See also Liang et.al. : arXiv 2011.13352

Elastic nuclear recoil kinematics

Momentum conservation implies

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

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



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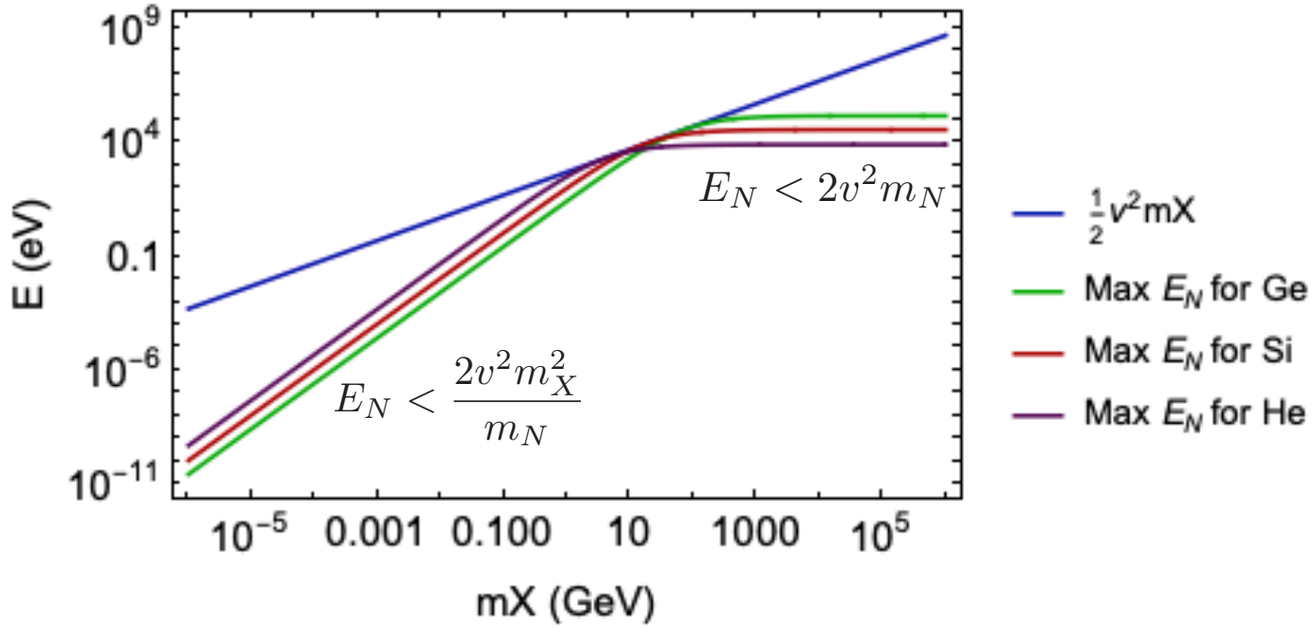

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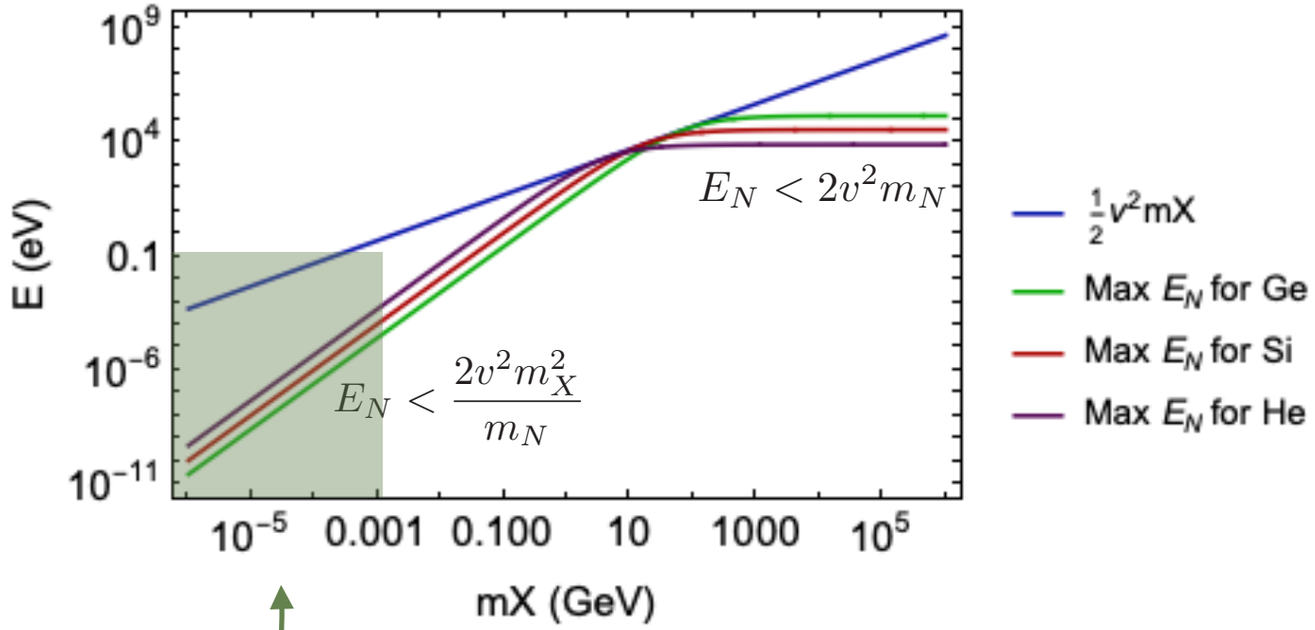

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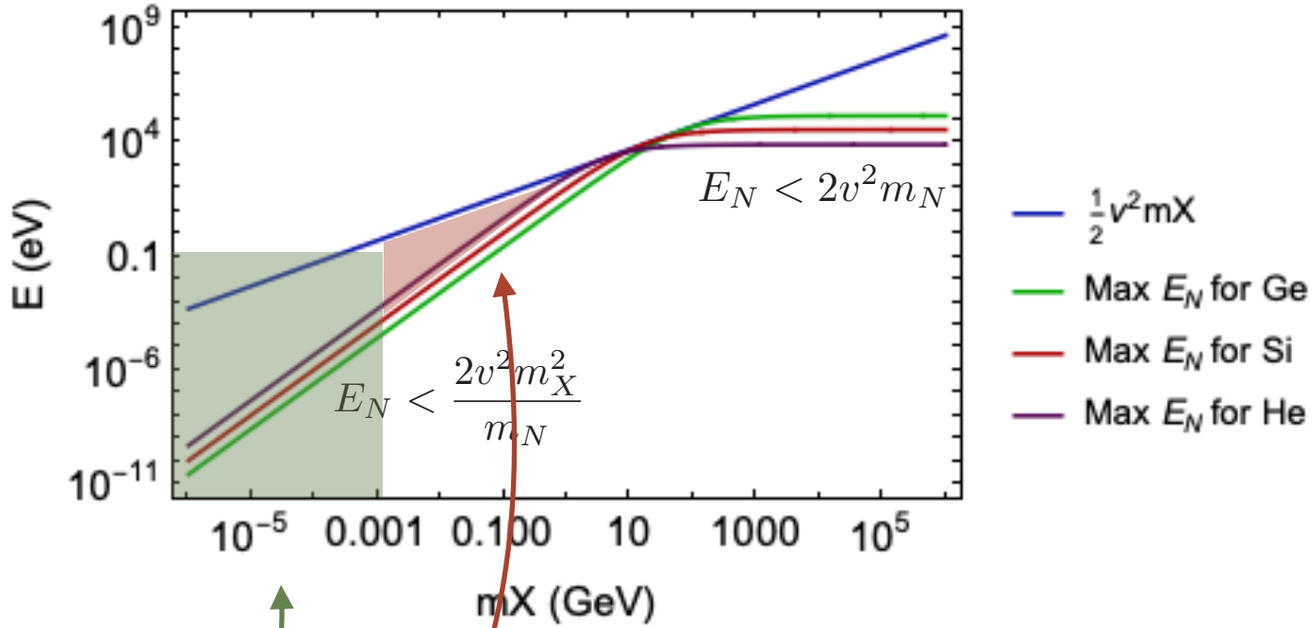

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The Migdal effect

A. Migdal (1939)
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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

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Ionization

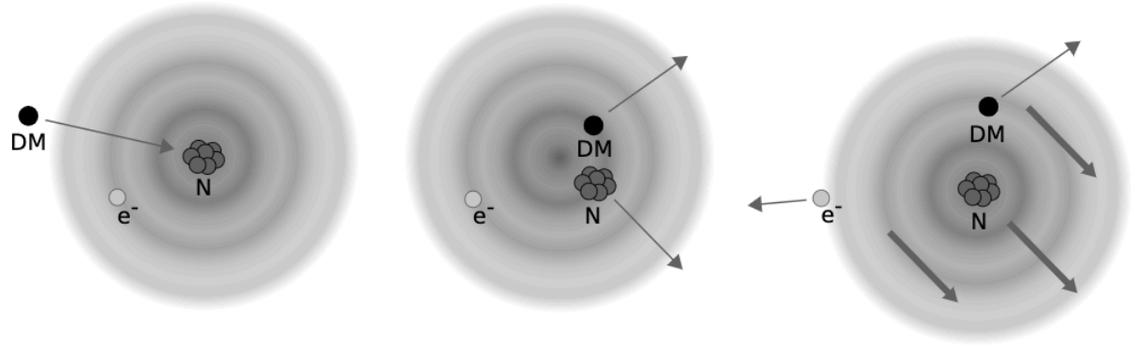

Figure from arXiv 1711.09906

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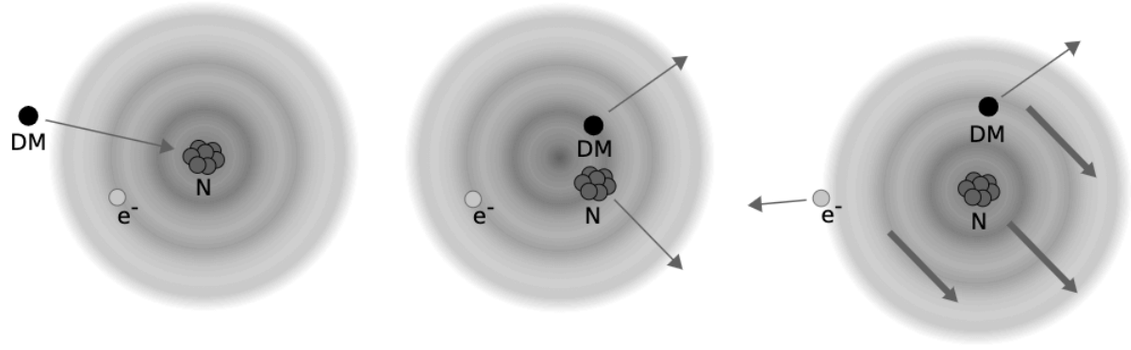
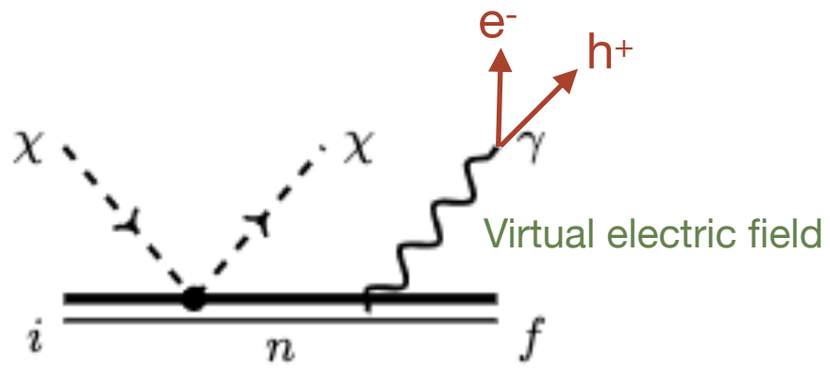


Figure from arXiv 1711.09906

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 brehmstrallung, but energy is dissipated into e^- h^+ pairs instead of a photon



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 α
ω, k	Energy and momentum deposited to the electrons

Migdal's trick

A. Migdal (1939)

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

The excited electron wave functions in the rest frame of the recoiling nucleus

→

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The ground state wave function, boosted to the frame of the recoiling nucleus.

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Boosting the wave function with a velocity v_N:

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

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

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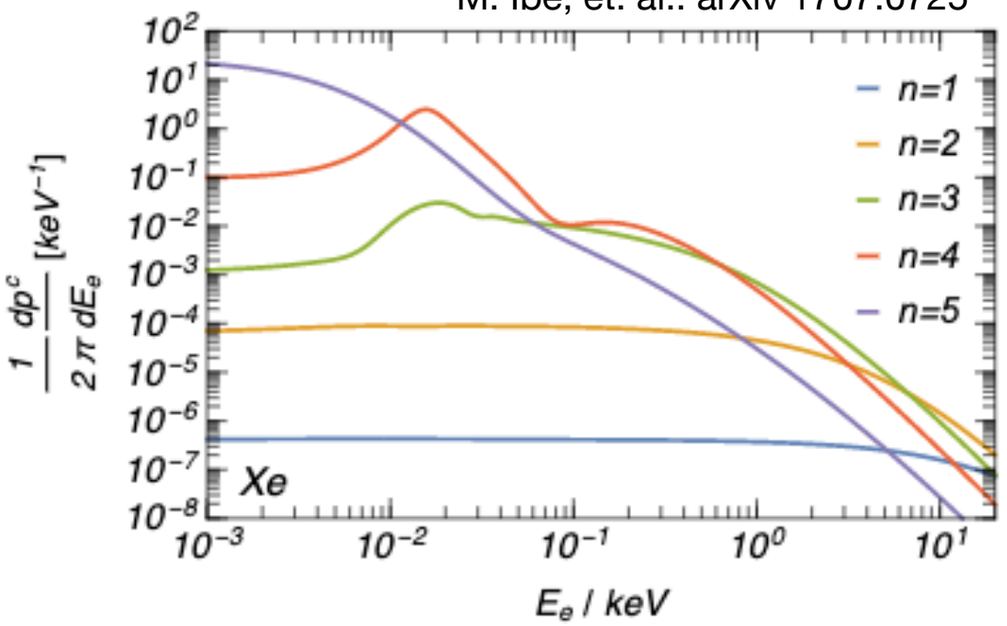

Alternative calculation

Migdal's trick has a few drawbacks:

- The "brehmstrallung" 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?

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

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

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

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

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

→ Dipole potential

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

Alternative calculation

The transition probability is

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

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

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

Perturbation theory

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

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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!

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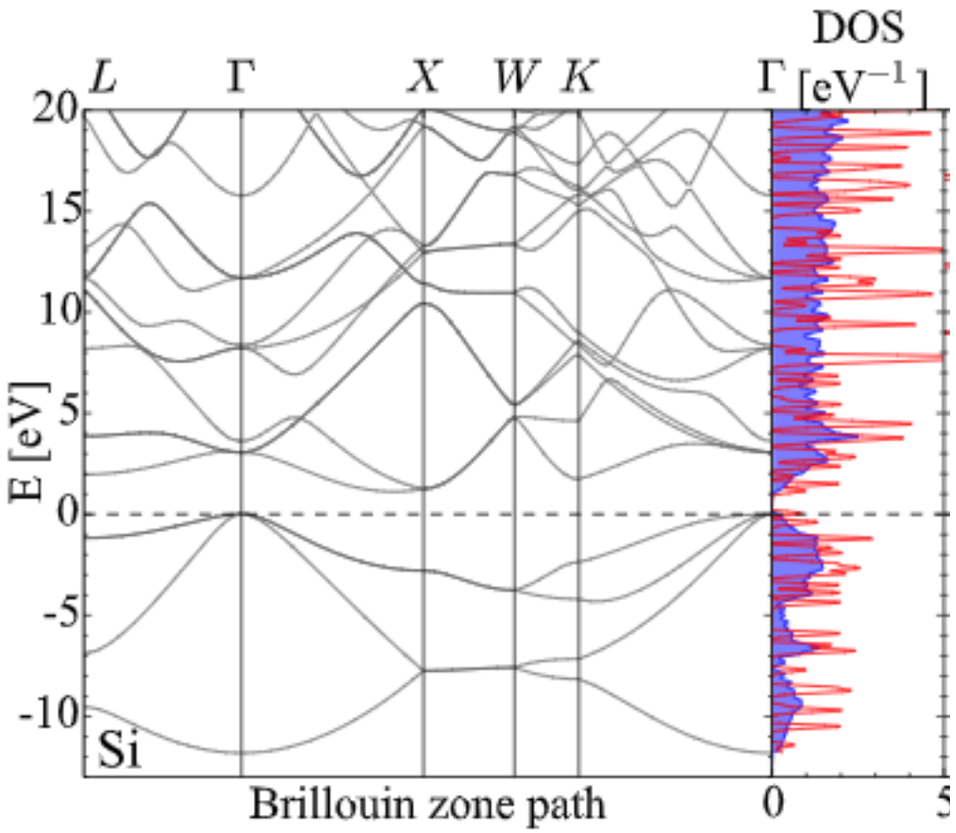
Use this for crystals!

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!

Electrons in crystals are complicated



e⁻ are not free

e⁻ are not at rest

e⁻ are not localized

e⁻ are not alone

→ screening

Bloch wave functions

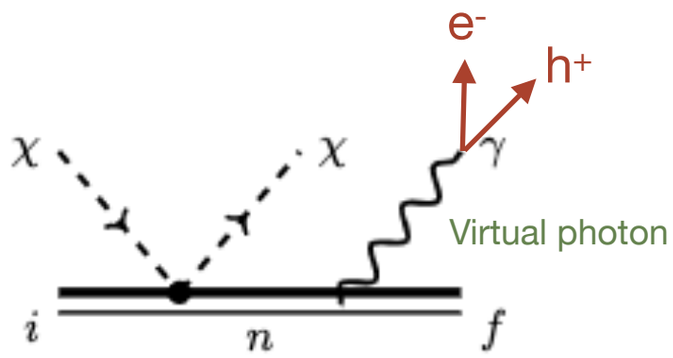
Obtain with density functional theory (DFT)

There is a shortcut however!

Figure from Essig et. al. 1509.01598

The energy loss function (ELF)

Process:



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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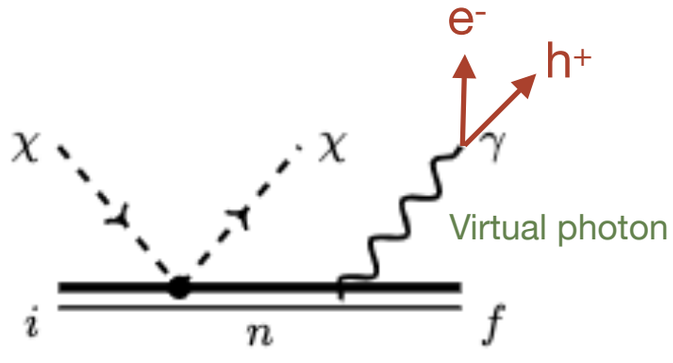

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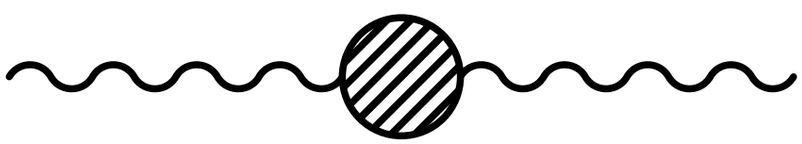

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(Non-relativistic limit)

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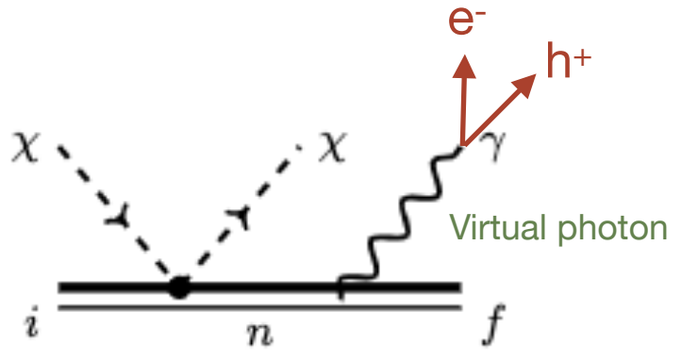

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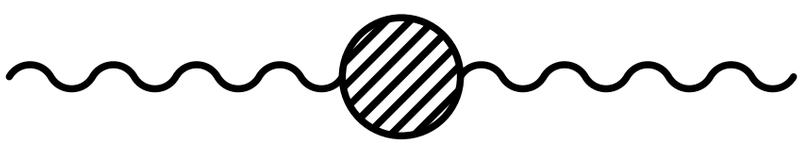

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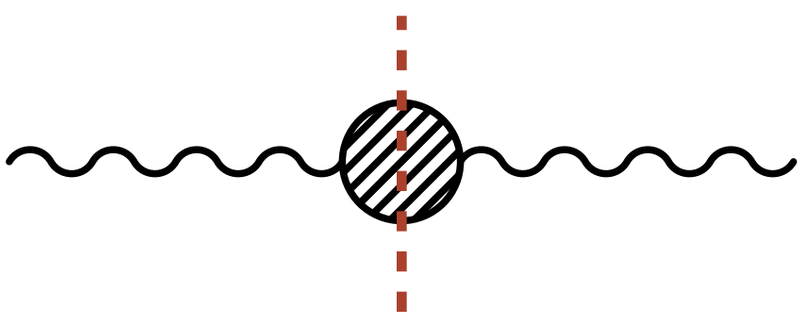
We are interested in energy dissipation:



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

“Energy Loss Function” (ELF)

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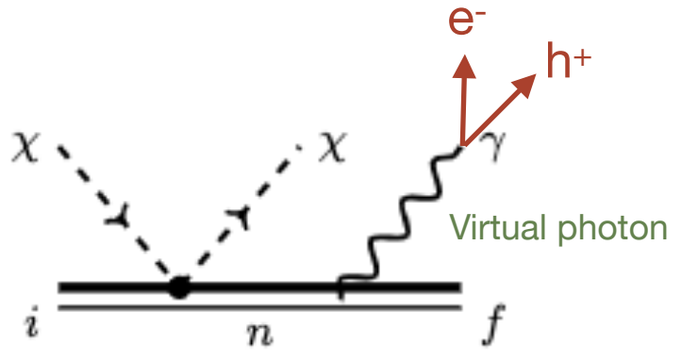

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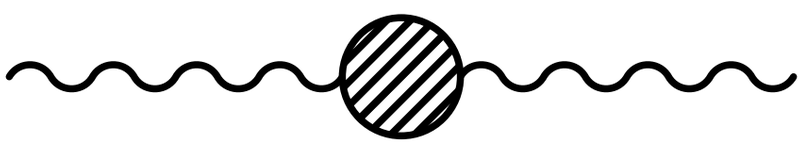

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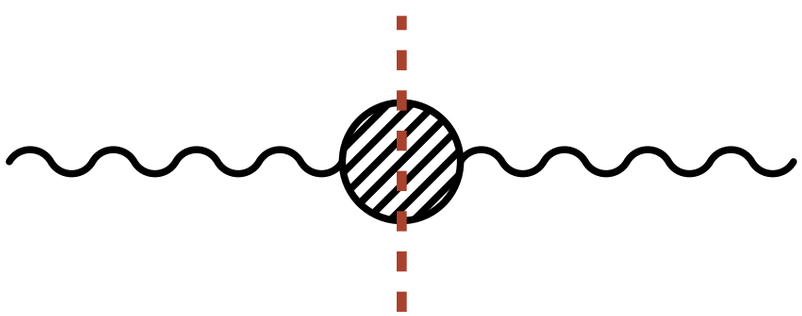

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e- excitation matrix element

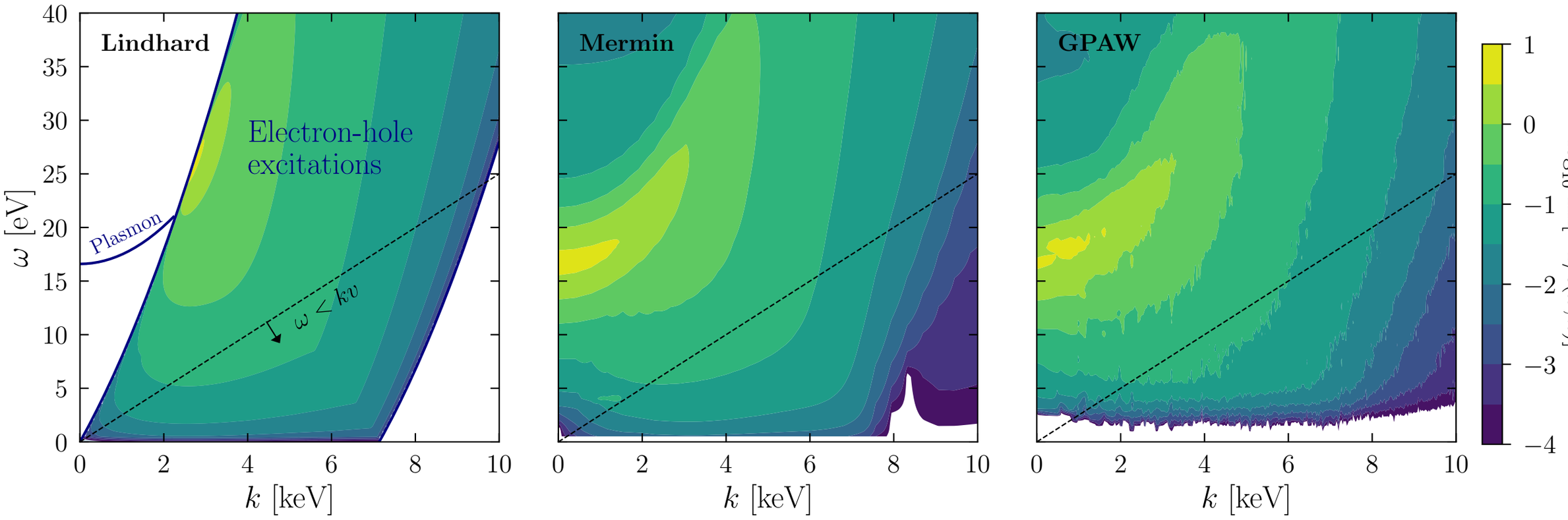
Lindhard (1954)

Screening

“Energy Loss Function” (ELF)

Calculating the ELF

Simple → Sophisticated



Free electron gas approximation

100% analytic

Phenomenological model fit to data

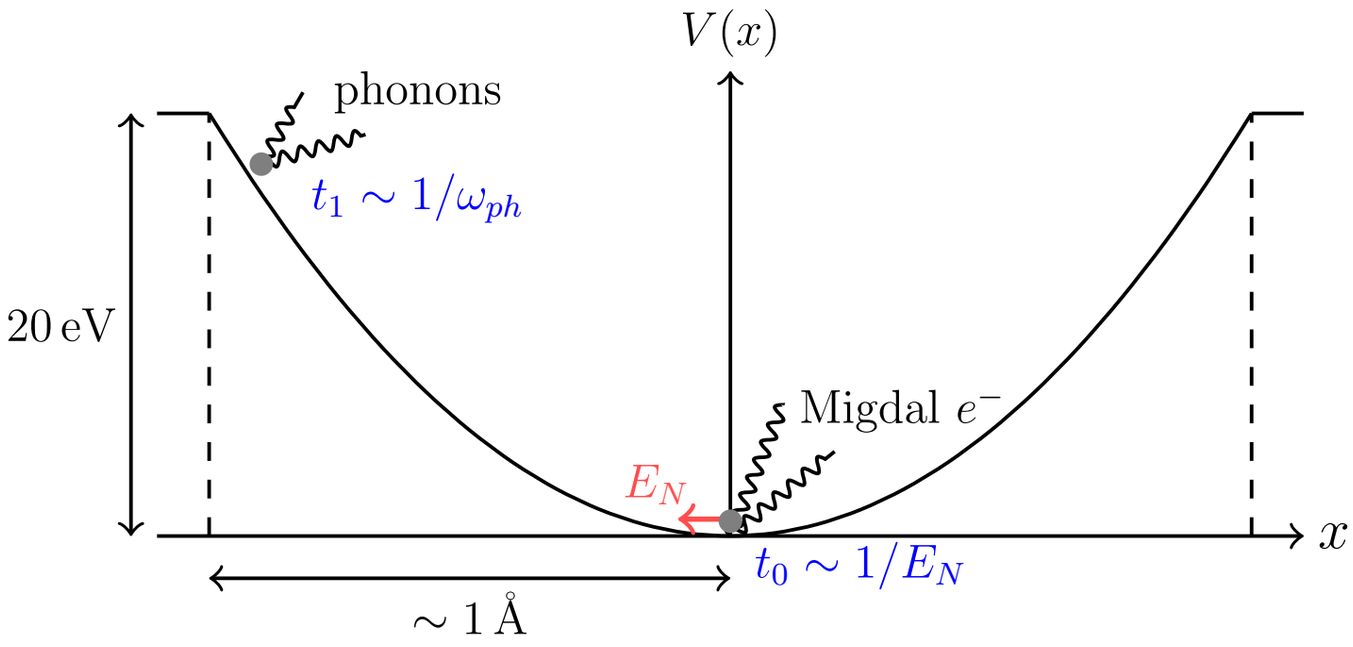
semi-analytic

First principles DFT calculation

Fully numerical

More details in back-up slides

Nucleus response: The impulse approximation



If the DM is heavy enough, most collisions take place at an energy well above the typical phonon energy (~ 30 meV)

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

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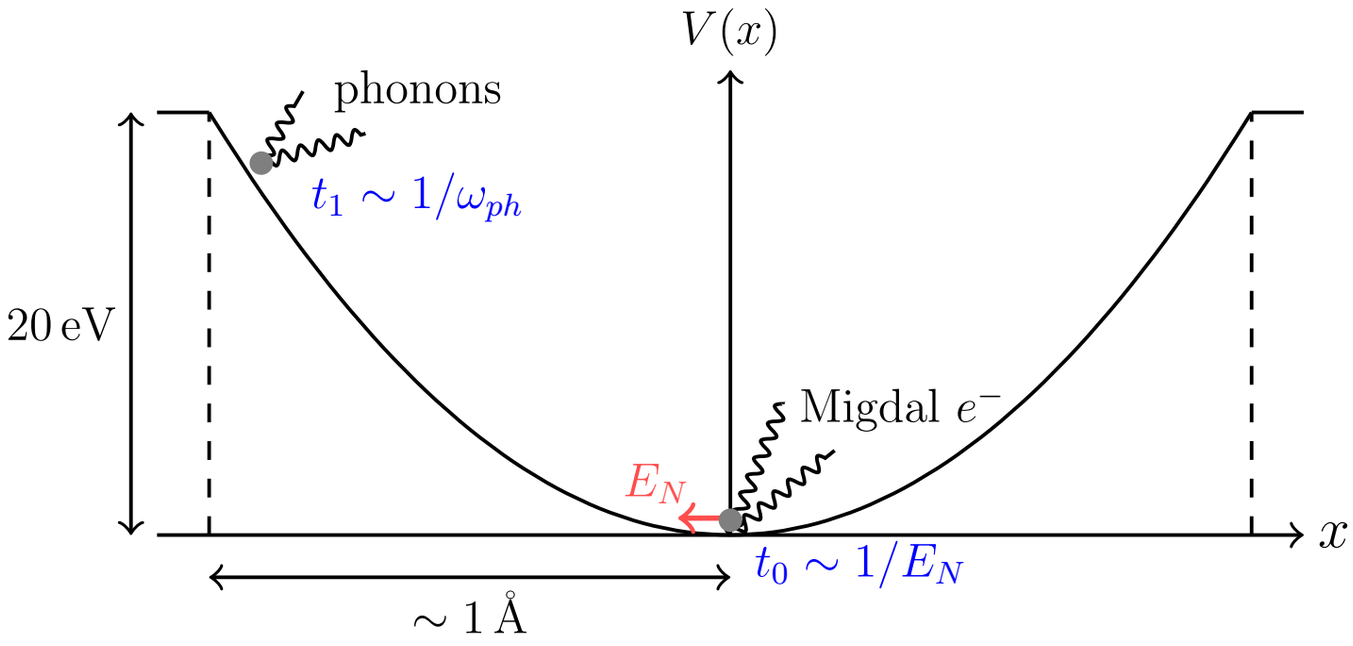

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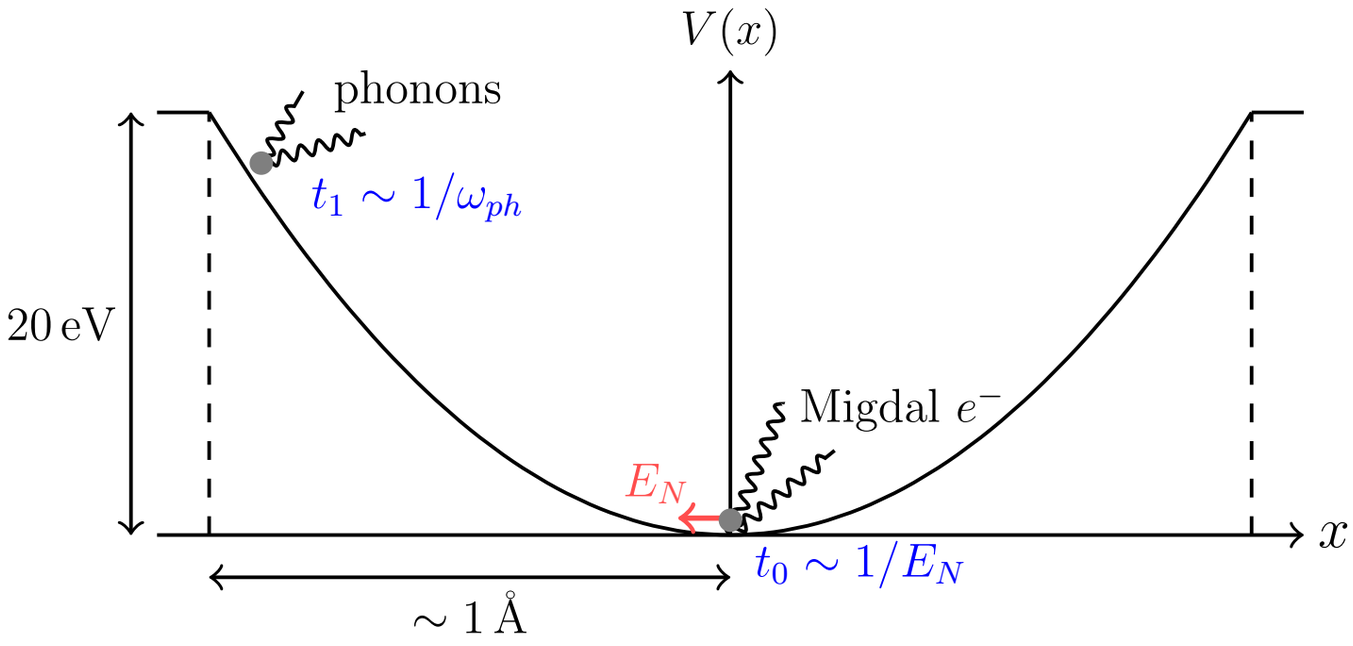

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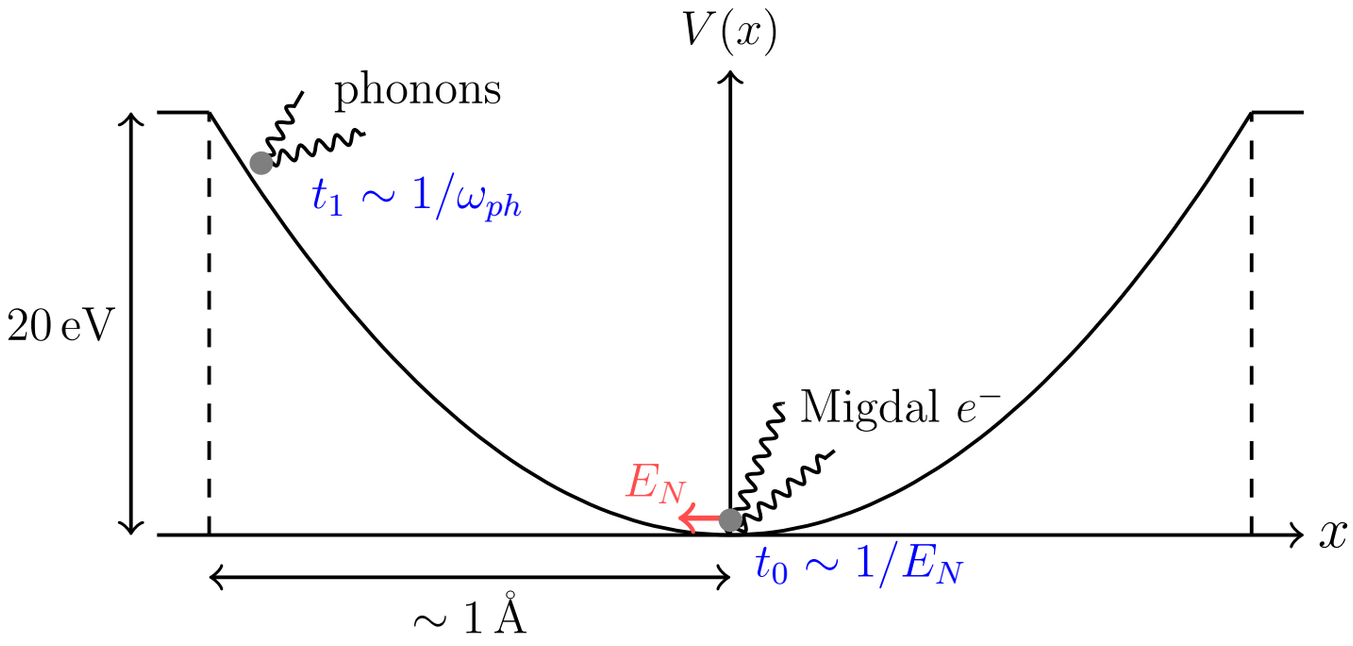

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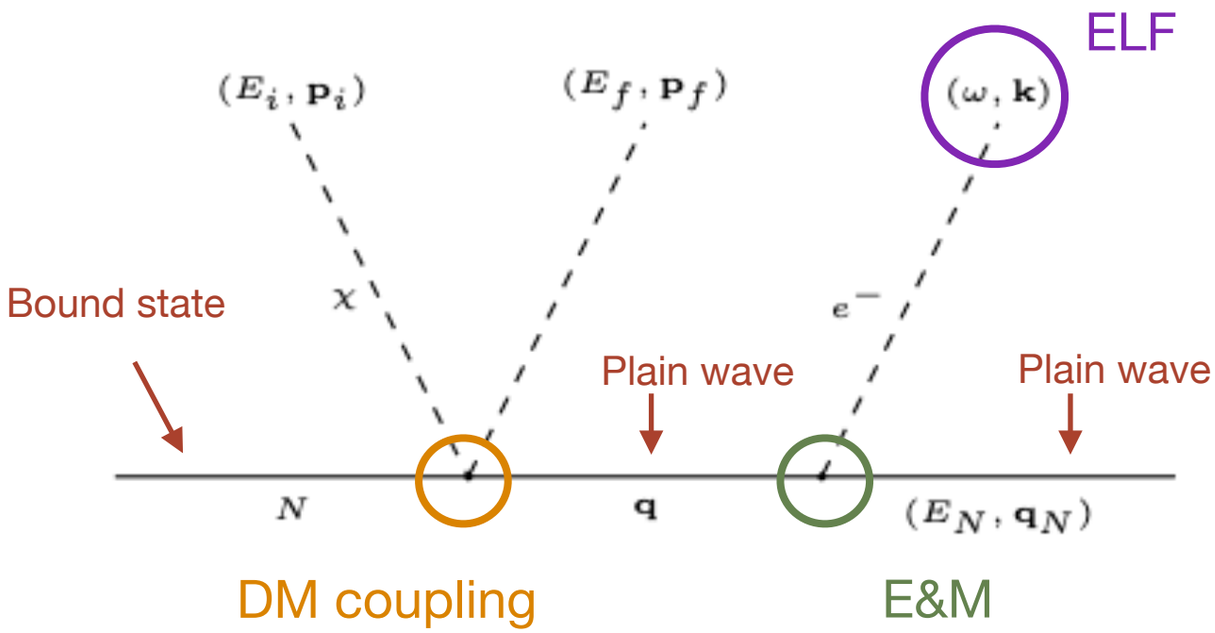
When it is valid we can factorize the long distance physics (phonons) from the short distance physics (Migdal effect).

Full result

With impulse approximation:



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

Result:

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

Full derivation in appendix A of SK, J. Kozaczuk, T. Lin: arXiv 2011.09496
See also Liang et.al. : arXiv 2011.13352

Full result

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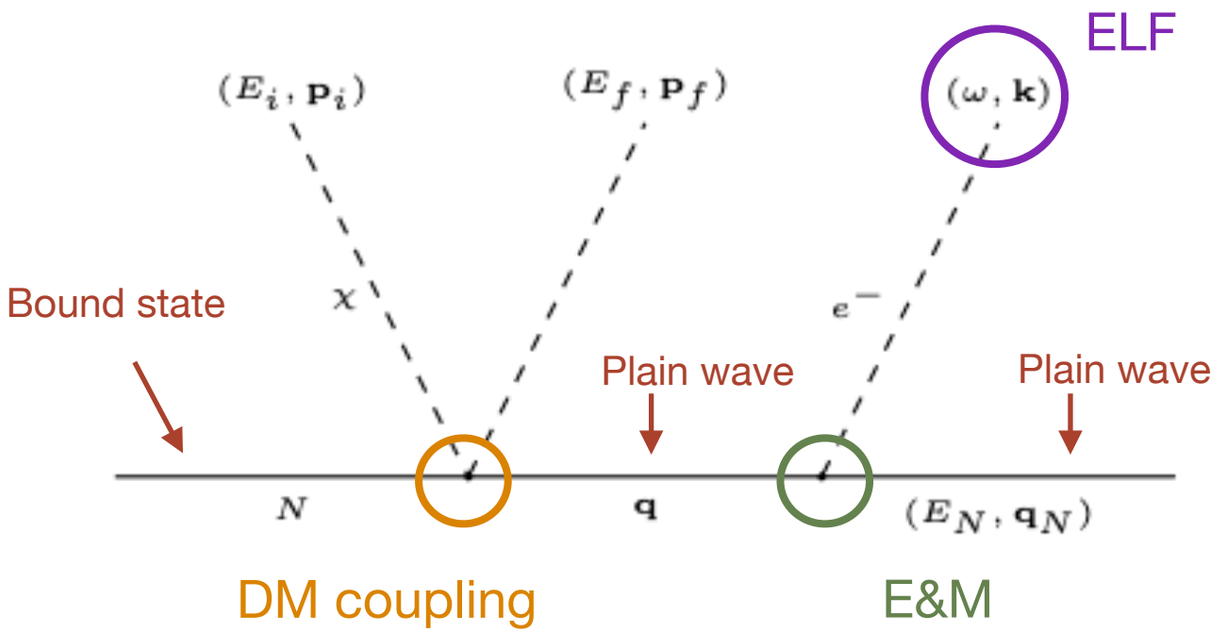

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ELF Nucleus propagator

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DM form factor Crystal form factor

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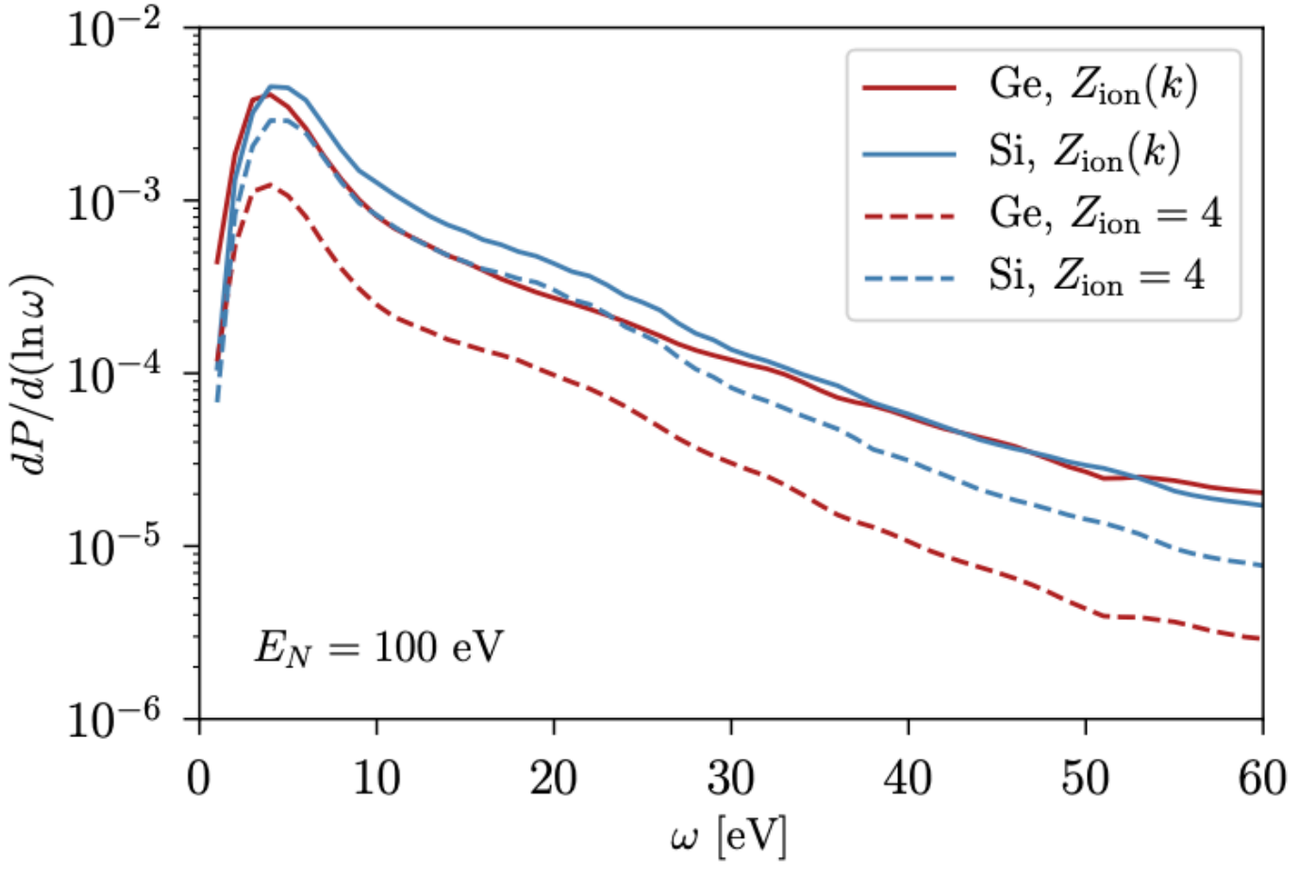
In the soft limit

For k << v m_X, we can factorize the rate into elastic recoil x excitation probability:

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

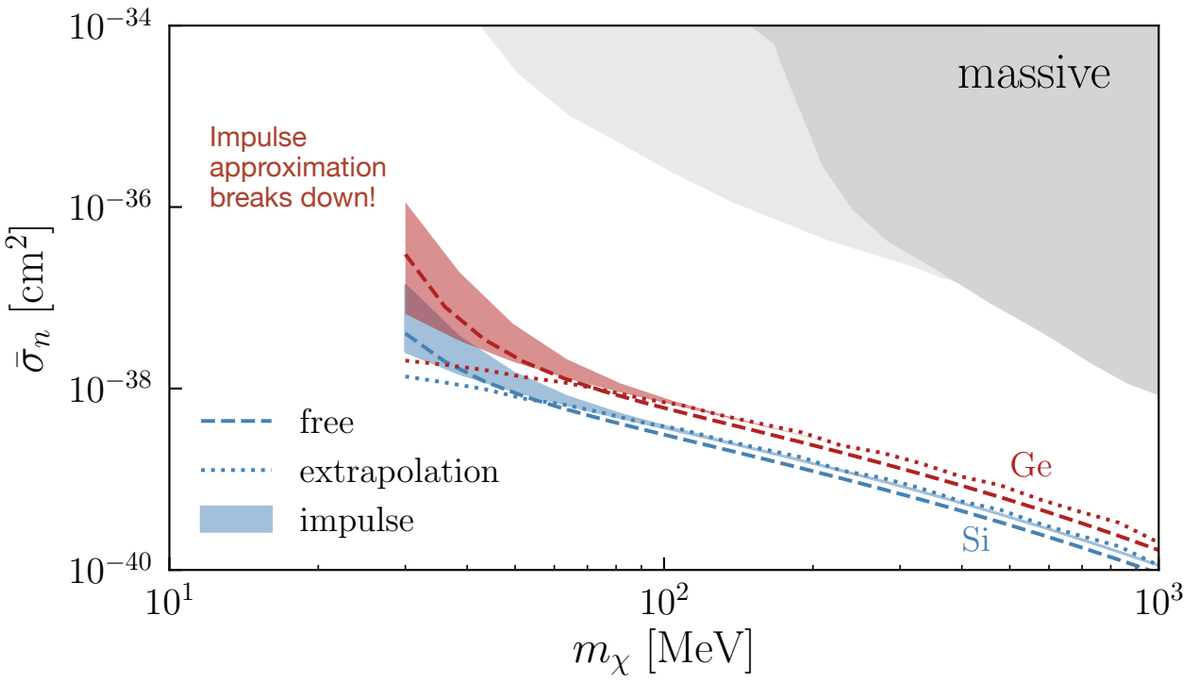
$$\frac{dP}{d\omega} = 4\alpha \int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{Z^2_{\rm ion}(k)}{k^2}\frac{|\mathbf{v}_N\cdot\mathbf{k}|^2}{\omega^4}{\rm Im}\left[\frac{-1}{\epsilon(\mathbf{k},\omega)}\right].$$

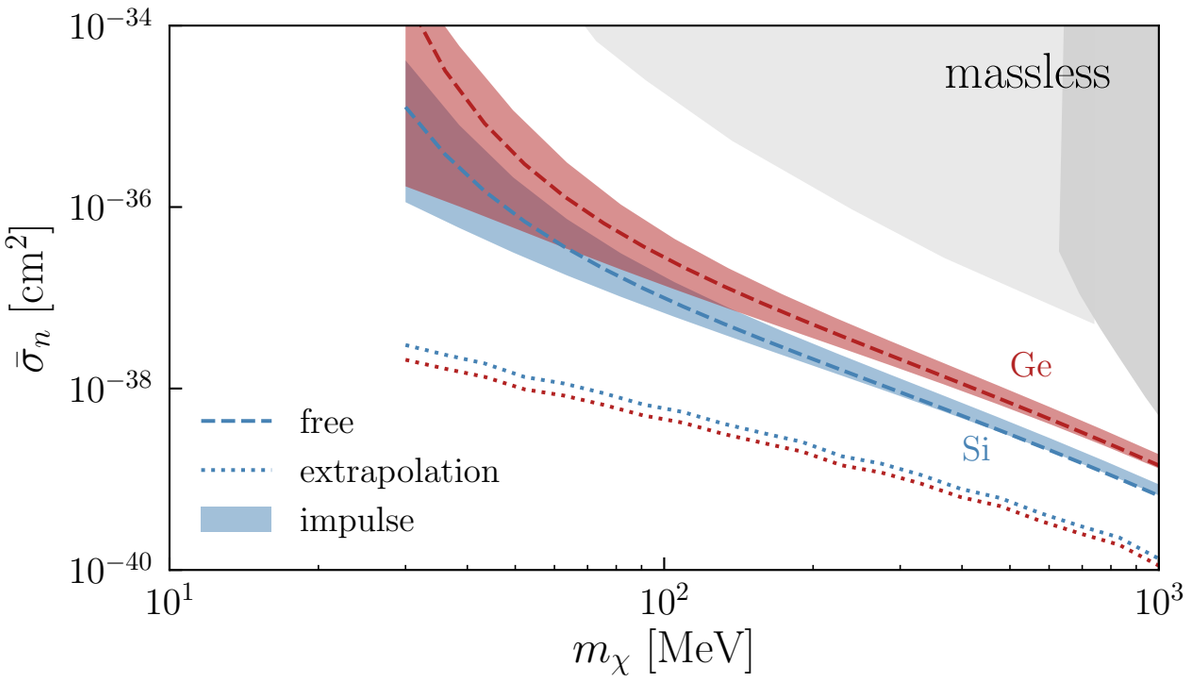


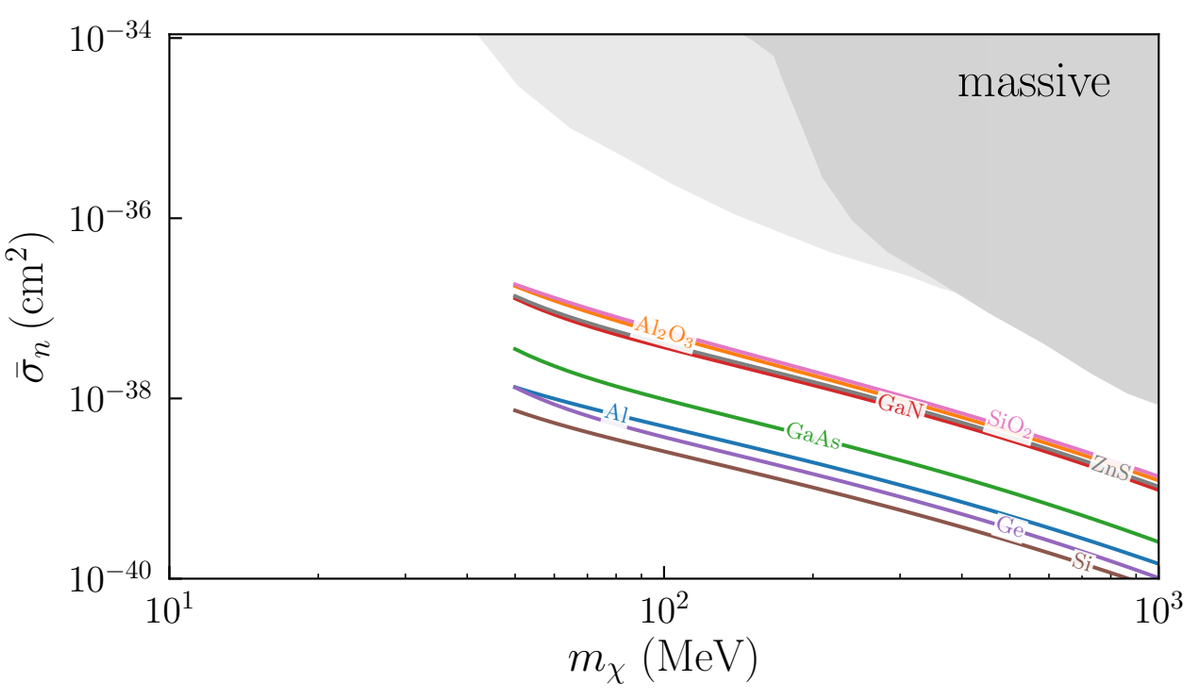
The momentum dependence of the effective charge is quite important.

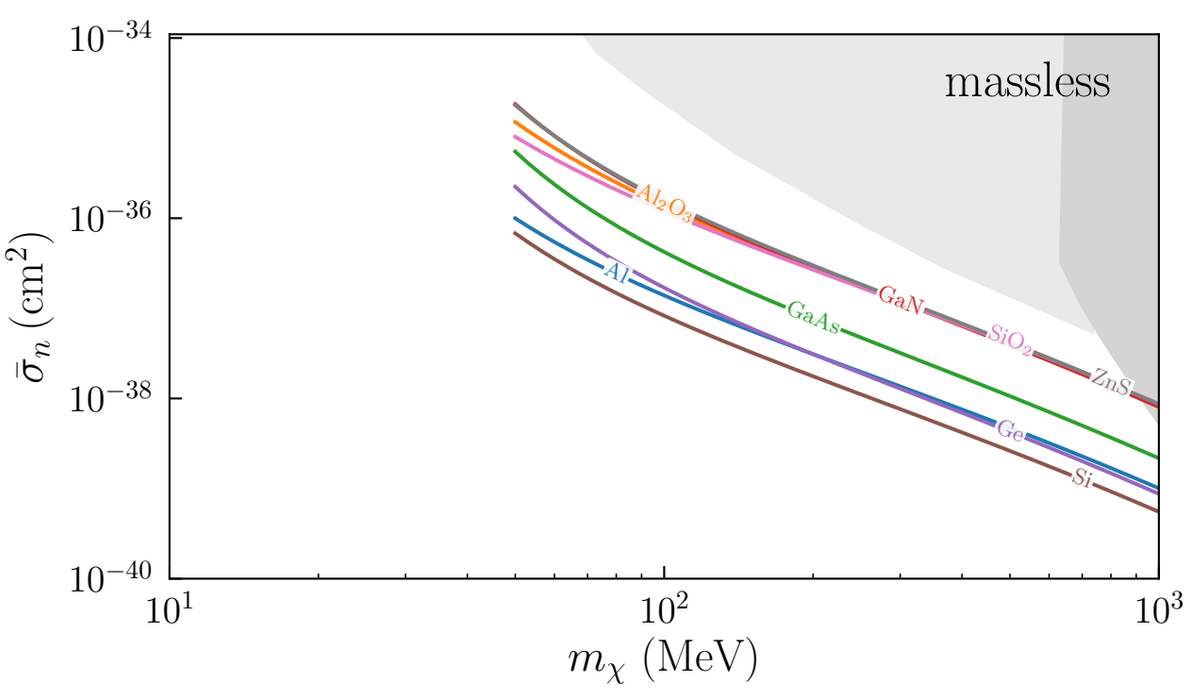
(Because the probability is weighted towards fairly high k, screening isn't as effective)

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 Add file 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

No releases published
Create a new release

Packages

No packages published
Publish your first package

Contributors 2

simonknapen86

tongylin Tongyan Lin

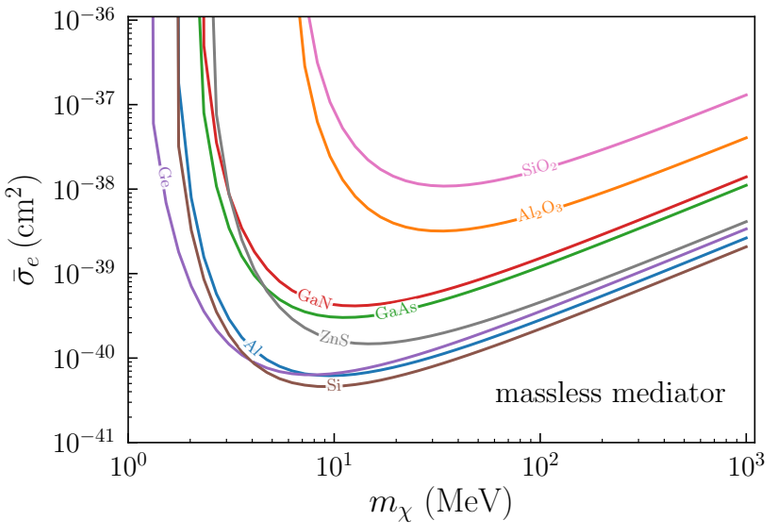
Languages

Python 100.0%

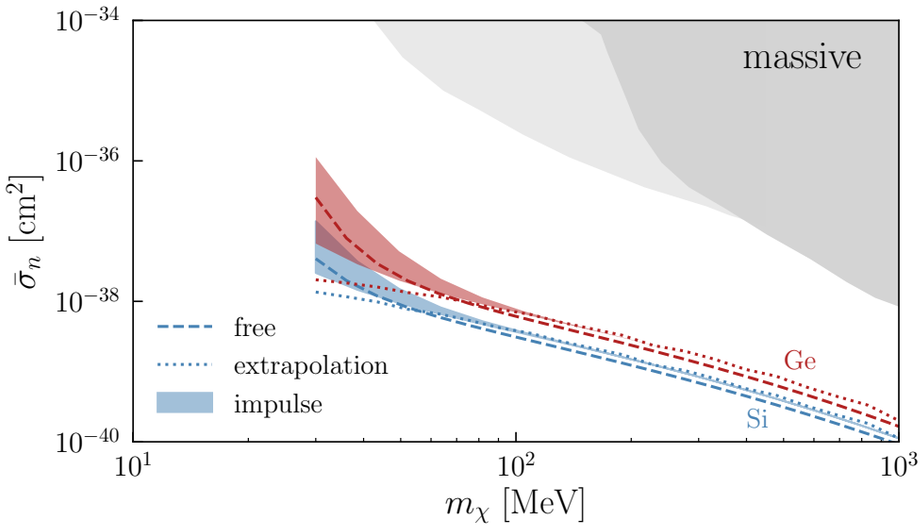
https://github.com/tongylin/DarkELF

DarkELF functions

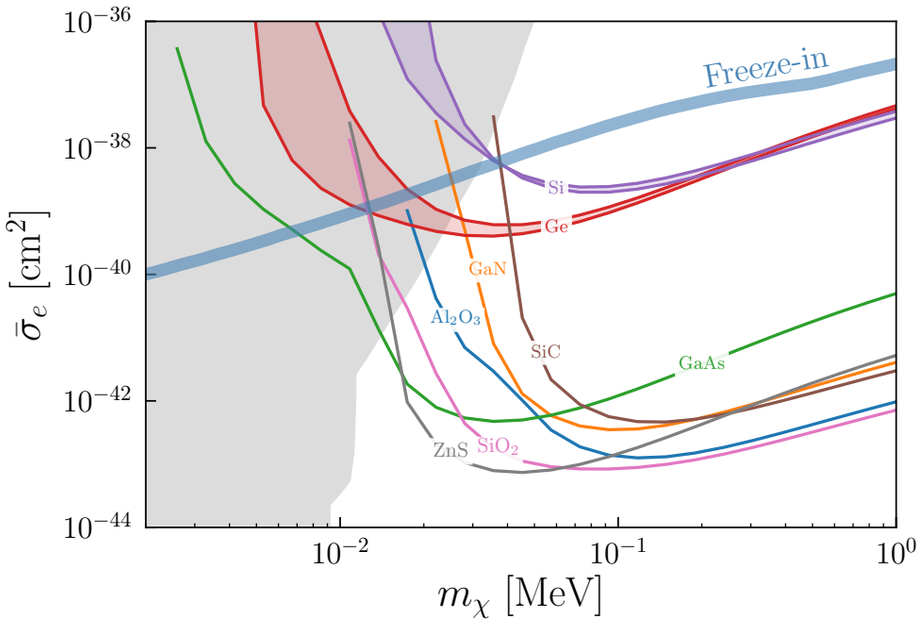
DM - electron scattering



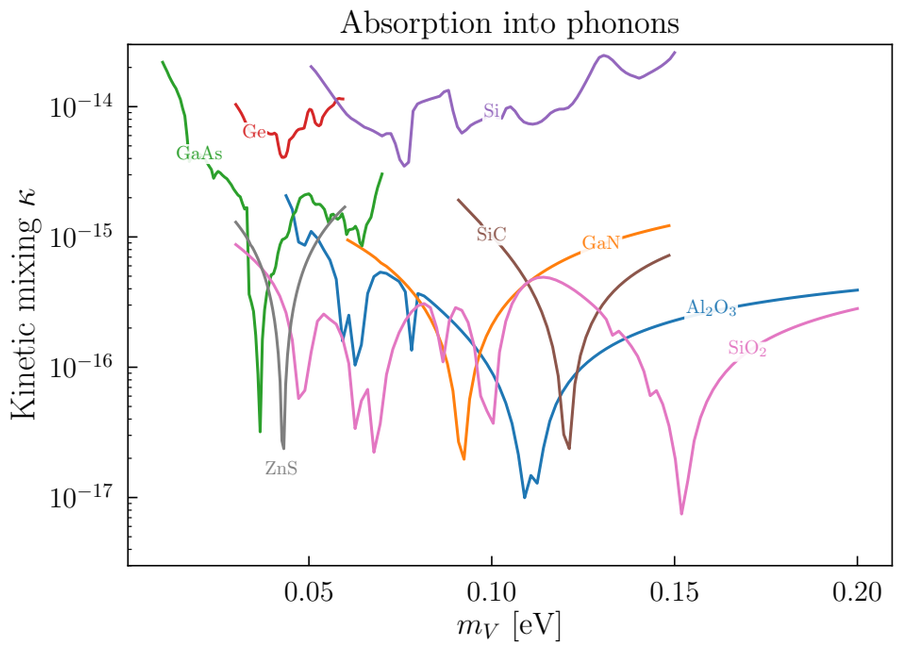
Migdal effect



DM - phonon scattering



Dark photon absorption



Summary

- 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 nobel liquids and crystals. In this regime the correct answer is not yet known.
- Calculations available at https://github.com/tongylin/DarkELF

Summary

- 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 nobel liquids and crystals. In this regime the correct answer is not yet known.
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Questions?

Back up

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:

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

And

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

Total force exerted on the electron

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

Making sense of this

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

$$= -i\frac{m_e}{\omega}\mathbf{v}_N \cdot \langle f| \sum_\beta [\mathbf{r}_\beta, H_0] |i\rangle \qquad \text{used} \qquad \omega = E_f - E_i$$

$$= \frac{1}{\omega}\mathbf{v}_N \cdot \langle f| \sum_\beta \mathbf{p}_\beta |i\rangle$$

$$= -\frac{1}{\omega^2}\mathbf{v}_N \cdot \langle f| \sum_\beta [\mathbf{p}_\beta, H_0] |i\rangle$$

$$= i\frac{1}{\omega^2}\mathbf{v}_N \cdot \langle f| \sum_\beta \frac{dV}{d\mathbf{r}_\beta} |i\rangle \longrightarrow$$

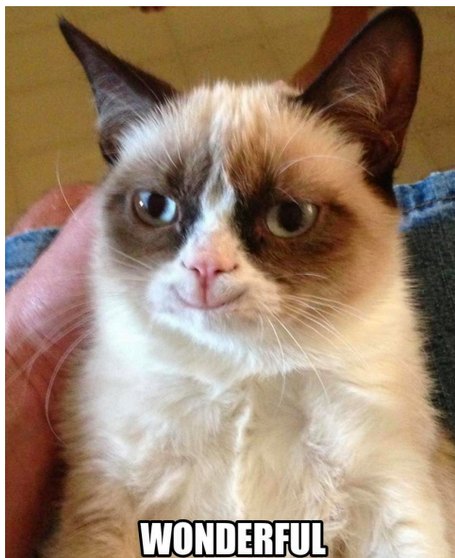
Proportional to total force exerted in the electron

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

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

$$= i\frac{Z_N\alpha}{\omega^2}\mathbf{v}_N \cdot \langle f| \sum_\beta \frac{\hat{\mathbf{r}}_\beta}{|\mathbf{r}_\beta|^2} |i\rangle \qquad \text{taking} \qquad \mathbf{r}_\beta \gg \mathbf{r}_N$$

$$= \mathcal{M}_{if}^{(pert)}$$



A closer look…

Just removing some intermediate steps here, same derivation…

$$\mathcal{M}_{if}^{(Migdal)} = i\frac{1}{\omega^2}\mathbf{v}_N \cdot \langle f| \sum_\beta \frac{dV}{d\mathbf{r}_\beta} |i\rangle$$

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

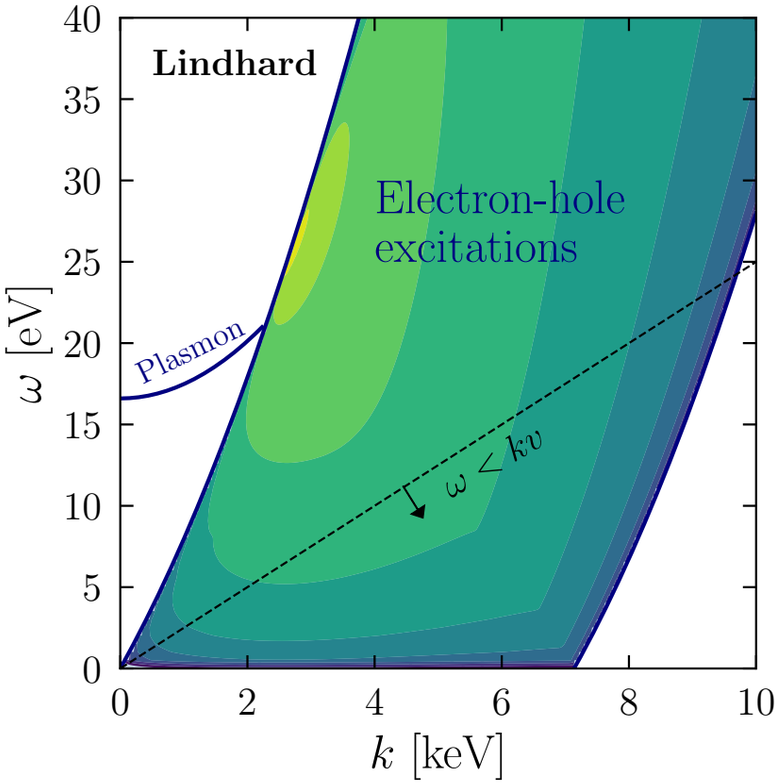
$$= \mathcal{M}_{if}^{(pert)}$$

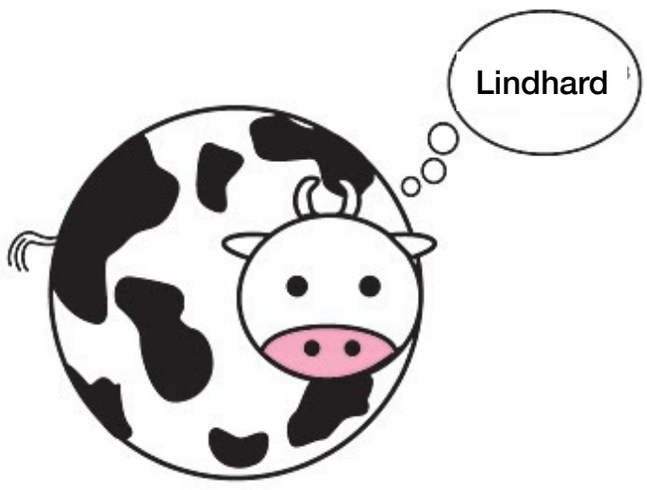
This step assumes that only the recoiling nucleus exerts a force on the electrons!

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

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.

Lindhard model





Homogenous, free electron gas:

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

with

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

Plasmon frequency

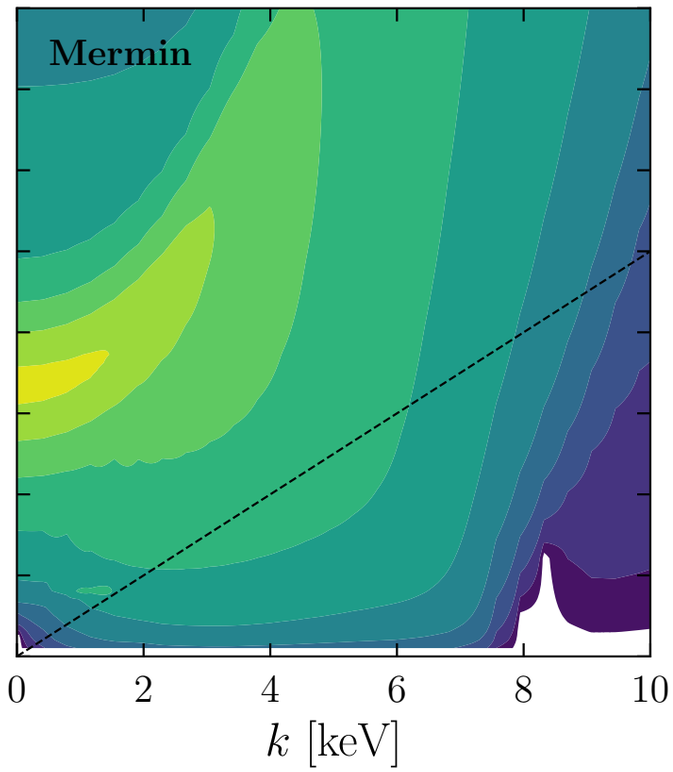
$$f(u,z) = \frac{1}{2} + \frac{1}{8z}\left[g(z-u) + g(z+u) \right]$$

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

Features:

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

Mermin model

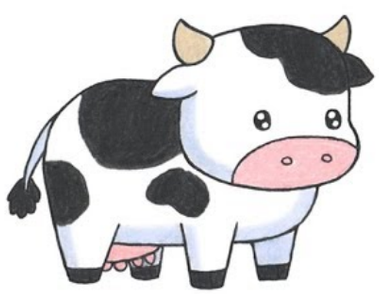


Homogenous, free electron gas with dissipation (Γ)

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

Fit a linear combination of Mermin oscillators to optical data:

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

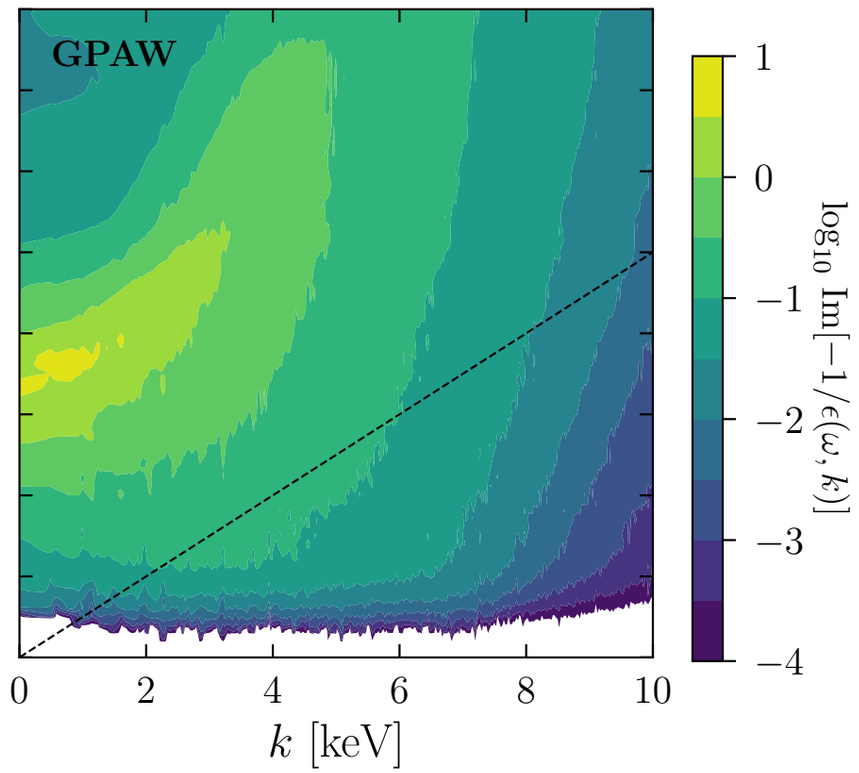


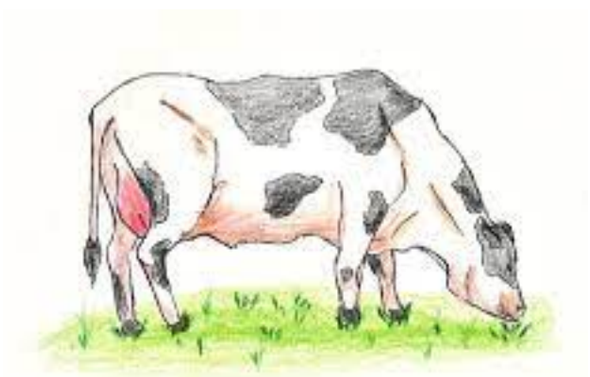
M. Vos, P. Grande: chapidif package
Data from Y. Sun et. al. Chinese Journal of Chemical Physics 9, 663 (2016)

Features:

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

GPAW method





GPAW: https://wiki.fysik.dtu.dk/gpaw/

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

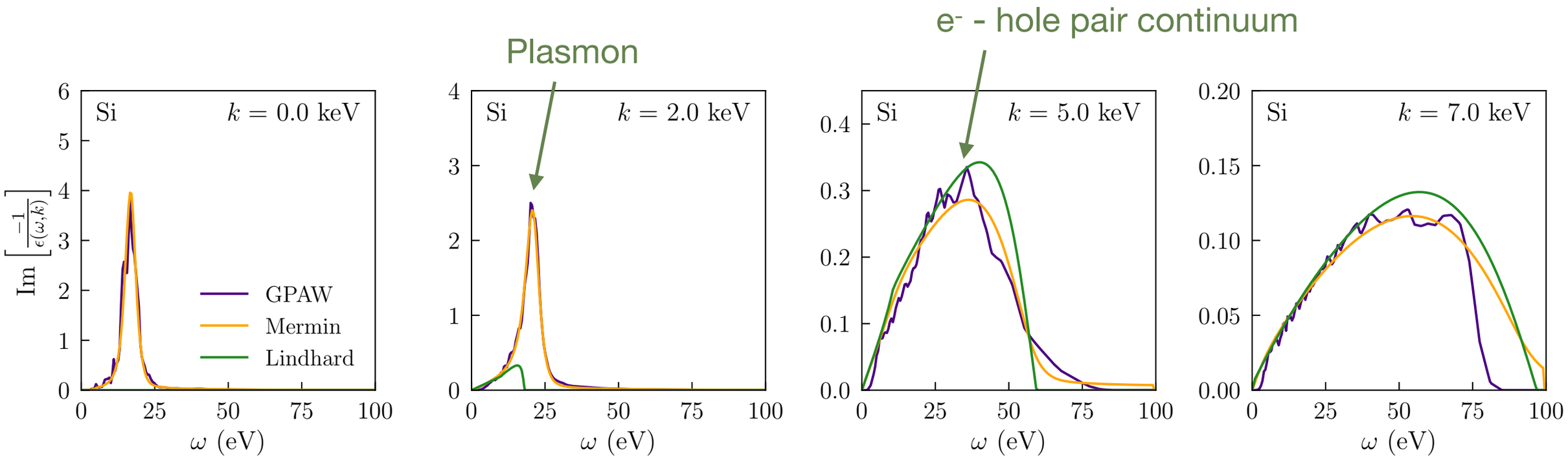
Puts atoms on periodic lattice and model interacting e^- as non-interacting e^- + effective external potential (Kohn-Sham method)

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

Features:

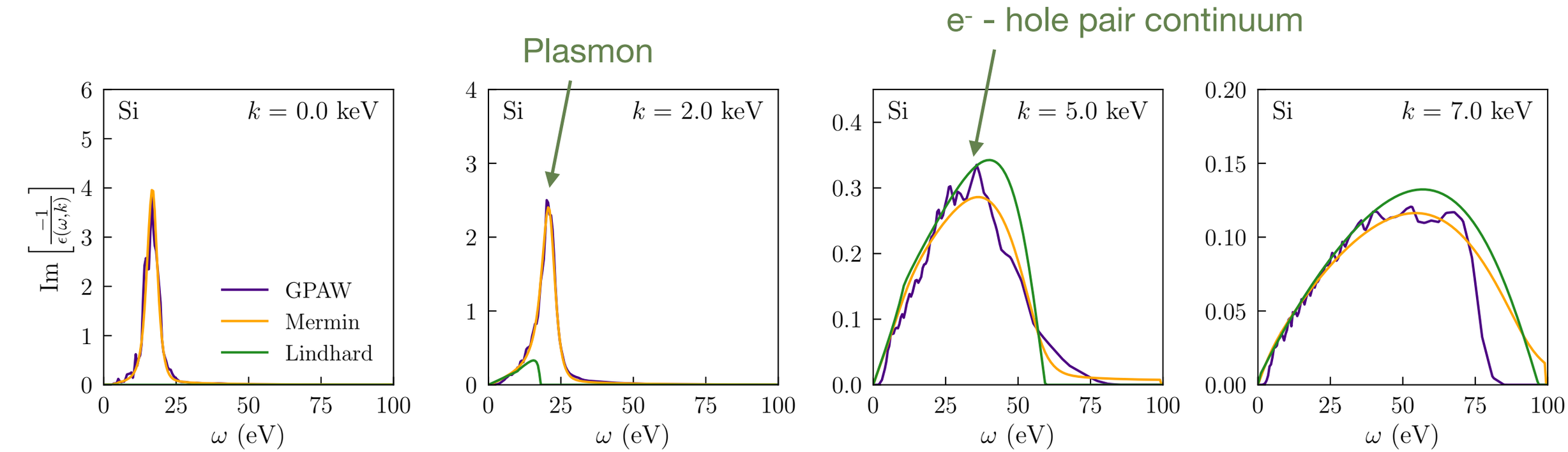
- ☑ Pauli blocking
- ☑ e-h pair continuum
- ☑ Plasmon width
- ☑ Low k region
- ☑ Bandgap

Comparing all three methods



Generally very good agreement, especially between Mermin and GPAW!

Comparing all three methods



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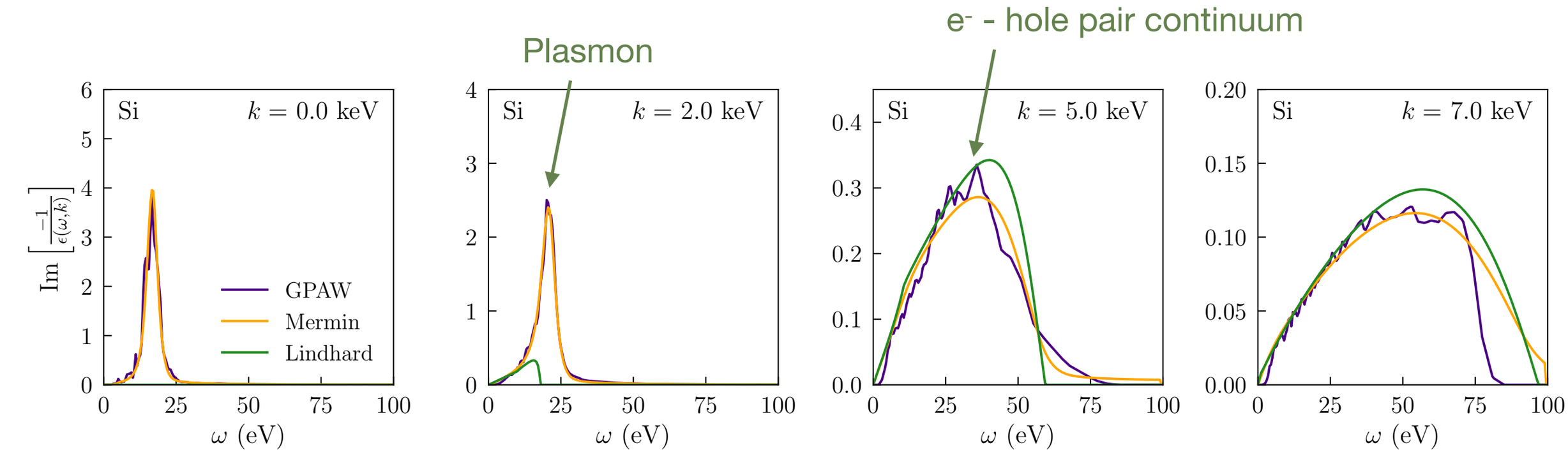
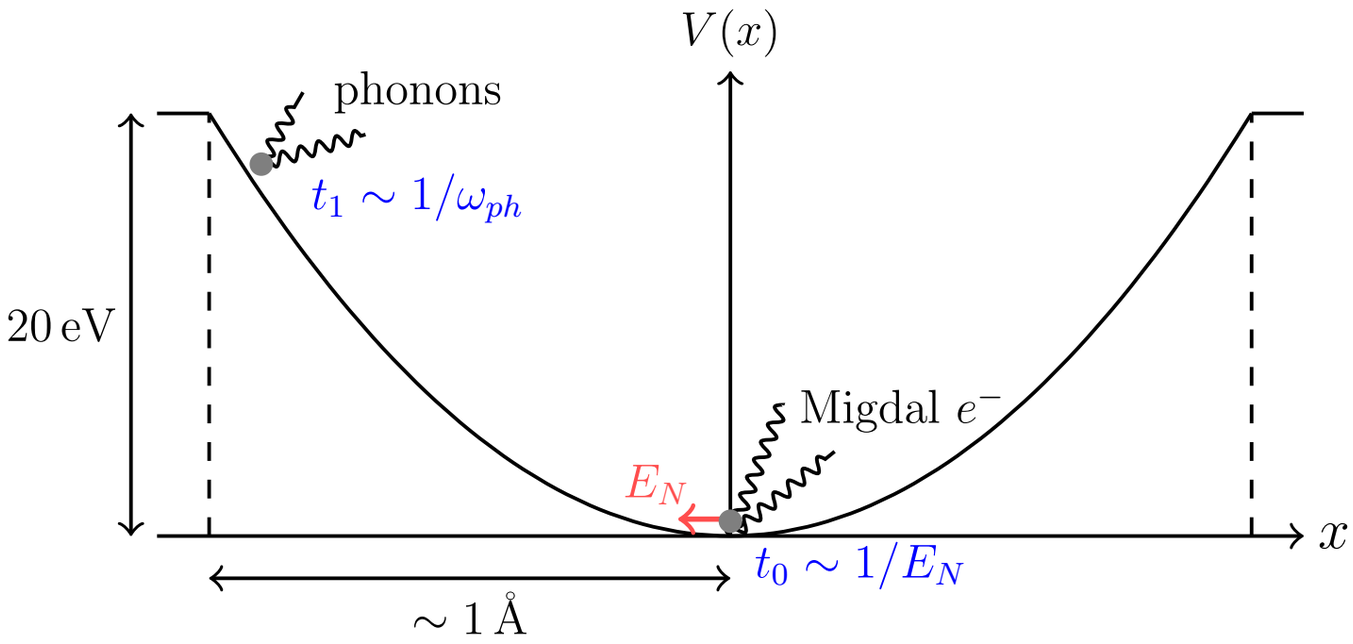
Comparing all three methods



To be understood further

Generally very good agreement, especially between Mermin and GPAW!

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:

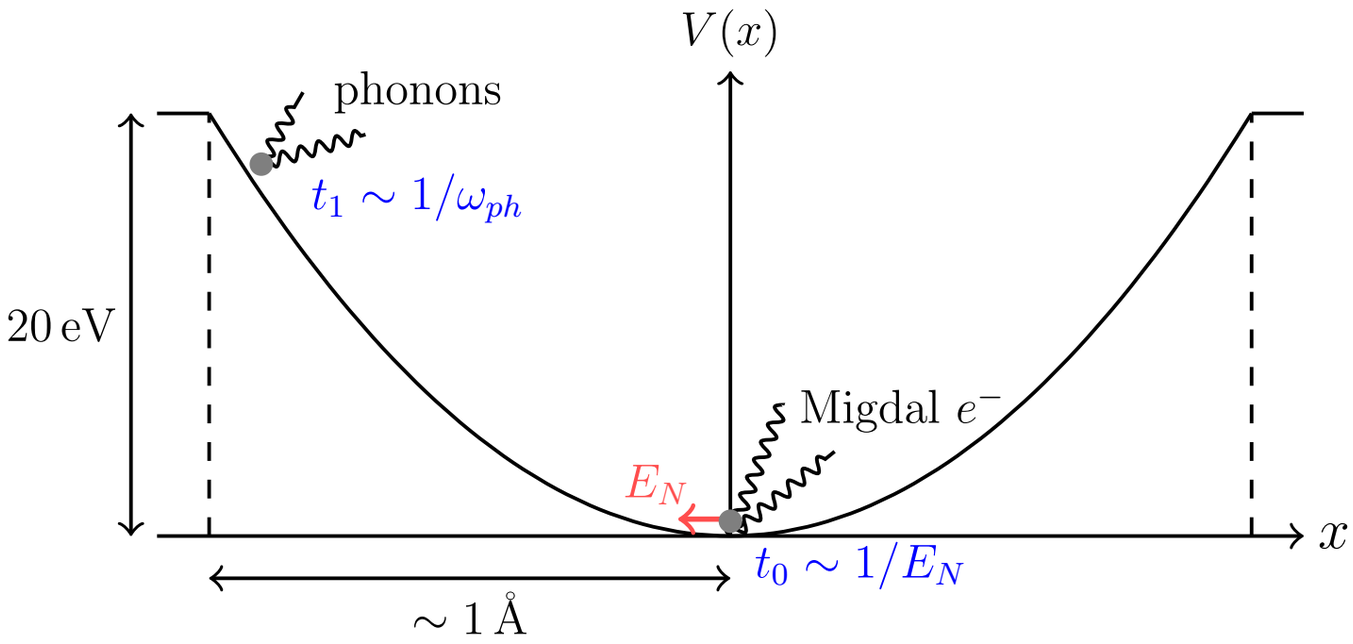
$$\mathcal{V}(\mathbf{r}) = V_0 \delta(\mathbf{r}_N - \mathbf{r}) \rightarrow \tilde{V}(\mathbf{q}) = \tilde{V}_0 e^{i\mathbf{q}\cdot\mathbf{r}_N}$$

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

Soft nuclear recoils

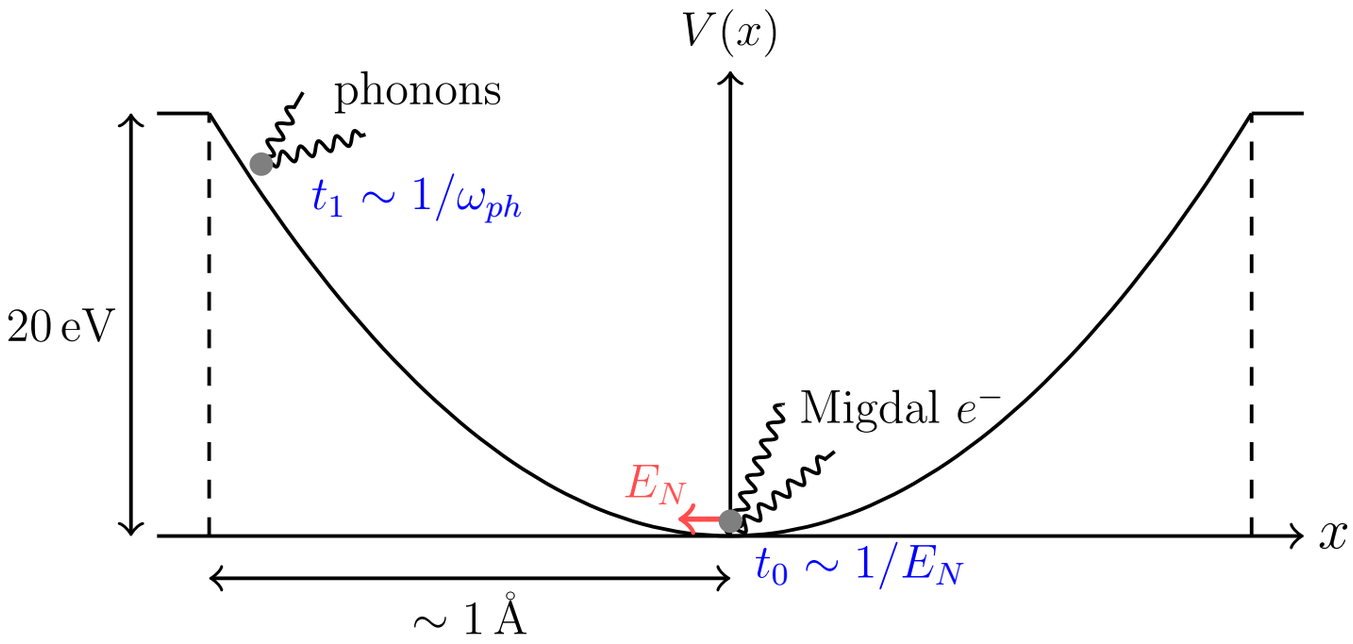


$$
\begin{aligned}
S(\mathbf{q},\omega) &\equiv \sum_{\lambda_f} \left| \langle \lambda_f | \, e^{-i\mathbf{q}\cdot\mathbf{r}_N} \, | \lambda_i \rangle \right|^2 \delta(E_{\lambda_f} - E_{\lambda_i} - \omega) \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \sum_{\lambda_f} \langle \lambda_i | \, e^{-i\mathbf{q}\cdot\mathbf{r}_N} \, | \lambda_f \rangle \langle \lambda_f | \, e^{iE_{\lambda_f} t} e^{i\mathbf{q}\cdot\mathbf{r}_N} e^{-iE_{\lambda_i} t} \, | \lambda_i \rangle \, e^{-i\omega t} \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, \langle e^{-i\mathbf{q}\cdot\mathbf{r}_N(0)} e^{i\mathbf{q}\cdot\mathbf{r}_N(t)} \rangle e^{-i\omega t} \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, e^{-2W(\mathbf{q})} e^{\langle \mathbf{q}\cdot\mathbf{r}_N(0) \, \mathbf{q}\cdot\mathbf{r}_N(t) \rangle} e^{-i\omega t}
\end{aligned}
$$

(This step is a page of algebra)

Appendix B of SK, J. Kozaczuk, T. Lin: arXiv 2011.09496

Soft nuclear recoils



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\begin{aligned}
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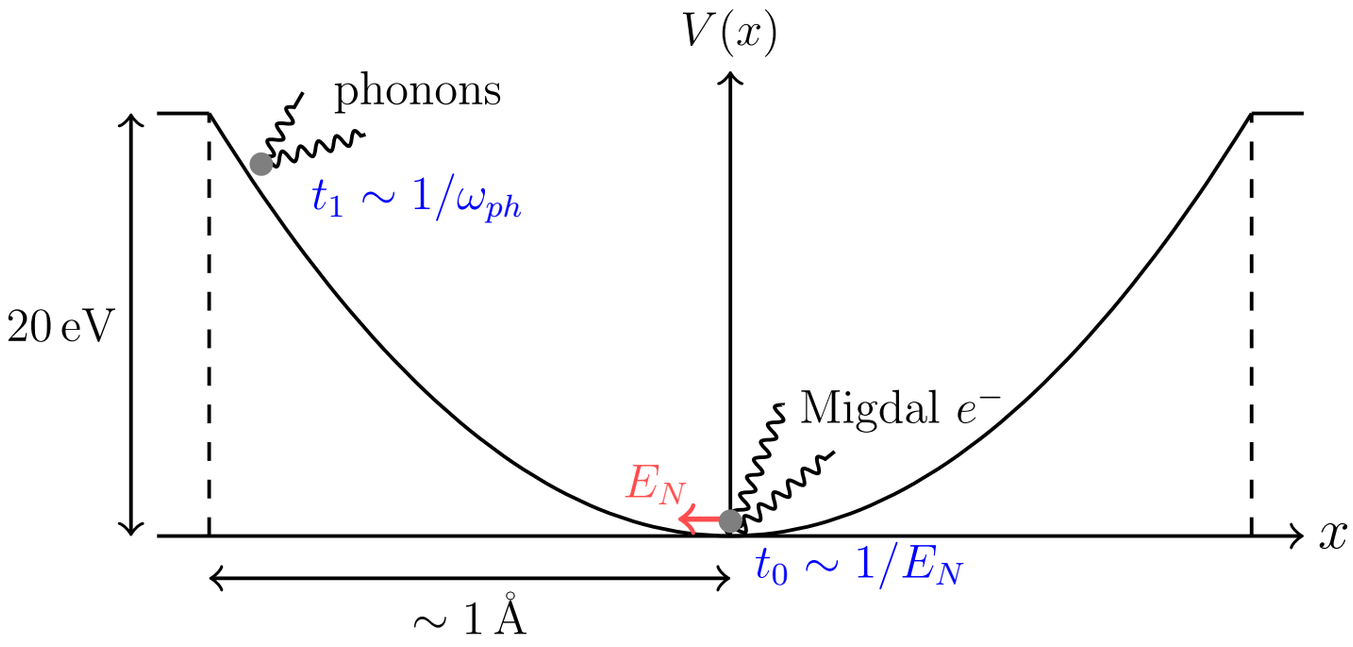
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, \langle e^{-i\mathbf{q}\cdot\mathbf{r}_N(0)} e^{i\mathbf{q}\cdot\mathbf{r}_N(t)} \rangle e^{-i\omega t} \\
&= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, e^{-2W(\mathbf{q})} e^{\langle \mathbf{q}\cdot\mathbf{r}_N(0) \, \mathbf{q}\cdot\mathbf{r}_N(t) \rangle} e^{-i\omega t}
\end{aligned}
$$

(This step is a page of algebra)

Debeye-Waller factor, measures how delocalized the nucleus is

Appendix B of SK, J. Kozaczuk, T. Lin: arXiv 2011.09496

Soft nuclear recoils



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$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \sum_{\lambda_f} \langle \lambda_i | \, e^{-i\mathbf{q}\cdot\mathbf{r}_N} \, | \lambda_f \rangle \langle \lambda_f | \, e^{iE_{\lambda_f} t} e^{i\mathbf{q}\cdot\mathbf{r}_N} e^{-iE_{\lambda_i} t} \, | \lambda_i \rangle \, e^{-i\omega t}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, \langle e^{-i\mathbf{q}\cdot\mathbf{r}_N(0)} e^{i\mathbf{q}\cdot\mathbf{r}_N(t)} \rangle e^{-i\omega t}$$

(This step is a page of algebra)

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, e^{-2W(\mathbf{q})} e^{\langle \mathbf{q}\cdot\mathbf{r}_N(0) \, \mathbf{q}\cdot\mathbf{r}_N(t) \rangle} e^{-i\omega t}$$

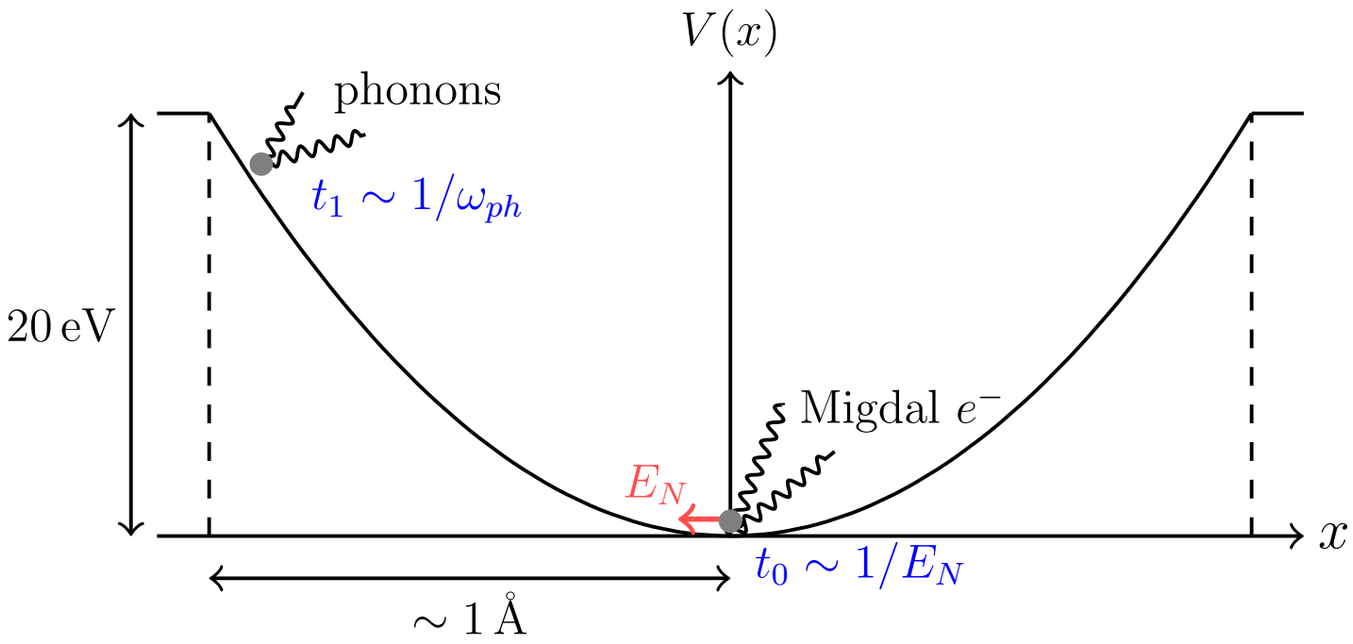
Debeye-Waller factor, measures how delocalized the nucleus is

In a harmonic potential

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

Appendix B of SK, J. Kozaczuk, T. Lin: arXiv 2011.09496

Soft nuclear recoils



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

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \sum_{\lambda_f} \langle \lambda_i | \, e^{-i\mathbf{q}\cdot\mathbf{r}_N} \, | \lambda_f \rangle \langle \lambda_f | \, e^{iE_{\lambda_f} t} e^{i\mathbf{q}\cdot\mathbf{r}_N} e^{-iE_{\lambda_i} t} \, | \lambda_i \rangle \, e^{-i\omega t}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, \langle e^{-i\mathbf{q}\cdot\mathbf{r}_N(0)} e^{i\mathbf{q}\cdot\mathbf{r}_N(t)} \rangle e^{-i\omega t}$$

(This step is a page of algebra)

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, e^{-2W(\mathbf{q})} e^{\langle \mathbf{q}\cdot\mathbf{r}_N(0) \, \mathbf{q}\cdot\mathbf{r}_N(t) \rangle} e^{-i\omega t}$$

Debeye-Waller factor, measures how delocalized the nucleus is

In a harmonic potential

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

Density of states

Appendix B of SK, J. Kozaczuk, T. Lin: arXiv 2011.09496

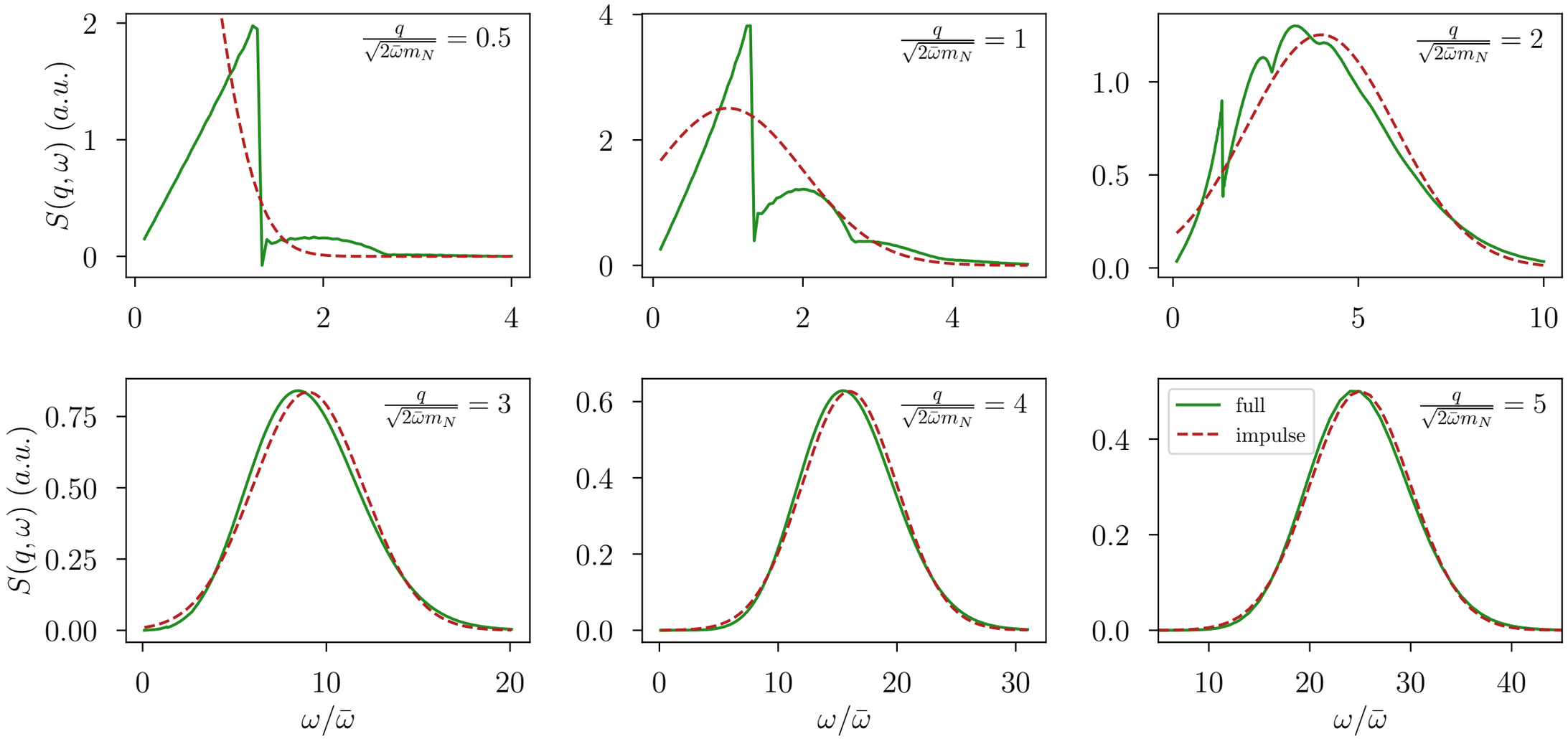
Soft nuclear recoils

In the impulse approximation, the response function is gaussian

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

Typical phonon frequency

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



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

Appendix B of SK, J. Kozaczuk, T. Lin: arXiv 2011.09496