Theory of DM-electron scattering and electronic excitation

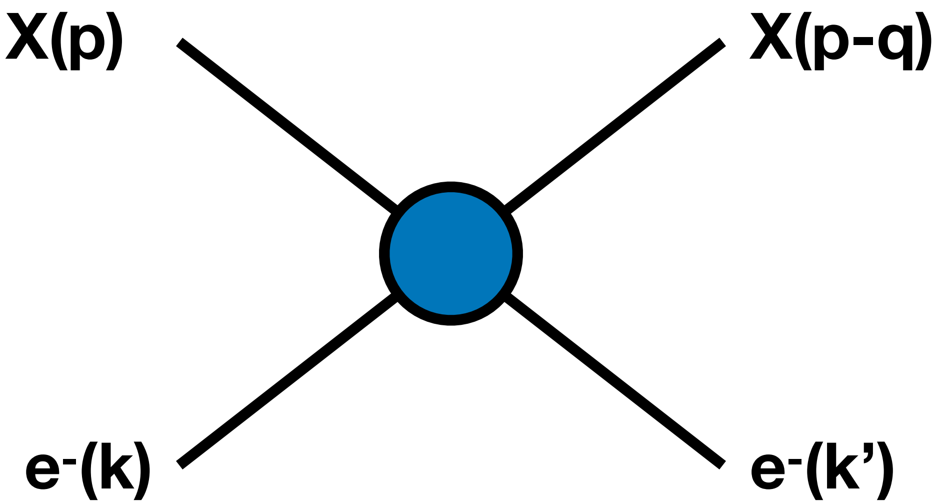
Tien-Tien Yu (University of Oregon)

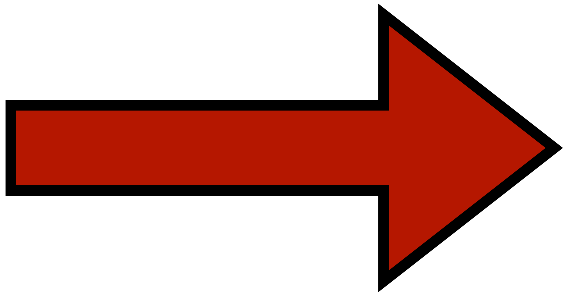
[arXiv:1108.5383,1509.01598, 1607.01009, 1703.00910]

New Directions in the Search for Light Dark Matter Particles

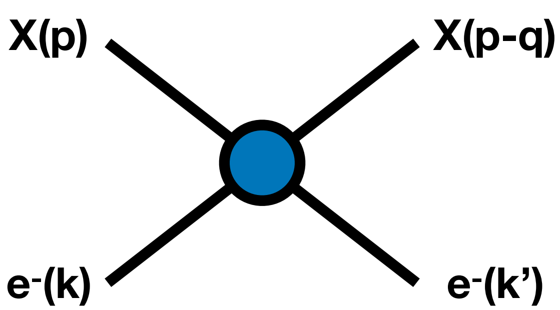
June 5, 2019 Fermilab

kinematics





typical momentum transfer



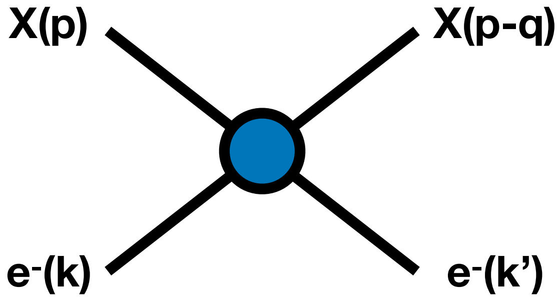
typical size of the momentum transfer is set by the electron's momentum

$$q_{\rm typ} \simeq m_e v_e \sim Z_{\rm eff}\,\alpha m_e$$

~ 4 keV

but q can be much larger than this (albeit suppressed)

typical energy transfer

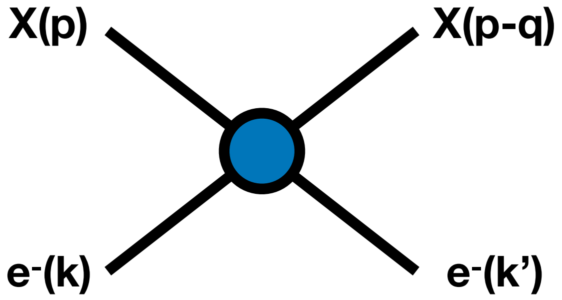


$$\Delta E_{e,\mathrm{typ}} \simeq q_{\mathrm{typ}}\, v \simeq 4\ \mathrm{eV}$$

~ 10^{-3}

in principle, all of the DM's kinetic energy is transferred to electron!

minimum mass

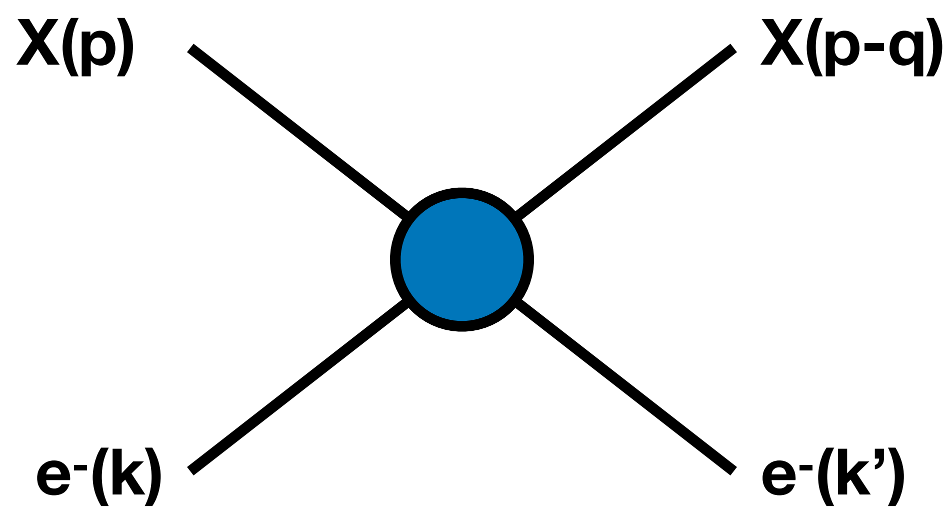


$$E_\chi = \frac{1}{2} m_\chi v_\chi^2 \geq \Delta E_e$$

$$v_\chi \lesssim v_{\rm esc} + v_{\rm E}$$

$$m_\chi \gtrsim 250 \text{ keV} \times \left(\frac{\Delta E_e}{1 \text{ eV}} \right)$$

General Formula



phase space of ionized electron

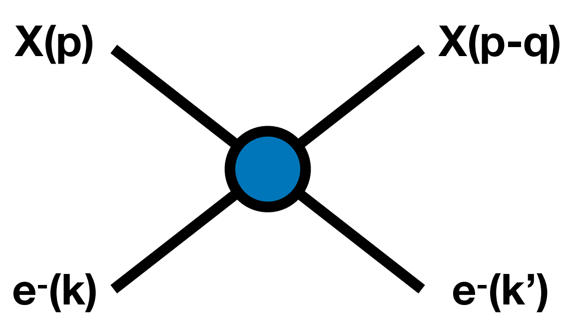
$$\sigma v_{\rm free} = \frac{1}{4E'_\chi E'_e} \int \frac{d^3q}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \frac{1}{4E_\chi E_e} (2\pi)^4 \delta(E_i - E_f) \delta^3(\vec{k} + \vec{q} - \vec{k}') \overline{|\mathcal{M}_{\rm free}(\vec{q})|^2}$$

momentum transfer

$$\overline{|\mathcal{M}_{\rm free}(\vec{q})|^2} \equiv \overline{|\mathcal{M}_{\rm free}(\alpha m_e)|^2} \times |F_{\rm DM}(q)|^2$$

$$\overline{\sigma}_e \equiv \frac{\mu_{\chi e}^2 \overline{|\mathcal{M}_{\rm free}(\alpha m_e)|^2}}{16\pi m_\chi^2 m_e^2}$$

General Formula



Non-relativistic scattering amplitude

for free electrons:

$$\langle \chi_{\vec{p}-\vec{q}}, e_{\vec{k}'} | H_{\text{int}} | \chi_{\vec{p}}, e_{\vec{k}} \rangle = C\,\mathcal{M}_{\text{free}}(\vec{q}) \times (2\pi)^3 \delta^3(\vec{k} - \vec{q} - \vec{k}')$$

plane waves

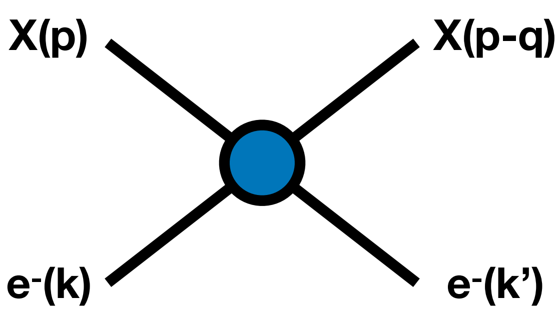
for bound electrons:

$$\langle \chi_{\vec{p}-\vec{q}}, e_2 | H_{\text{int}} | \chi_{\vec{p}}, e_1 \rangle = \left[\int \frac{\sqrt{V} d^3k'}{(2\pi)^3} \widetilde{\psi}_2^*(\vec{k}') \langle \chi_{\vec{p}'}, e_{\vec{k}'} | \right] H_{\text{int}} \left[\int \frac{\sqrt{V} d^3k}{(2\pi)^3} \widetilde{\psi}_1(\vec{k}) | \chi_{\vec{p}}, e_{\vec{k}} \rangle \right]$$

$$= C\,\mathcal{M}_{\text{free}}(\vec{q}) \times \int \frac{V d^3k}{(2\pi)^3} \widetilde{\psi}_2^*(\vec{k} + \vec{q}) \widetilde{\psi}_1(\vec{k})$$

momentum-space wavefunctions of electrons

General Formula



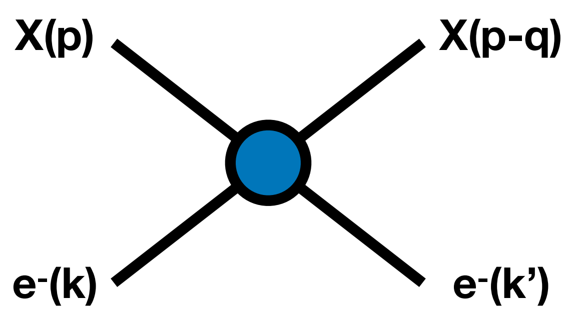
$$\sigma v_{\rm free} = \frac{1}{4E'_\chi E'_e}\int \frac{d^3q}{(2\pi)^3}\frac{d^3k'}{(2\pi)^3}\frac{1}{4E_\chi E_e}(2\pi)^4\delta(E_i - E_f)\delta^3(\vec{k}+\vec{q}-\vec{k}')\overline{|\mathcal{M}_{\rm free}(\vec{q})|^2}$$

$$\sigma v_{1\to 2} = \frac{1}{4E'_\chi E'_e}V\int \frac{d^3q}{(2\pi)^3}\frac{d^3k'}{(2\pi)^3}\frac{1}{4E_\chi E_e}2\pi\delta(E_i - E_f)\overline{|\mathcal{M}_{\rm free}(\vec{q})|^2}\times|f_{1\to 2}(\vec{q})|^2$$

=1
if only one final electron state

$$\left|\int \frac{d^3k}{(2\pi)^3}\widetilde{\psi}_2^*(\vec{k}')\widetilde{\psi}_1(\vec{k})\right|^2$$

General Formula



Non-relativistic scattering amplitude

$$E_i = m_\chi + m_e + \frac{1}{2} m_\chi v^2 + E_{e,1}$$

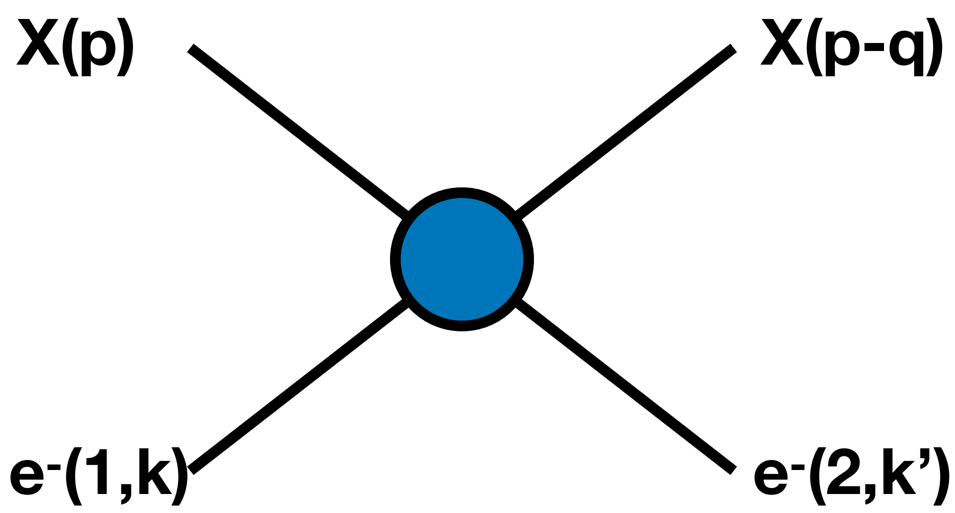
$$E_f = m_\chi + m_e + \frac{|m_\chi \vec{v} - \vec{q}\,|^2}{2m_\chi} + E_{e,2}$$

choice of parameterization of scattering

$$\overline{|\mathcal{M}_{\rm free}(\vec{q}\,)|^2} \equiv \overline{|\mathcal{M}_{\rm free}(\alpha m_e)|^2} \times |F_{\rm DM}(q)|^2$$

$$\overline{\sigma}_e \equiv \frac{\mu_{\chi e}^2 \overline{|\mathcal{M}_{\rm free}(\alpha m_e)|^2}}{16\pi m_\chi^2 m_e^2}\,,$$

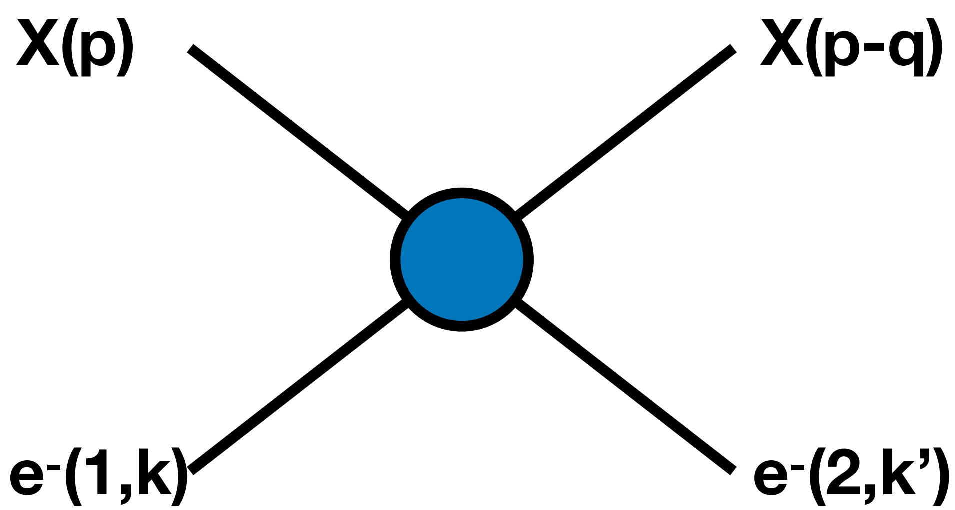
General Formula



$$\sigma v_{1\to 2} = \frac{1}{4E'_\chi E'_e} V \int \frac{d^3q}{(2\pi)^3}\frac{d^3k'}{(2\pi)^3}\frac{1}{4E_\chi E_e} 2\pi\delta(E_i - E_f)\overline{|\mathcal{M}_{\rm free}(\vec{q})|^2} \times |f_{1\to 2}(\vec{q})|^2$$

$$\sigma v_{1\to 2} = \frac{\overline{\sigma}_e}{\mu_{\chi e}^2} V \int \frac{d^3q}{4\pi}\frac{d^3k'}{(2\pi)^3}\,\delta\Big(\Delta E_{1\to 2} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\Big) \times |F_{\rm DM}(q)|^2 |f_{1\to 2}(\vec{q})|^2$$

General Formula



$$\sigma v_{1\to 2} = \frac{1}{4E'_\chi E'_e} V \int \frac{d^3q}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \frac{1}{4E_\chi E_e} 2\pi\delta(E_i - E_f) \overline{|\mathcal{M}_{\rm free}(\vec{q})|^2} \times |f_{1\to 2}(\vec{q})|^2$$

$$\left| \int \frac{d^3k}{(2\pi)^3} \widetilde{\psi}_2^*(\vec{k}+\vec{q}) \widetilde{\psi}_1(\vec{k}) \right|^2$$

$$\sigma v_{1\to 2} = \frac{\overline{\sigma}_e}{\mu_{\chi e}^2} V \int \frac{d^3q}{4\pi} \frac{d^3k'}{(2\pi)^3} \delta\left(\Delta E_{1\to 2} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right) \times |F_{\rm DM}(q)|^2 |f_{1\to 2}(\vec{q})|^2$$

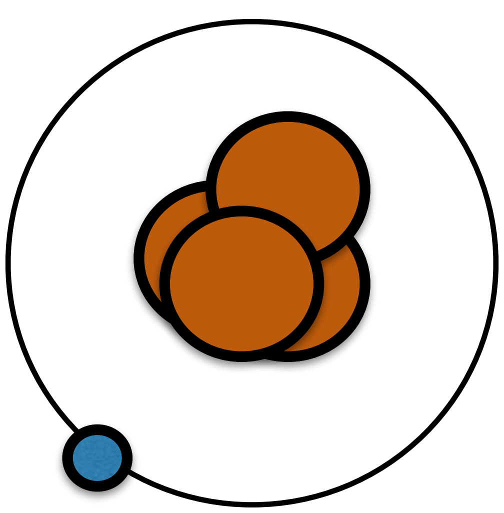
phase space

transition probability

Isolated Atom

Hydrogen
Xenon
Argon

$$\Delta E_B \sim 10 \text{ eV}$$
$$m_\chi \gtrsim 2.5 \text{ MeV}$$



Isolated Atom

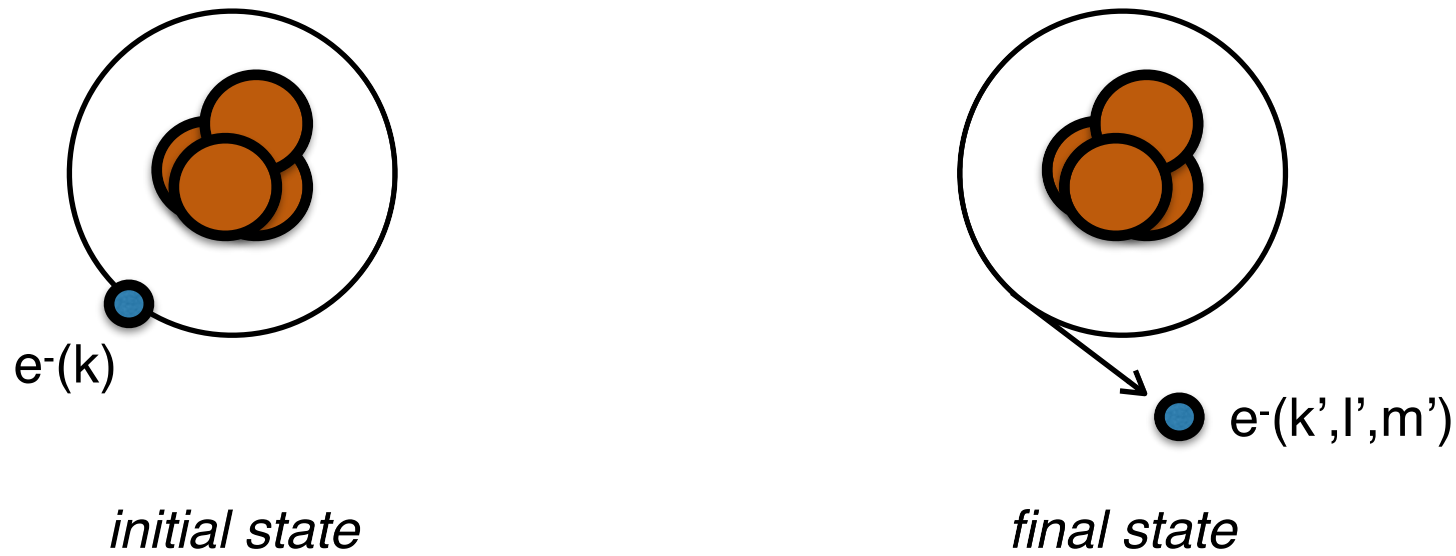
initial state *final state*

final state is a "free" electron with angular quantum numbers l', m', and momentum k'

$$\psi_{k'l'm'}(\vec{x}) = 4\pi j_{\ell'}(k'x) Y^*_{\ell' m'}(\theta_{\vec{x}}, \phi_{\vec{x}})$$

normalization: $\langle \psi_{k'l'm'} | \psi_{klm} \rangle = (2\pi)^3 \delta_{l'l} \delta_{m'm} \frac{1}{k^2} \delta(k - k') \equiv V$

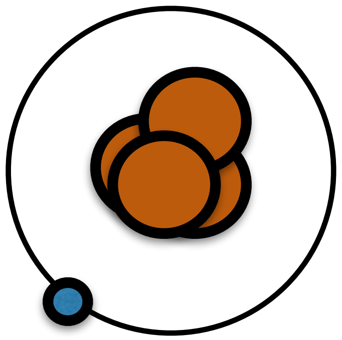
Isolated Atom



final state is a "free" electron with angular quantum numbers l', m', and momentum k'

$$\widetilde{\psi}_{k'l'm'}(\vec{x}) = 4\pi j_{\ell'}(k'x) Y^*_{\ell' m'}(\theta_{\vec{x}}, \phi_{\vec{x}})$$

$$|f_{i\to k'l'm'}|^2 = \left| \int d^3x \, 4\pi j_{\ell'}(k'x) Y^*_{\ell' m'}(\theta_{\vec{x}}, \phi_{\vec{x}}) \psi_i(\vec{x}) e^{i\vec{q}\cdot\vec{x}} \right|^2$$



Isolated Atom

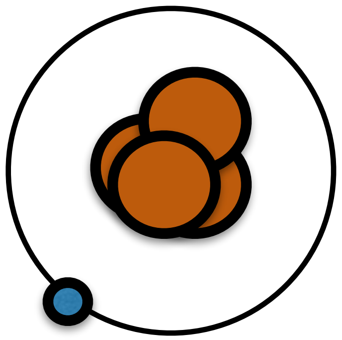
$$E_R \equiv \frac{k'^2}{2m_e}$$

$$\text{ionized electron phase space} = \sum_{l'm'} \int \frac{k'^2 dk'}{(2\pi)^3} = \frac{1}{2} \sum_{l'm'} \int \frac{k'^3 d\ln E_R}{(2\pi)^3}$$

$$\sigma v_{i\to k'l'm'} = \frac{\overline{\sigma}_e}{\mu_{\chi e}^2} \int \frac{d^3q}{8\pi} \frac{k'^3 d\ln E_R}{(2\pi)^3} \delta\left(\Delta E_{1\to 2} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right) \times |F_{\rm DM}(q)|^2 |f_{i\to k'l'm'}(\vec{q})|^2$$

We assume the potential is spherically symmetric and we ionize a full atomic shell therefore, sum over all initial and final angular momentum variables

$$\sigma v_{\rm ion} = \frac{\overline{\sigma}_e}{\mu_{\chi e}^2} \sum_{\substack{\text{occupied}\\\text{states}}} \sum_{l'm'} \int \frac{d^3q}{8\pi} \frac{k'^3 d\ln E_R}{(2\pi)^3} \delta\left(\Delta E_{i\to k'l'm'} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right) |F_{\rm DM}(q)|^2 |f_{i\to k'l'm'}(\vec{q})|^2$$



Isolated Atom

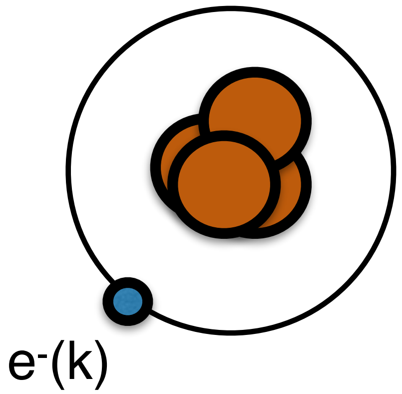
$$\sigma v_{\text{ion}} = \frac{\overline{\sigma}_e}{\mu_{\chi e}^2} \sum_{\substack{\text{occupied}\\ \text{states}}} \sum_{l'm'} \int \frac{d^3q}{8\pi} \frac{k'^3 d\ln E_R}{(2\pi)^3} \delta\left(\Delta E_{i\to k'l'm'} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right) |F_{\text{DM}}(q)|^2 |f_{i\to k'l'm'}(\vec{q})|^2$$

we can also define an "ionization form factor"

$$\left|f_{\text{ion}}(k', q)\right|^2 = \frac{2k'^3}{(2\pi)^3} \sum_{\substack{\text{occupied}\\ \text{states}}} \sum_{l'm'} \left| \int d^3x\, \psi^*_{k'l'm'}(\vec{x})\psi_i(\vec{x}) e^{i\vec{q}\cdot\vec{x}} \right|^2$$

$$\left| \int d^3x\, 4\pi j_{\ell'}(k'x) Y^*_{\ell'm'}(\theta_{\vec{x}}, \phi_{\vec{x}}) \psi_i(\vec{x}) e^{i\vec{q}\cdot\vec{x}} \right|^2$$

Isolated Atom



$$\left|f_{\rm ion}(k',q)\right|^2 = \frac{2k'^3}{(2\pi)^3} \sum_{\substack{\rm occupied \\ \rm states}} \sum_{l'm'} \left| \int d^3x \, \psi^*_{k'l'm'}(\vec{x})\psi_i(\vec{x})e^{i\vec{q}\cdot\vec{x}} \right|^2$$

example: outgoing electron is free plane wave,
initial electron is part of a spherically symmetric atom with full shells

$$\left|f^i_{ion}(k',q)\right|^2 = \frac{(2\ell+1)k'^2}{4\pi^3 q} \int k dk \left|\chi_{nl}(k)\right|^2$$

integration limits: $|k' \pm q|$

RHF wavefunctions

spherically symmetric atom with full shells

in practice: solve radial Schrödinger equation for the exact unbound wavefunctions, using the effective potential extracted from the bounded wavefunctions

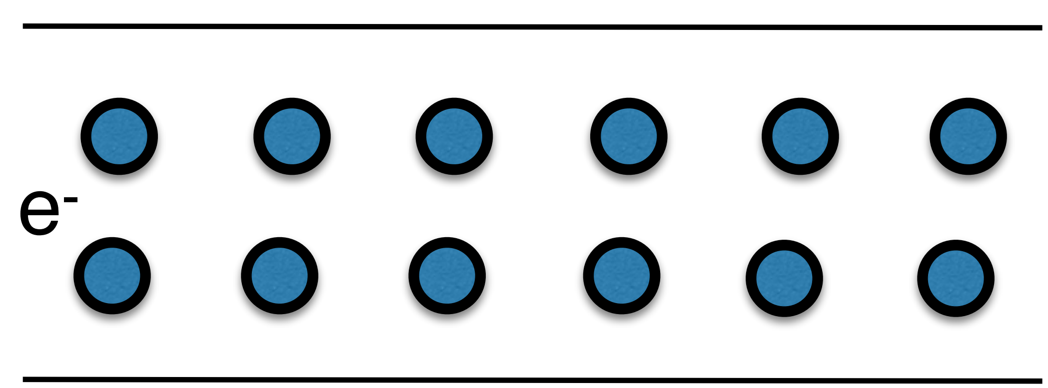
Crystals

Semiconductors: silicon, germanium

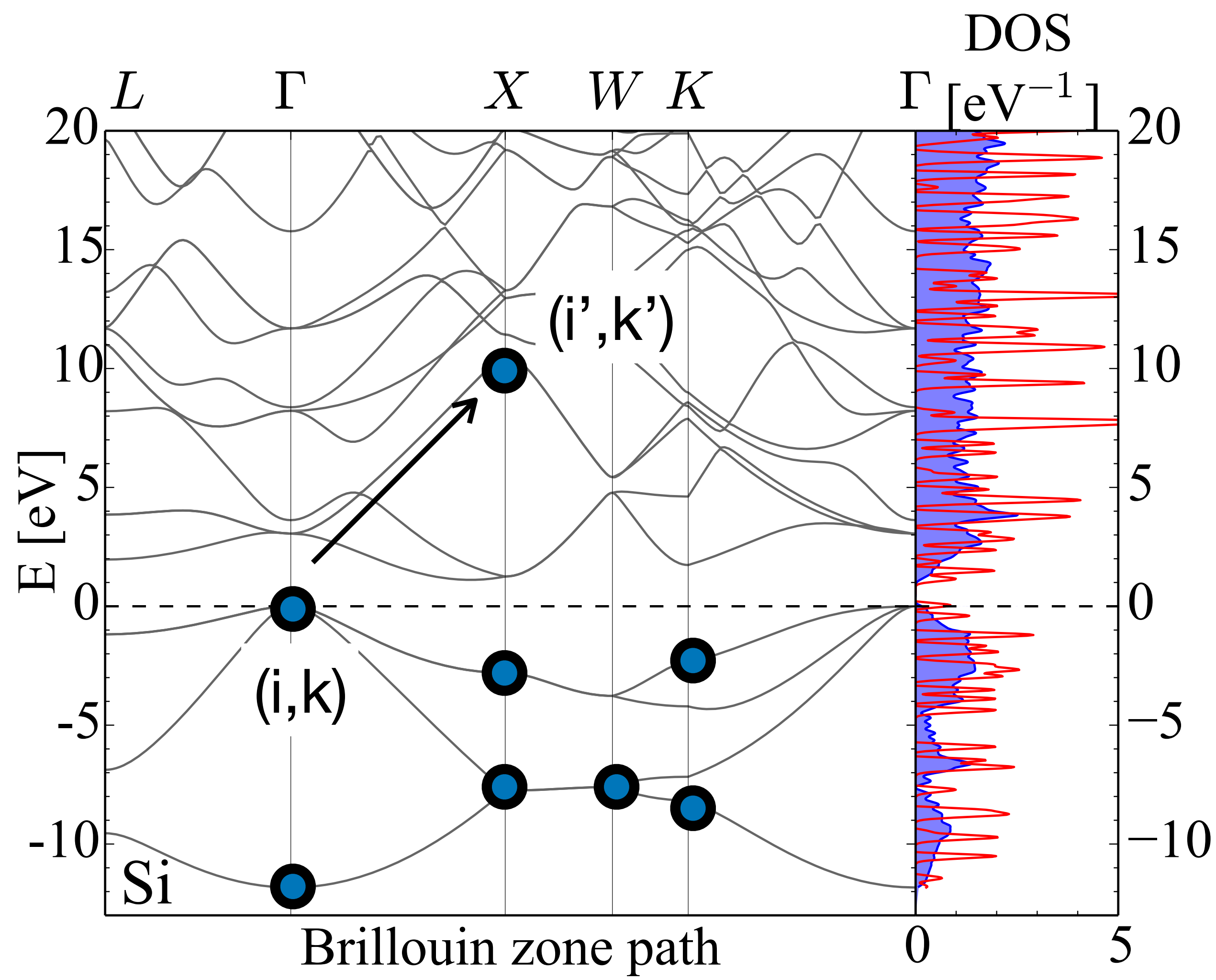
Scintillators: NaI, CsI, GaAs

$$\Delta E_B \sim 1 \text{ eV}$$

$$m_\chi \gtrsim 250 \text{ keV}$$



Crystals

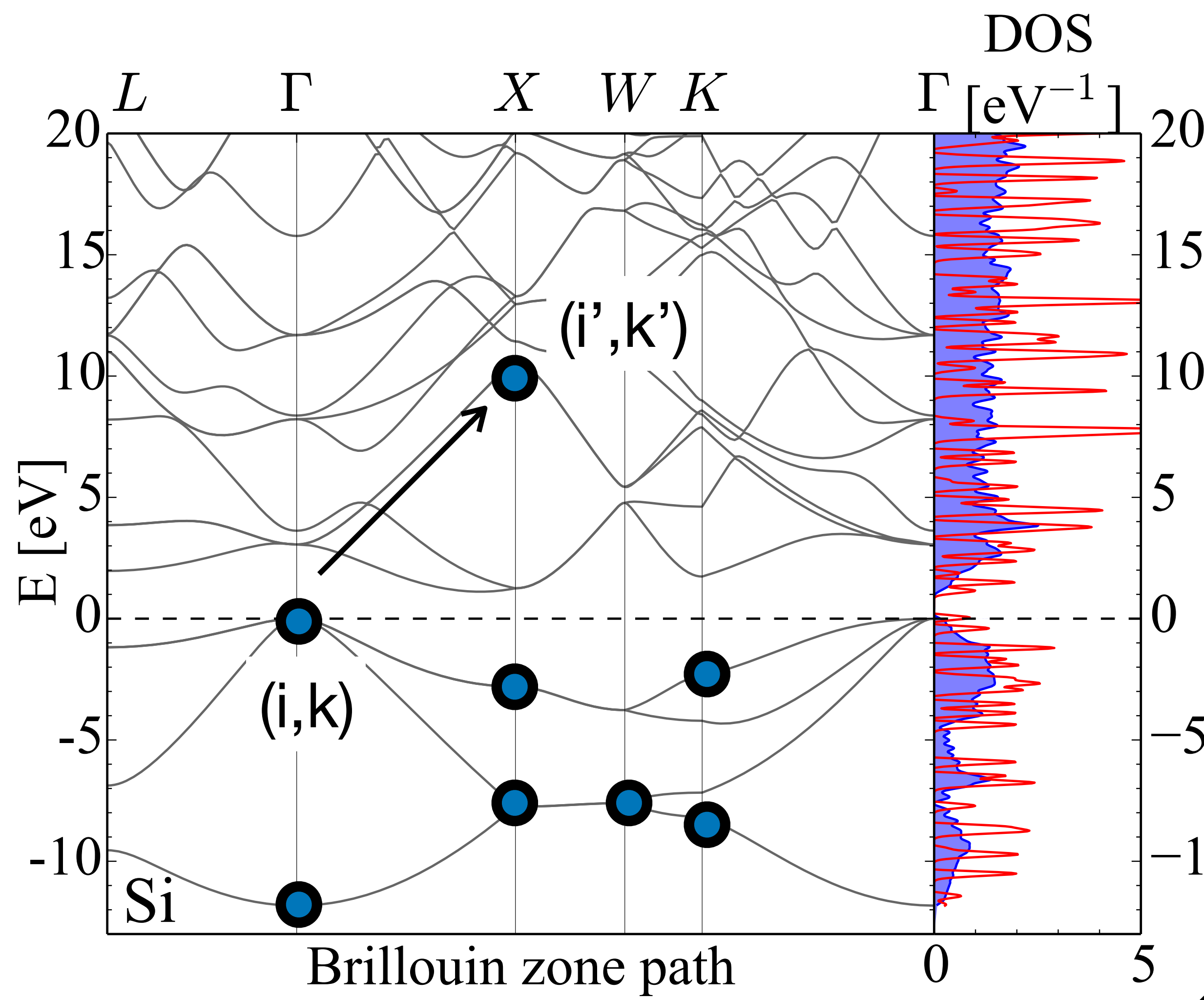


electrons are labeled by
band index i and wavevector k

$$\psi_{i\vec{k}}(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{\vec{G}} u_i(\vec{k}+\vec{G}) e^{i(\vec{k}+\vec{G})\cdot\vec{x}}$$

normalization: $\sum_{\vec{G}} \left| u_i(\vec{k}+\vec{G}) \right|^2 = 1$

Crystals



Use DFT techniques, i.e. QuantumEspresso

electrons are labeled by band index i and wavevector k

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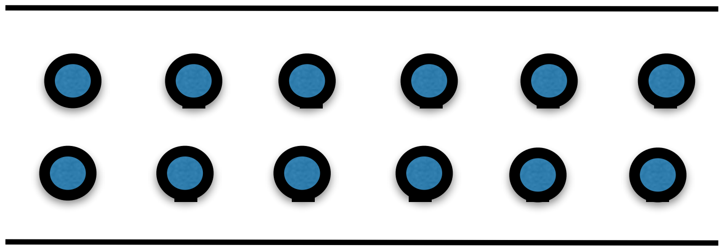
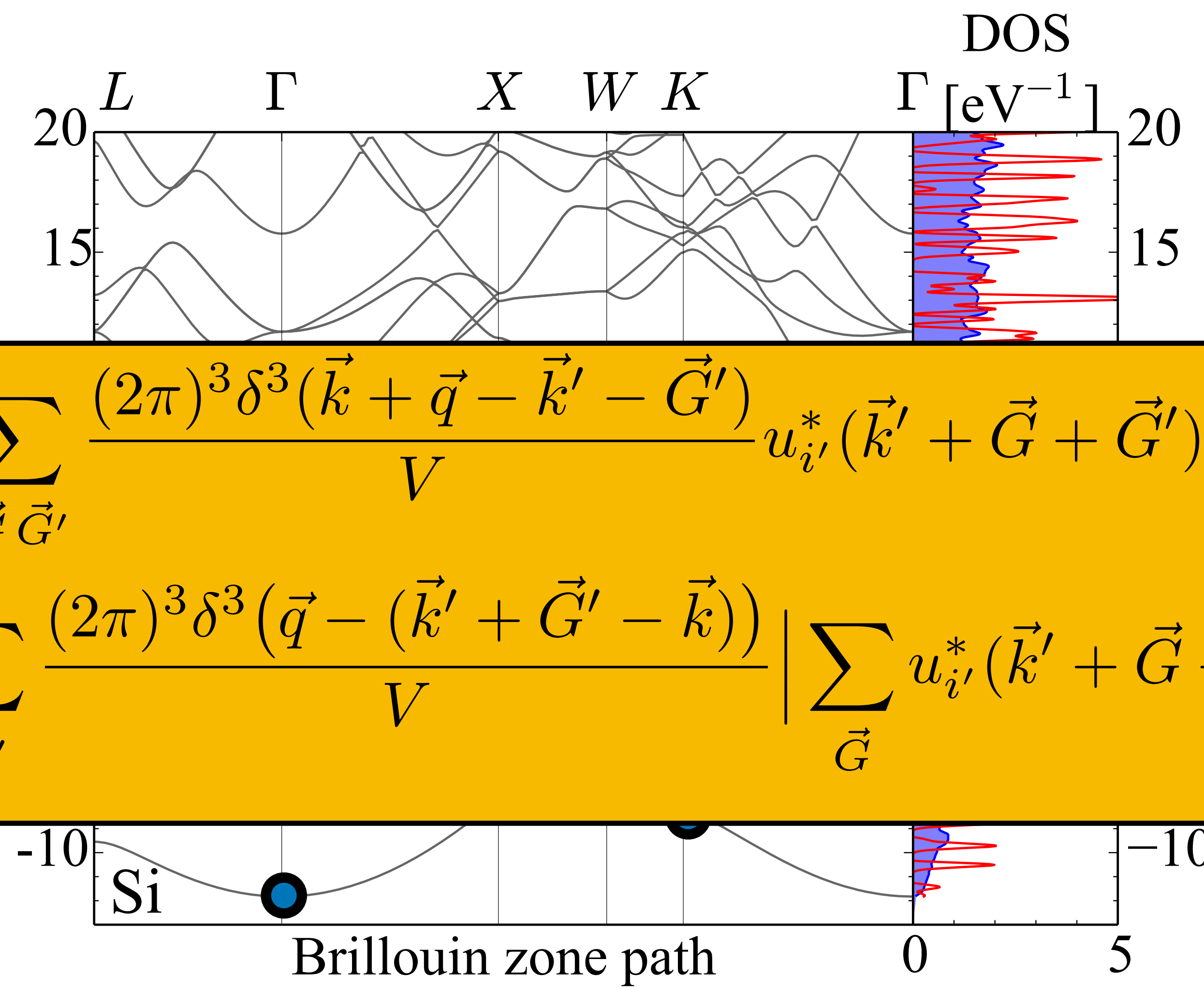


Crystals



$$\left|f_{i\vec{k}\to i'\vec{k}'}(\vec{q})\right|^2 = \left|\sum_{\vec{G}\,\vec{G}'} \frac{(2\pi)^3\delta^3(\vec{k}+\vec{q}-\vec{k}'-\vec{G}')}{V} u^*_{i'}(\vec{k}'+\vec{G}+\vec{G}')u_i(\vec{k}+\vec{G})\right|^2$$

$$= \sum_{\vec{G}'} \frac{(2\pi)^3\delta^3\big(\vec{q}-(\vec{k}'+\vec{G}'-\vec{k})\big)}{V}\left|\sum_{\vec{G}} u^*_{i'}(\vec{k}'+\vec{G}+\vec{G}')u_i(\vec{k}+\vec{G})\right|^2$$

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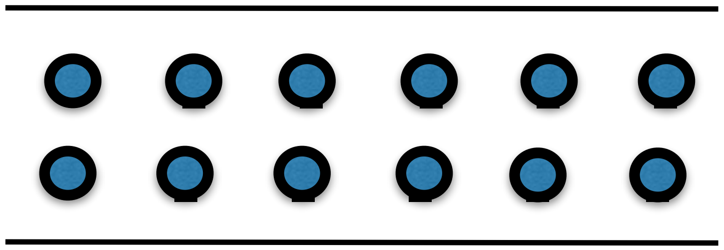
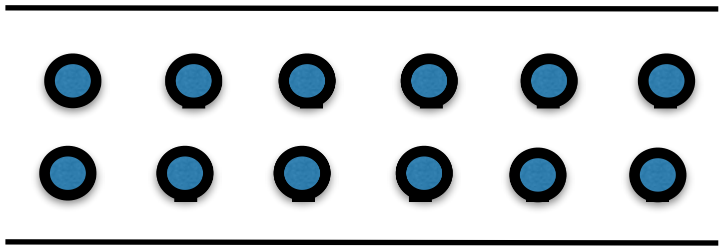


Crystals

$$\text{final electron phase space} = \sum_{i'} \int_{\text{BZ}} \frac{V d^3k'}{(2\pi)^3}$$

$$\sigma v_{ik\to\text{any}} = \frac{2\pi^2 \overline{\sigma}_e}{\mu_{\chi e}^2} \sum_{i'} \int_{\text{BZ}} \frac{d^3k'}{(2\pi)^3} \delta\left(\Delta E_{ik\to i'k'} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right)$$
$$\times |F_{\text{DM}}(q)|^2 \sum_{\vec{G}',\vec{G}} |u_{i'}^*(\vec{k}' + \vec{G} + \vec{G}')u_i(\vec{k} + \vec{G})|^2$$



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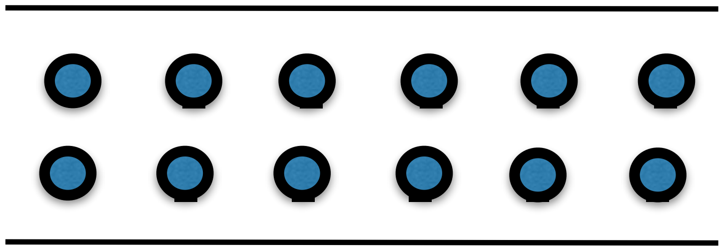
$$\text{initial electron phase space} = 2 \sum_{i} \int_{\text{BZ}} \frac{V d^3k}{(2\pi)^3}$$

electron spin

$$\sigma v_{\text{crystal}} = \frac{4\pi^2 \overline{\sigma}_e}{\mu_{\chi e}^2} V \sum_{ii'} \int_{\text{BZ}} \frac{d^3k d^3k'}{(2\pi)^6} \delta\left(\Delta E_{ik\to \text{i'k'}} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right) |F_{\text{DM}}(q)|^2$$
$$\times \sum_{\vec{G}',\vec{G}} |u_{i'}^*(\vec{k}' + \vec{G} + \vec{G}')u_i(\vec{k} + \vec{G})|^2$$



Crystals

$$\text{initial electron phase space} = 2\sum_i \int_{\text{BZ}} \frac{V d^3k}{(2\pi)^3}$$

electron spin

$$\sigma v_{\text{crystal}} = \frac{4\pi^2 \overline{\sigma}_e}{\mu_{\chi e}^2} V \sum_{ii'} \int_{\text{BZ}} \frac{d^3k\, d^3k'}{(2\pi)^6} \delta\left(\Delta E_{ik\to \text{i}'\text{k}'} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right) |F_{\text{DM}}(q)|^2 \times \sum_{\vec{G}',\vec{G}} |u_{i'}^*(\vec{k}' + \vec{G} + \vec{G}')u_i(\vec{k} + \vec{G})|^2$$

Dark Matter Halo

$$\sigma v_{1\to 2} = \frac{\overline{\sigma}_e}{\mu_{\chi e}^2} \int \frac{d^3 q}{4\pi}\, \delta\Big(\Delta E_{1\to 2} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\Big) \times |F_{\rm DM}(q)|^2 |f_{1\to 2}(\vec{q})|^2$$

need to average over DM velocity

Dark Matter Halo

$$\sigma v_{1\to 2} = \frac{\overline{\sigma}_e}{\mu_{\chi e}^2} \int \frac{d^3q}{4\pi}\, \delta\left(\Delta E_{1\to 2} + \frac{q^2}{2m_\chi} - qv\cos\theta_{qv}\right) \times |F_{\rm DM}(q)|^2 |f_{1\to 2}(\vec{q}\,)|^2$$

need to average over DM velocity

$$R_{1\to 2} = \frac{\rho_\chi}{m_\chi} \int d^3v\, g_\chi(\vec{v})\, \sigma v_{1\to 2}$$

number of events/time/volume

multiply by exposure to get number of expected events per target

Cross-section reach