

Tutorial: Calculating scattering rates

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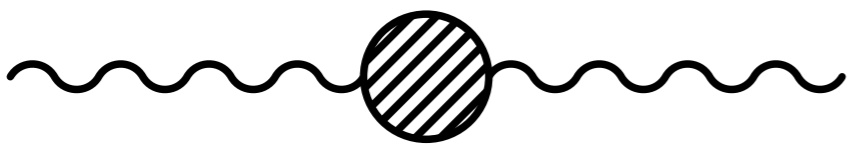
<http://dingercatadventures.blogspot.com/2012/08/>

Yesterday: The energy loss function (ELF)

Coulomb potential in a dielectric:

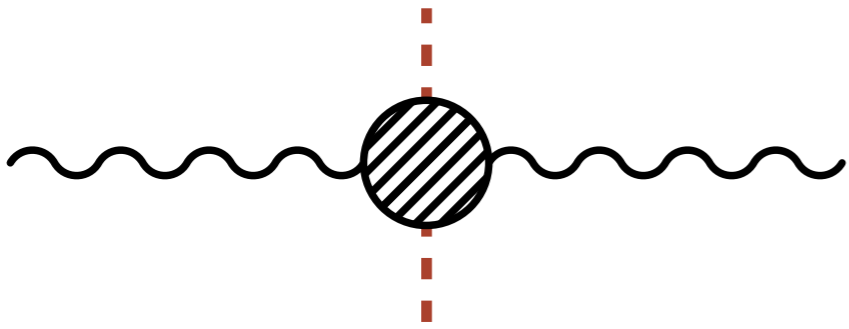
$$H = eQ_\chi \int \frac{d^3\mathbf{k}}{(2\pi)^2} \frac{1}{\epsilon(\mathbf{k}, \omega)} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{k^2}$$

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:



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

↗ Tien-Tien's matrix element
↘ Screening

“Energy Loss Function” (ELF)

DM-electron scattering rate

Lindhard dielectric function (see e.g. Dressel & Gruner textbook)

$$\epsilon(\mathbf{q}, \omega) = 1 - \frac{4\pi\alpha}{V} \lim_{\eta \rightarrow 0^+} \sum_{j, j', \mathbf{p}_e} \frac{|\langle \mathbf{p}_e + \mathbf{k} | \mathbf{p}_e \rangle_\Omega|^2}{|\mathbf{k}|^2} \frac{f_j(\mathbf{p}_e) - f_{j'}(\mathbf{p}_e + \mathbf{k})}{\omega_{j', \mathbf{p}_e + \mathbf{k}} - \omega_{j, \mathbf{p}_e} - \omega - i\eta}$$

Imaginary part

$$\text{Im}\epsilon(\mathbf{q}, \omega) = \frac{4\pi^2\alpha}{V} \sum_{\mathbf{p}_e} \frac{|\langle \mathbf{p}_e + \mathbf{k} | \mathbf{p}_e \rangle_\Omega|^2}{|\mathbf{k}|^2} (f(\mathbf{p}_e) - f(\mathbf{p}_e + \mathbf{k})) \delta(\omega_{\mathbf{p}_e + \mathbf{k}} - \omega_{\mathbf{p}_e} - \omega)$$

matrix element from Tien-Tien's lectures!

Full formula

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

Advantages of using the ELF:

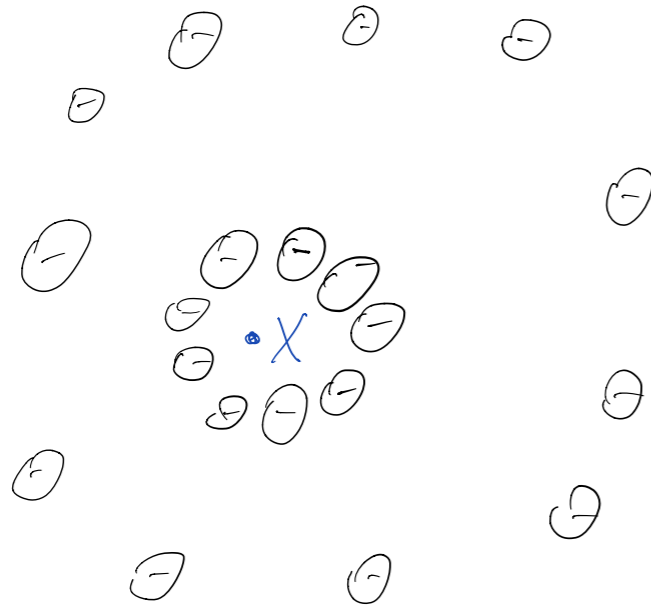
- Screening included automatically
- ELF has been measured and calculated extensively in the condensed matter literature

Sidebar: Screening is mediator independent

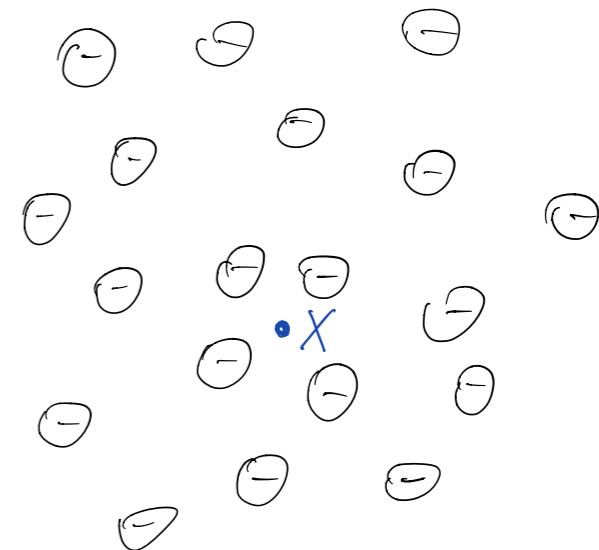
Consider a DM particle in the crystal, sourcing an external force

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

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

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

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

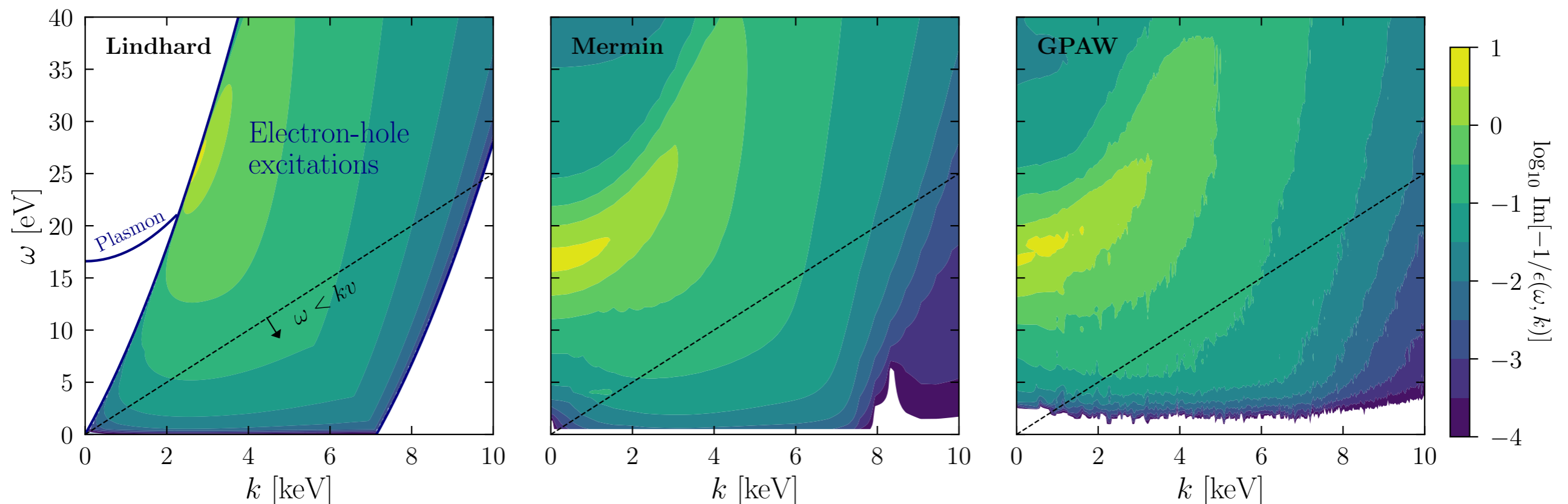
$$S(\omega, \mathbf{k}) = \frac{k^2}{2\pi\alpha_{em}} \frac{1}{1 - e^{-\beta\omega}} \text{Im} \left[\frac{-1}{\epsilon(\omega, \mathbf{k})} \right]$$

Energy Loss Function (ELF)

Calculating the ELF

Simple

Sophisticated



Free electron gas
approximation

100% analytic

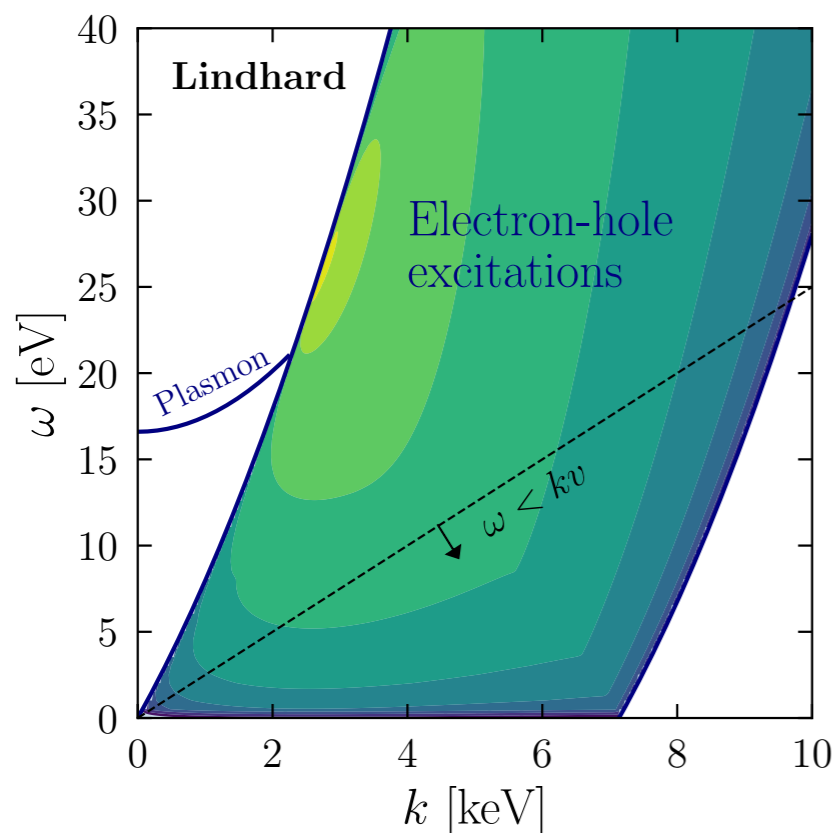
Phenomenological
model fit to data

semi-analytic

First principles DFT
calculation

Fully numerical

Lindhard model



Homogenous, free electron gas:

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

with

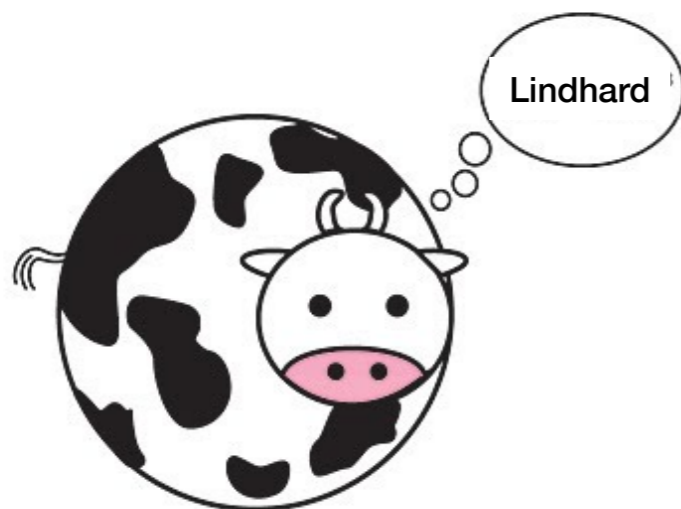
$$v_F = \left(\frac{3\pi\omega_p^2}{4\alpha m_e^2} \right)^{1/3} \text{ Plasmon frequency}$$

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

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

Features:

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



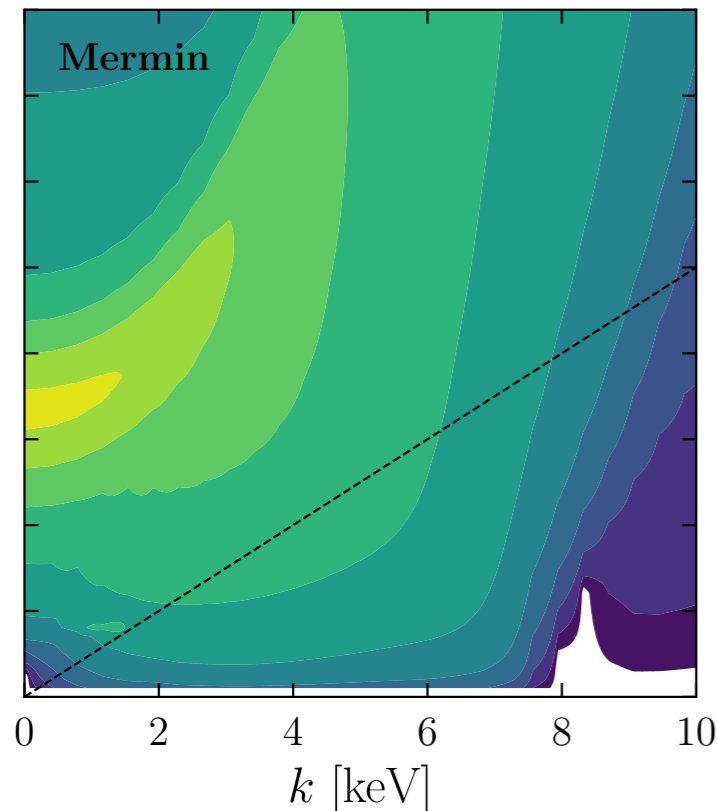
Mermin model

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:

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

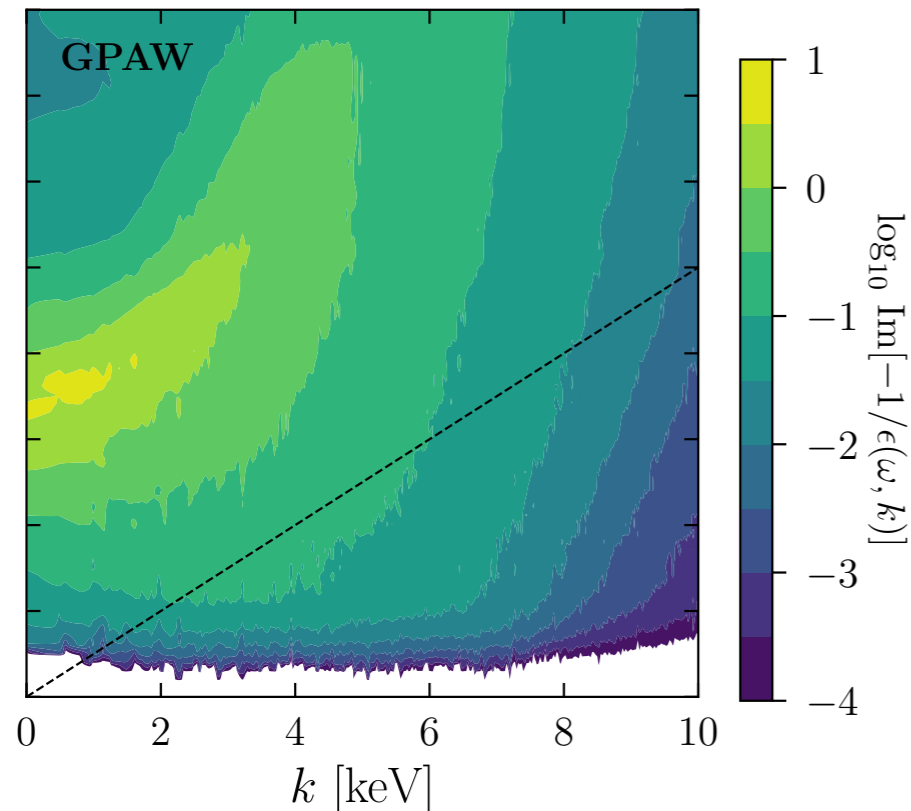


Features:

- ☒ 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



 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 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)

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
Packages

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Contributors

2

 **simonknapen86**

 **tongylin** Tongyan Lin

Languages

Python 100.0%

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

Let's do a few small problems

We'll be making a few plots, with data computed with darkELF

The easiest is to do this directly in python, but you can export the numbers to your favorite plotting tool, e.g. Mathematica, Matlab etc

Please open “vienna_tutorial.ipynb”

Make sure darkELF is in your python path or copy “vienna_tutorial.ipynb” to the darkELF examples folder