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Dielectric functions and stopping powers in the RPA

Thomas Hentschel

Adviser: Dr. Stephanie Hansen

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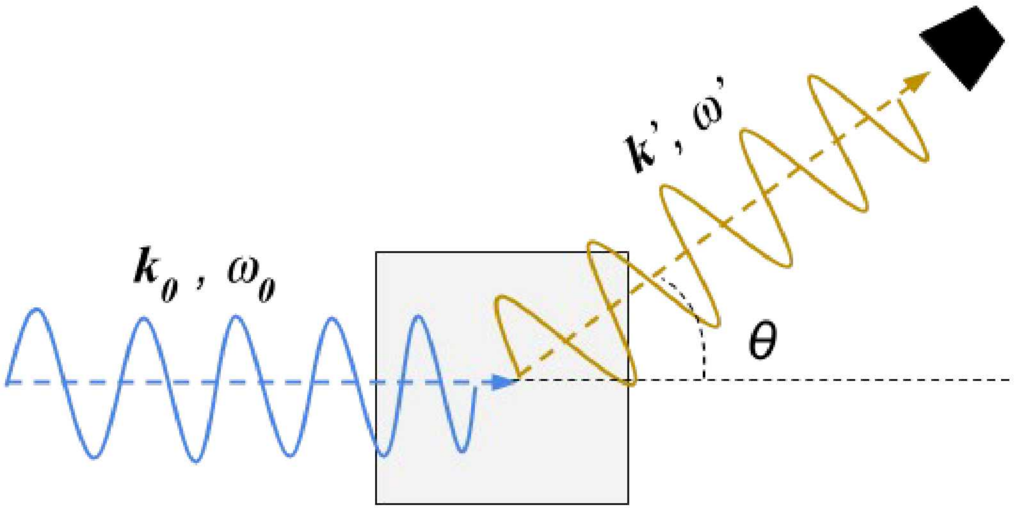
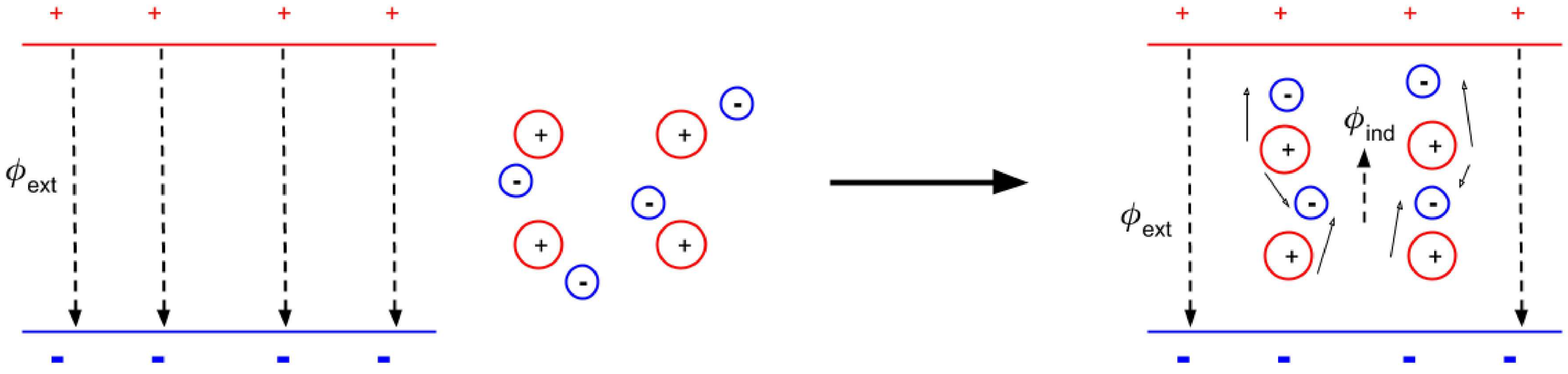
X-ray scattering experiments

- $k = |\mathbf{k}' - \mathbf{k_0}|$
- $\omega = \omega' - \omega_0$



Response to an electric field

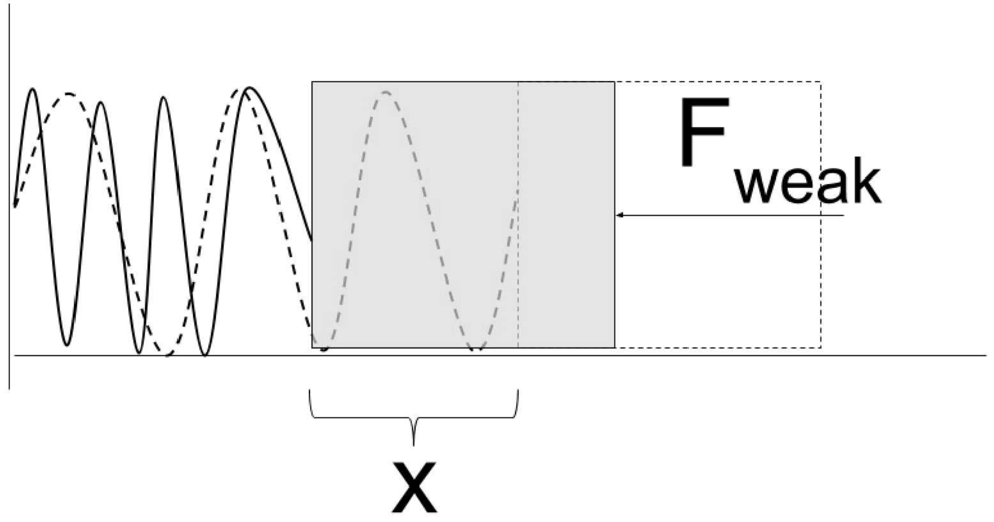


Measure: $\phi_{tot} = \phi_{ext} + \phi_{ind}$

$\rightarrow$ $\rho_{tot} = \rho_{ext} + \rho_{ind}$

Linear Response

- If ϕ_{ext} is weak, then $\rho_{\text{ind}} \sim \phi_{ext}$



Hooke's Law:
x ~ F_{weak}

- The response, $\chi\left(\mathbf{r}, t; \mathbf{r}', t'\right)$, can be non-local in space and time:

$$\rho_{\text{ind}}(\mathbf{r}, t) = \int d\mathbf{r}' \int_{-\infty}^{t} dt' \chi\left(\mathbf{r}, t; \mathbf{r}', t'\right) \phi_{\text{ext}}(\mathbf{r}', t')$$

Dielectric Function

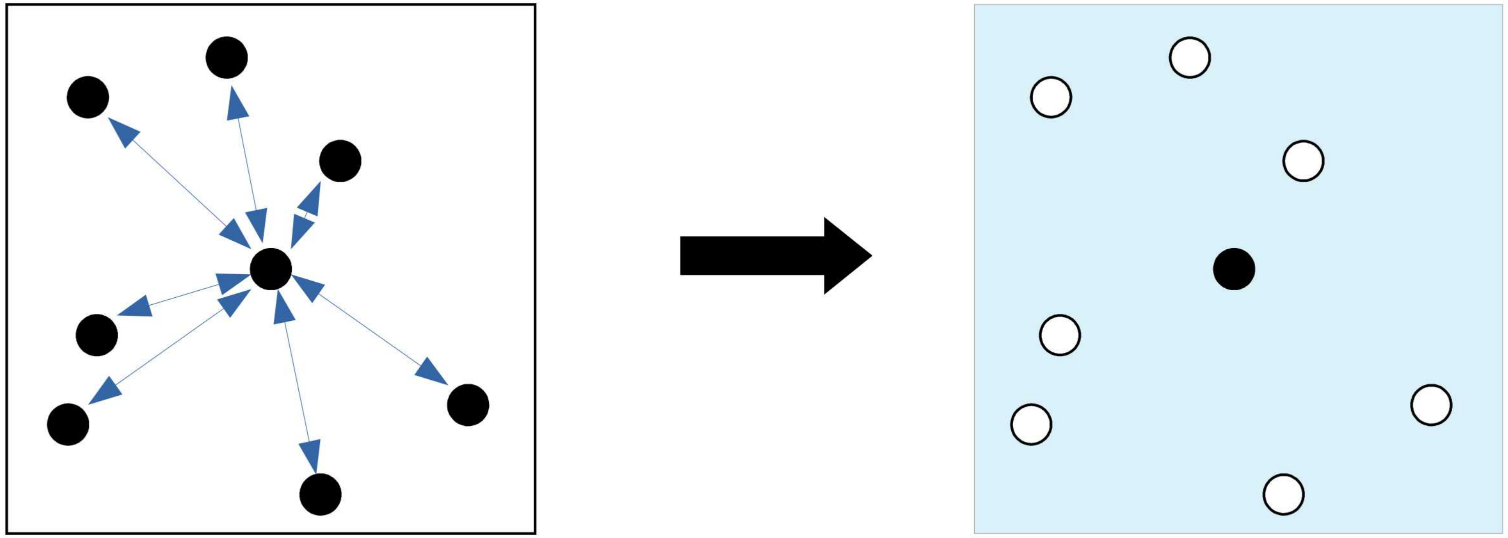
- $\varepsilon(\mathbf{k},\omega)$, the dielectric function, is related to the response function. In frequency space:

$$\varepsilon(\mathbf{k},\omega) = \frac{1}{1 + V_C(\mathbf{k})\chi(\mathbf{k},\omega)}$$

The dielectric function tells us how the electrons respond to an external potential

Random Phase Approximation

- $\varepsilon(\mathbf{k}, \omega)$ is (currently) too difficult to determine
- RPA is a type of mean field approximation

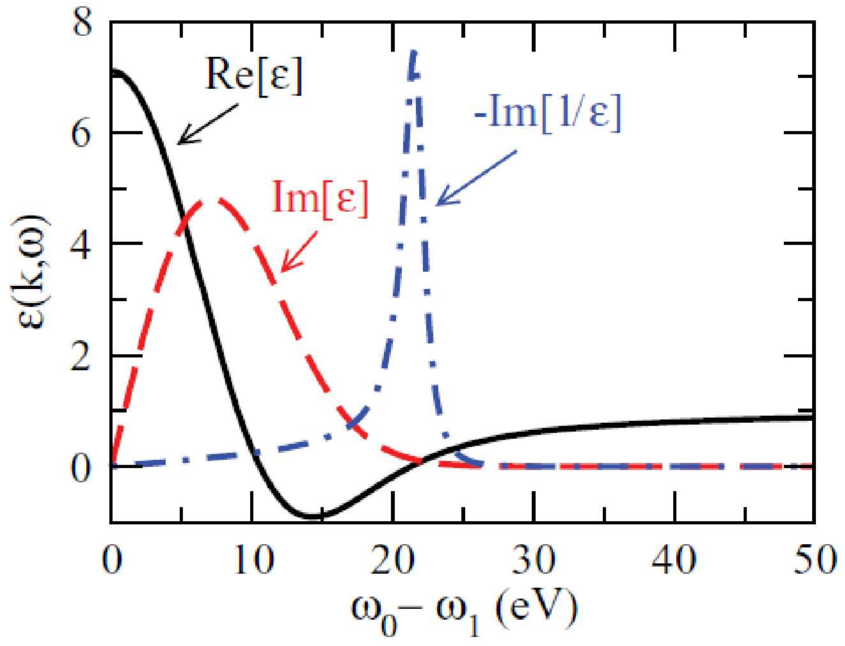


RPA Dielectric function

$$\varepsilon^{\mathrm{RPA}}(\mathbf{k},\omega) = \varepsilon_1 + i\varepsilon_2$$

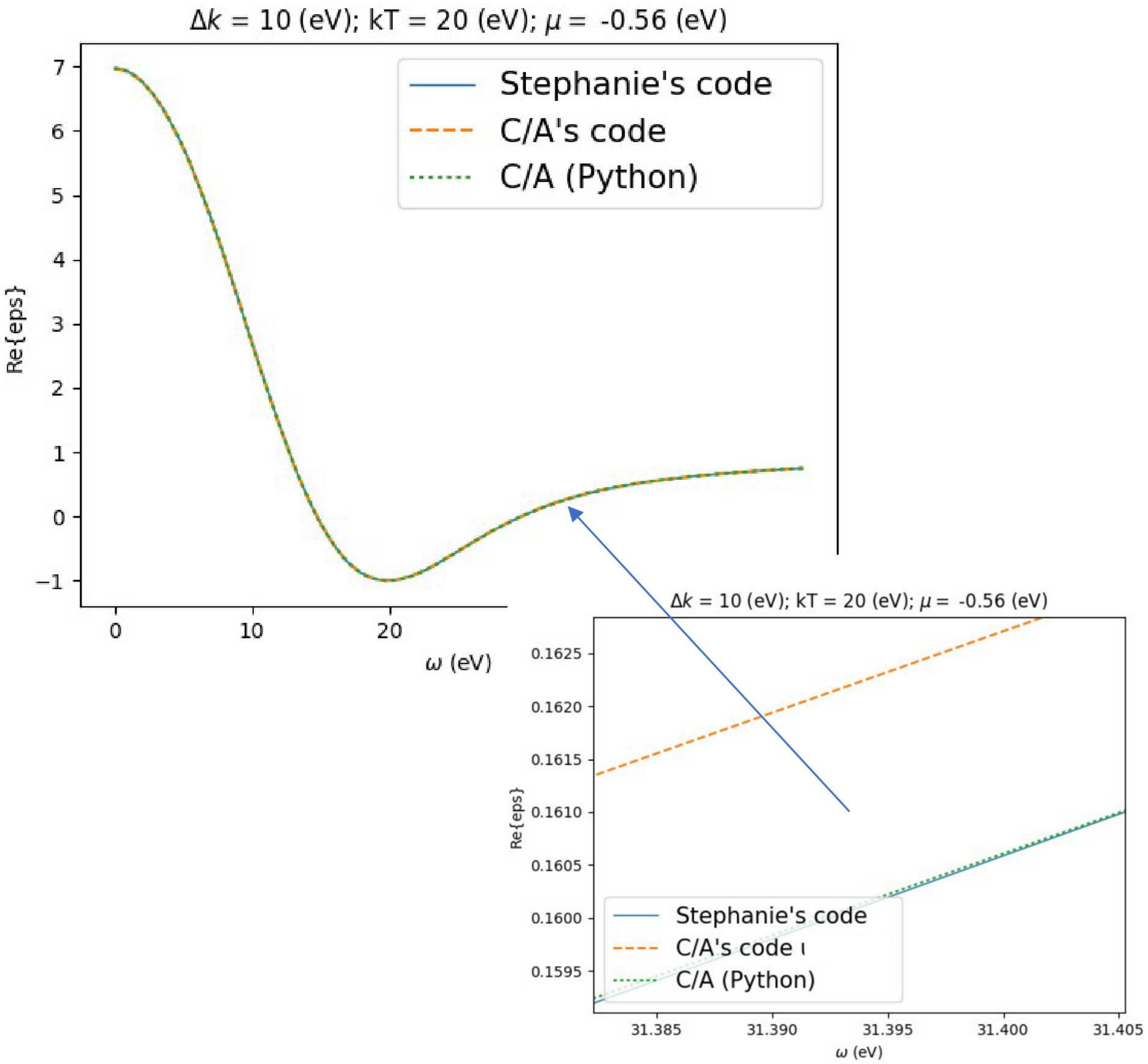
$$\varepsilon_1 = Re\{\varepsilon\} = 1 + \frac{2}{\pi k^3}\int_0^\infty dp\, p\, f(p)\left[\log\frac{|k^2+2pk+2\omega|}{|k^2-2pk+2\omega|} + \log\frac{|k^2-2pk+2\omega|}{|k^2-2pk-2\omega|}\right]$$

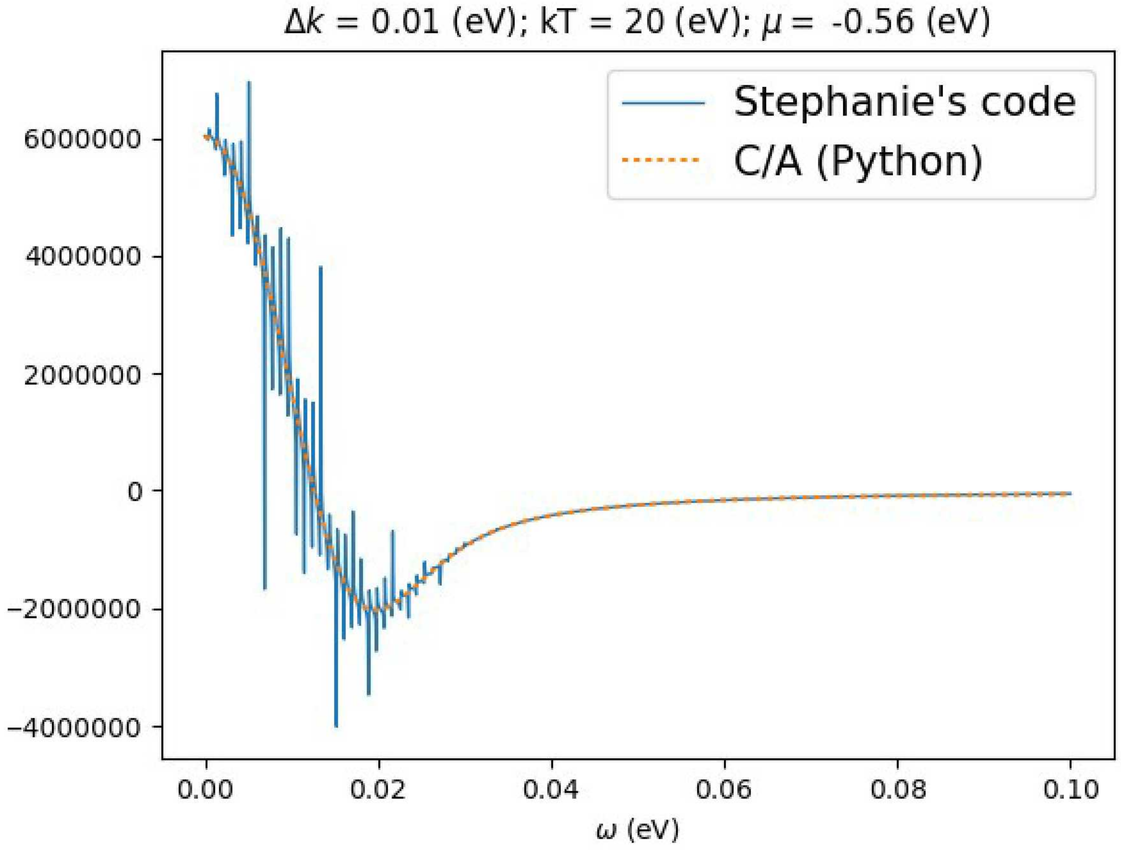
$$\varepsilon_2 = Im\{\varepsilon\} = \frac{2k_bT}{k^3}\log\left\{\frac{1+\exp\left[\left(\mu - \frac{(|2\omega-k^2|/2k)^2}{2}\right)/k_bT\right]}{1+\exp\left[\left(\mu - \frac{((2\omega+k^2)/2k)^2}{2}\right)/k_bT\right]}\right\}$$



Johnson et al., PRE 2012

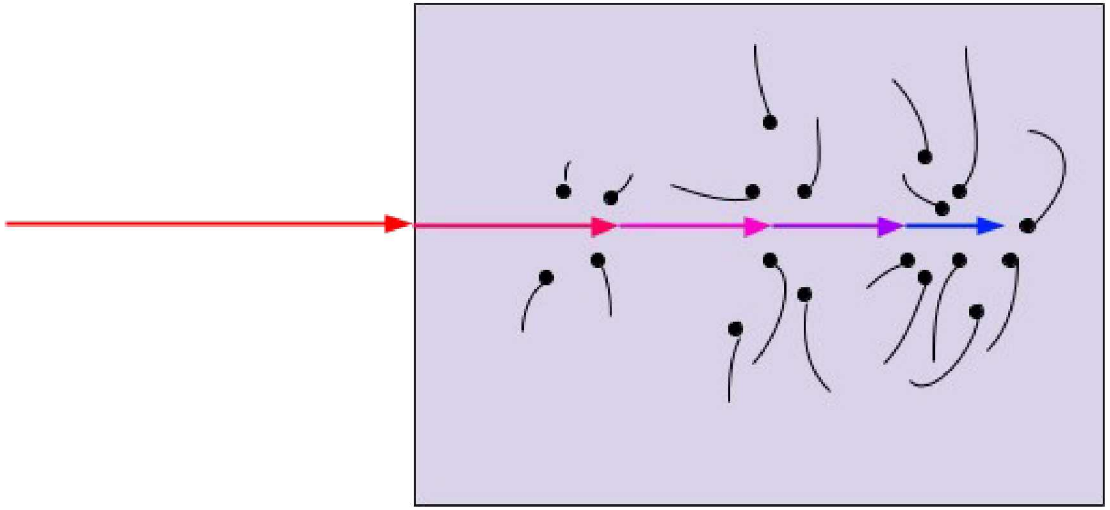
Numerically calculating ε_1





Stopping power

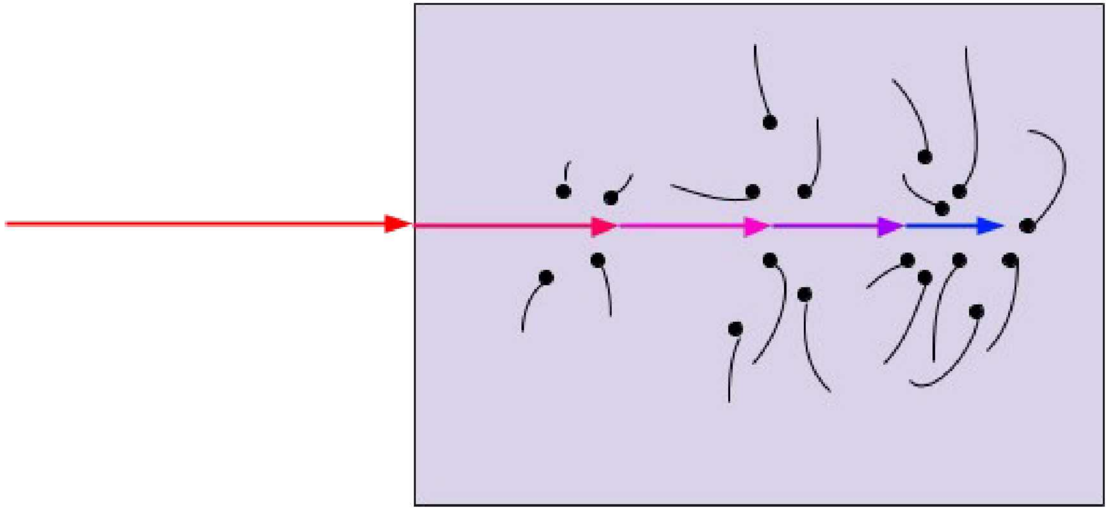
$$S_{\mathrm{e}}(v) = \frac{2Z^2}{\pi v^2}\int_0^{\infty}\frac{dk}{k}\int_0^{kv} d\omega\,\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon(k,\omega)}\right),$$



Stopping power

$$S_e(v) = \frac{2Z^2}{\pi v^2} \int_0^\infty \frac{dk}{k} \int_0^{kv} d\omega\,\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon(k,\omega)}\right)$$

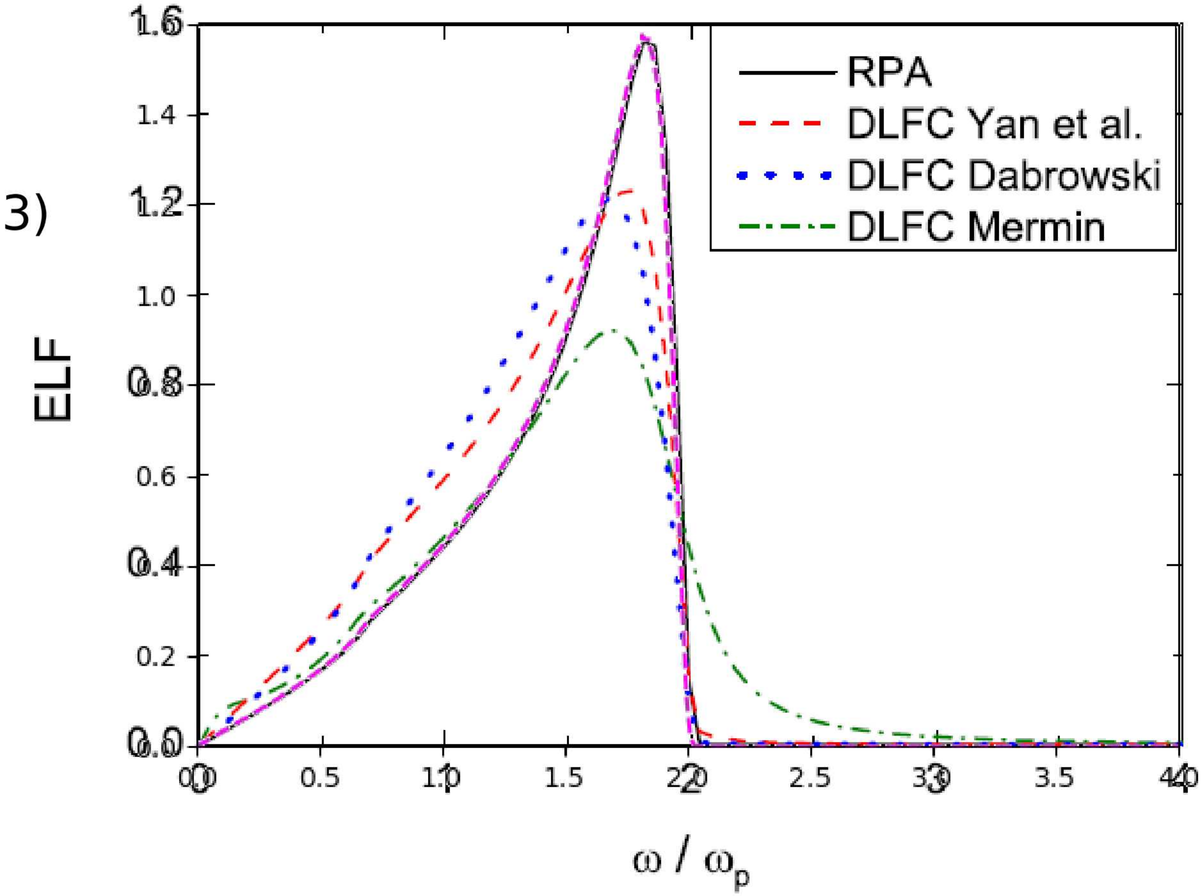
- Electron Loss Function = $\dfrac{\varepsilon_2}{\varepsilon_1^2 + \varepsilon_2^2}$



Electron loss function (ELF)

$$f_{ELF} = Im\left\{\frac{-1}{\varepsilon(k,\omega)}\right\} = \frac{Im\{\varepsilon\}}{\varepsilon^*\varepsilon}$$

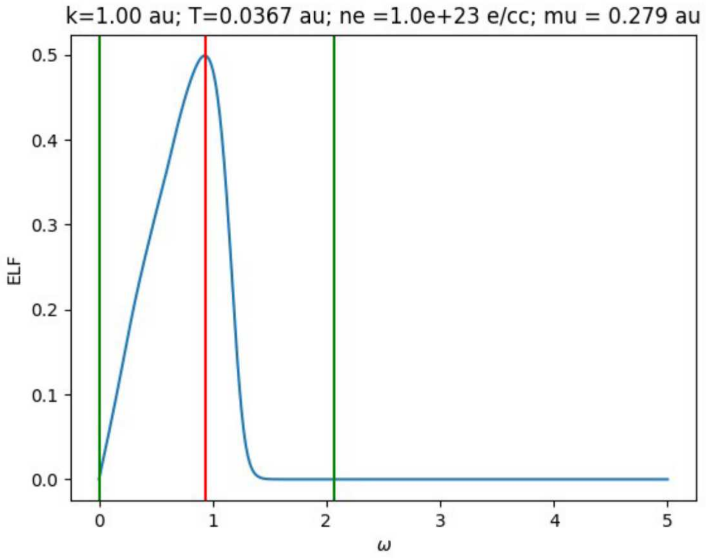
T = 0.1 eV
n_e = 10^23 e/cc
μ = 0.288 (for Al w/ Z*=3)

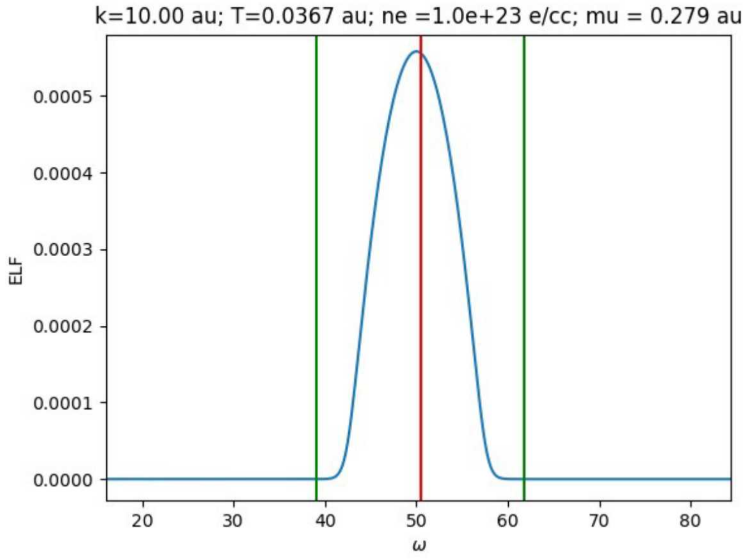


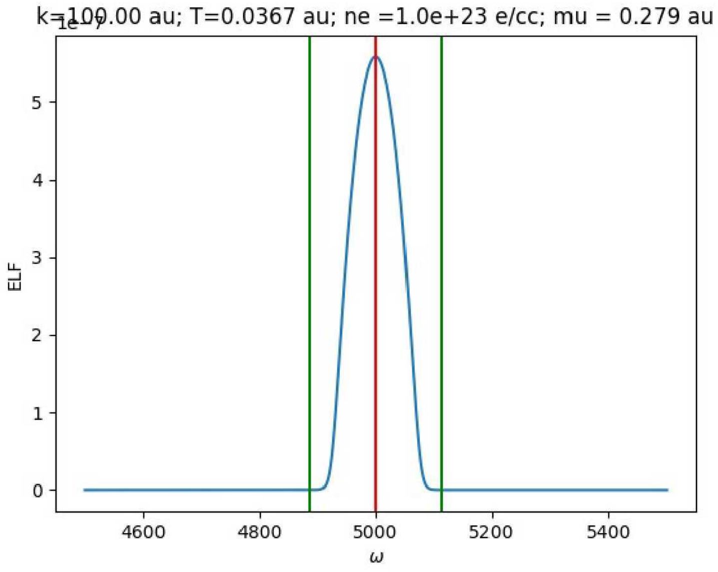
Barriga-Carrasco, PRE, 2009

ELF maximum

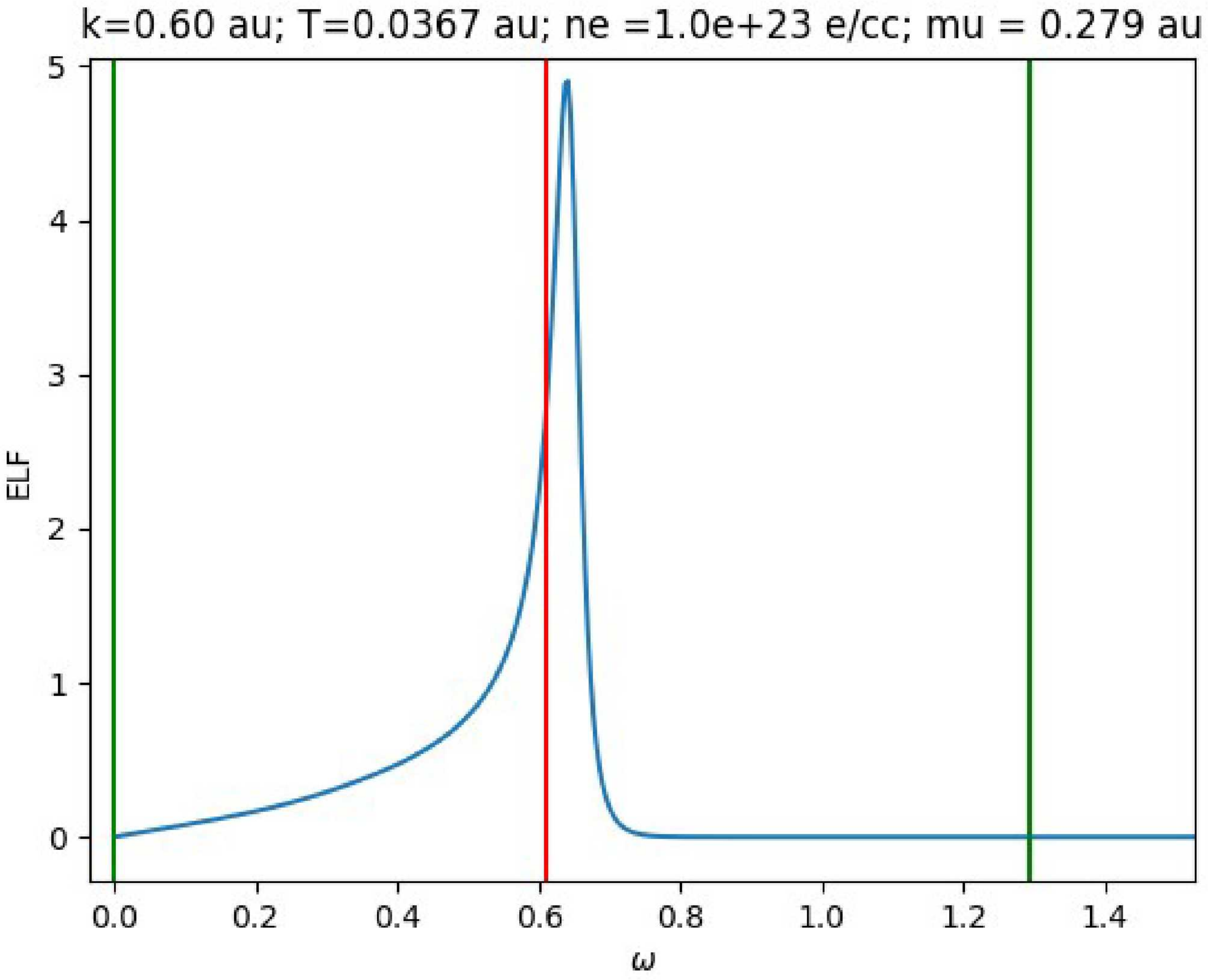
- Approximate function for max. position: $\omega_{max}(k, \mathrm{T}, n_e)$
- edges = $\omega_{max} \pm \gamma(\mathrm{T}, \mu, x)k$





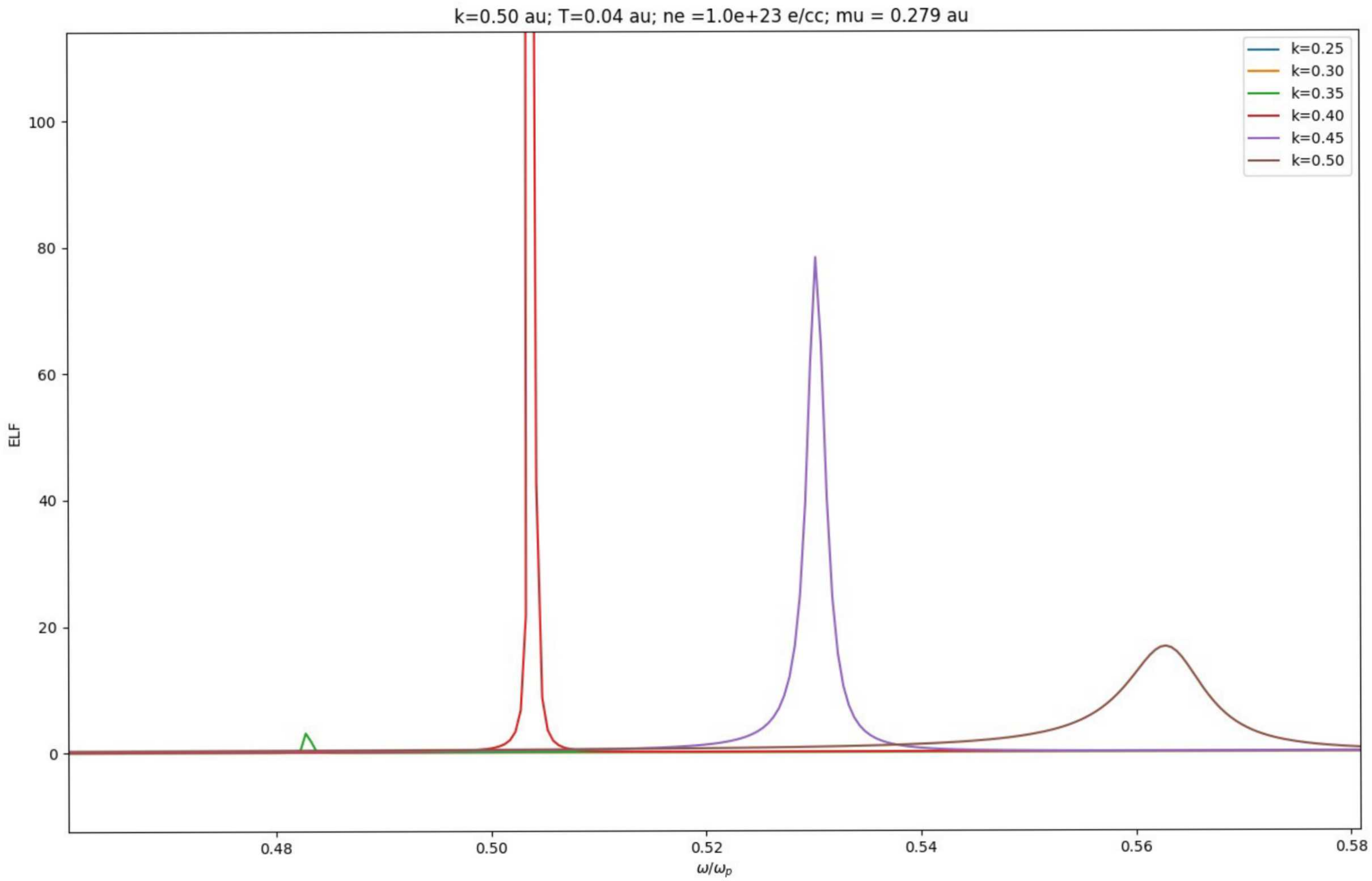


ELF maximum



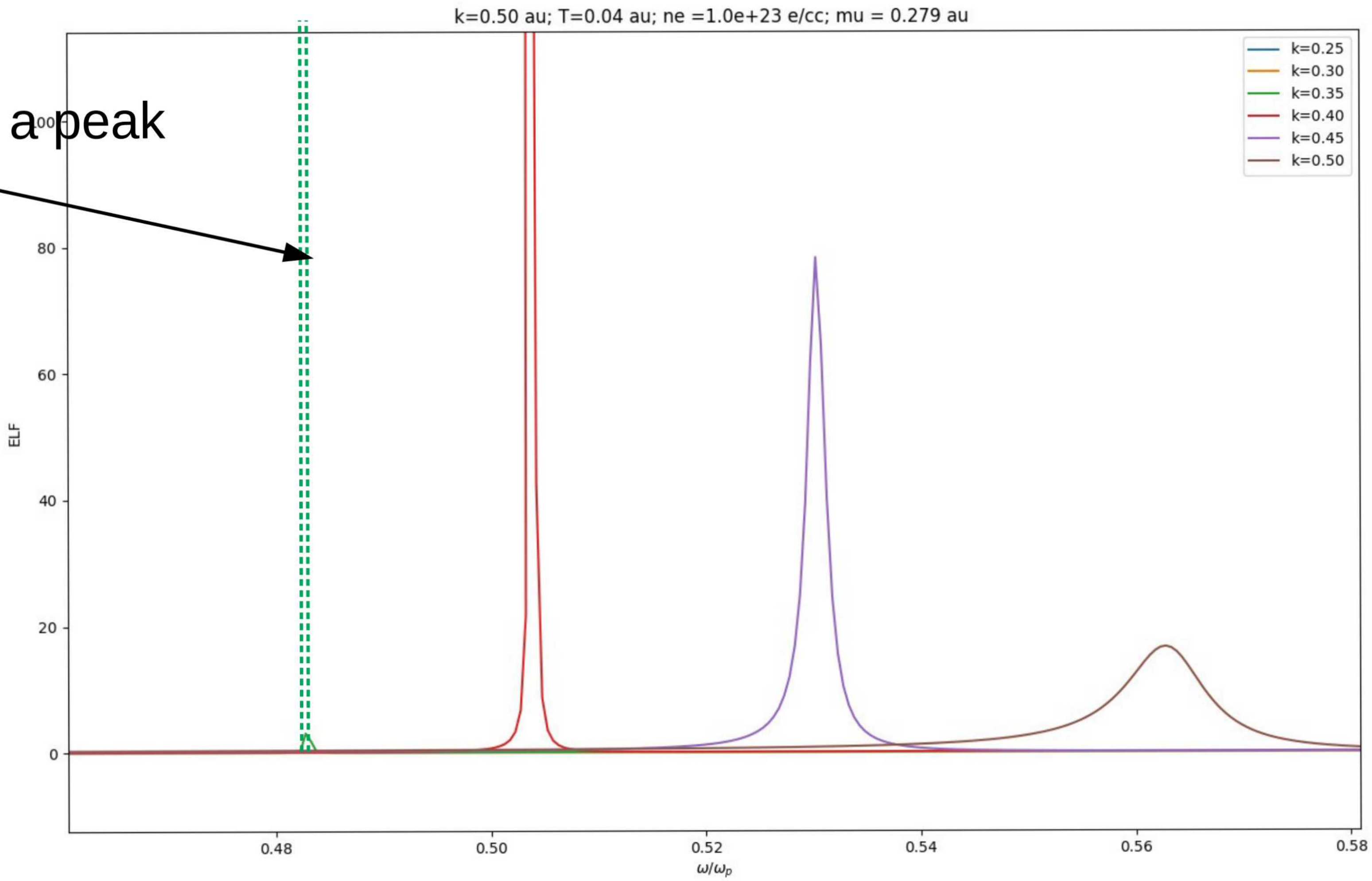
k=0.60 au; T=0.0367 au; ne =1.0e+23 e/cc; mu = 0.279 au
ELF
ω
0
1
2
3
4
5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4

Small k issues



Small k issues

There should be a peak here!

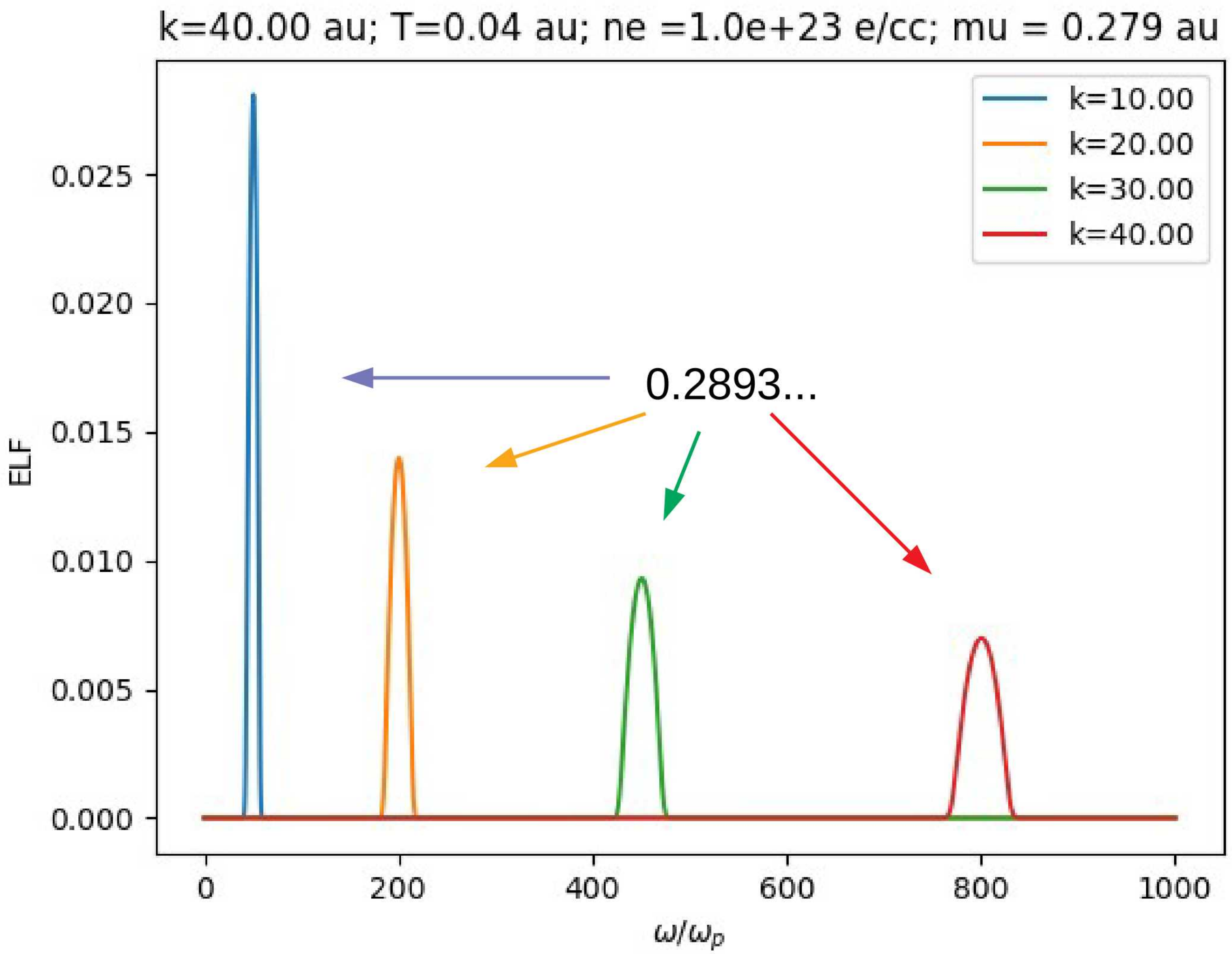


Sum rule

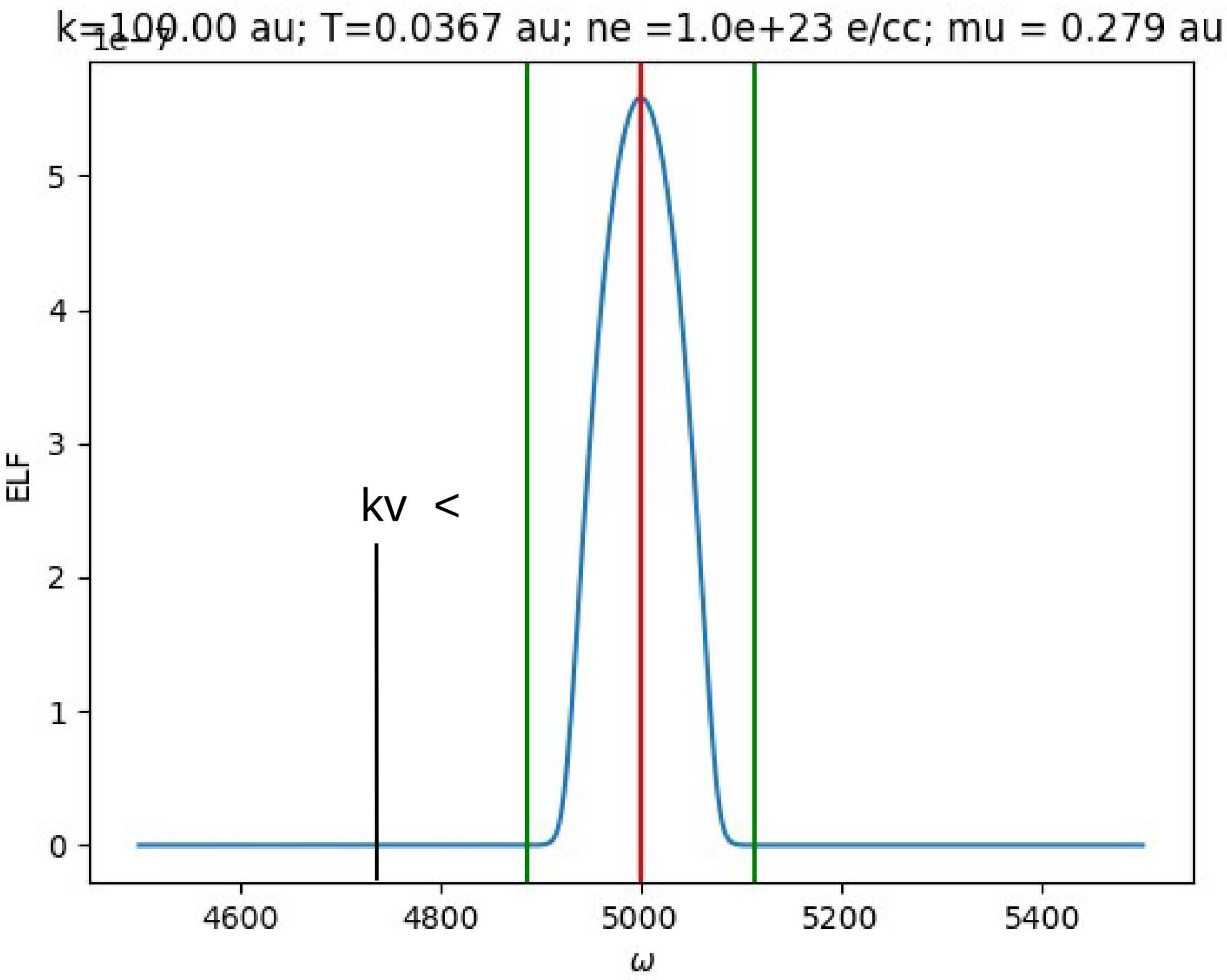
- F-sum rule:

$$\int_0^\infty d\omega\omega \mathrm{Im}\left(\frac{-1}{\epsilon}\right) = \frac{\pi}{2}\omega_p^2$$

= 0.2922...



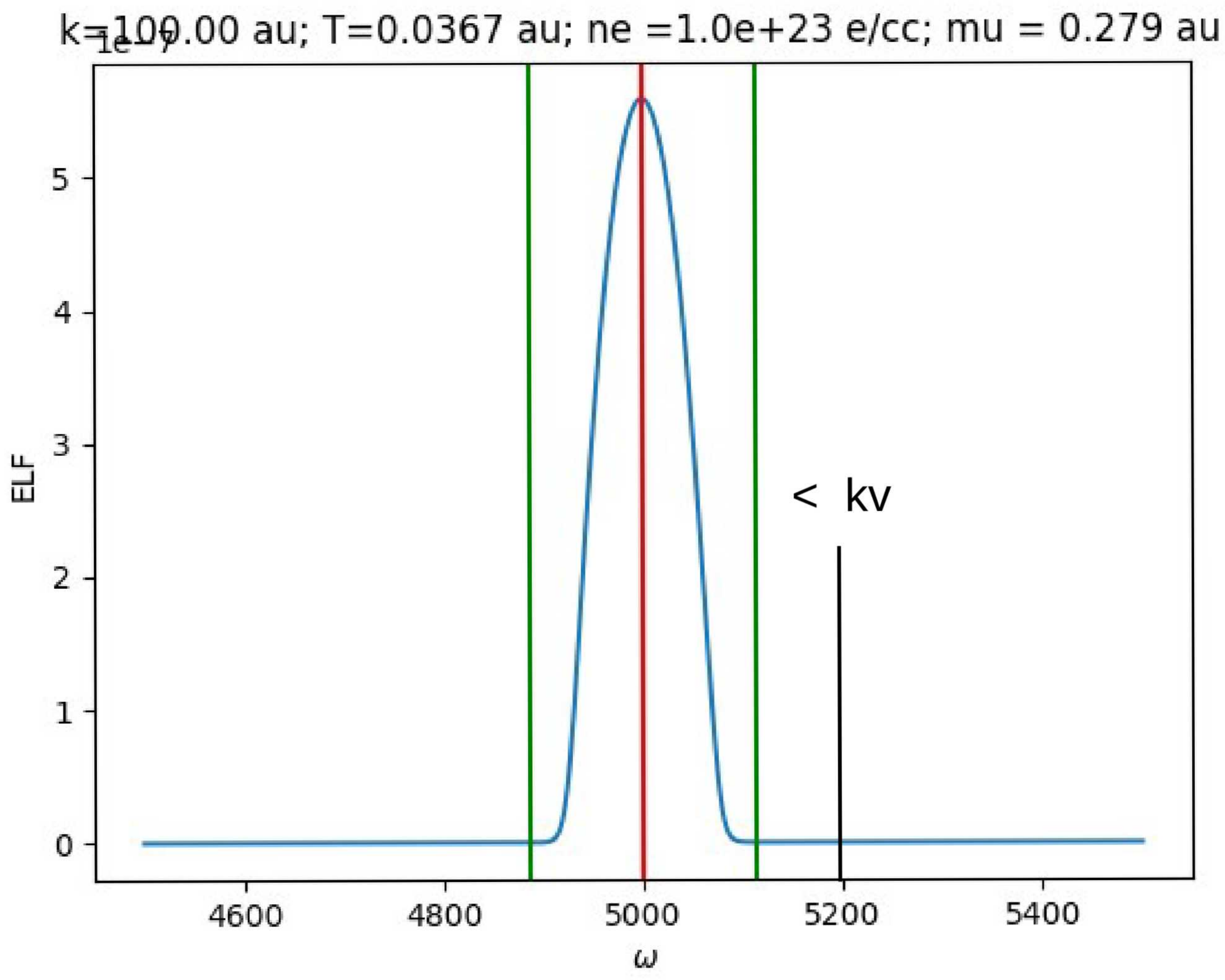
Stopping Power



$$S_e(v) = \frac{2Z^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon_x(k,\omega)}\right),$$

- If k*v < ω_{max} – γ(T, μ)*k*, then ω -integral = 0; true for **k < k1** or **k > k4**.

Stopping Power



$$S_e(v) = \frac{2Z^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon_x(k,\omega)}\right),$$

- If $k^*v < \omega_{max} - \gamma(T, \mu)k$, then ω-integral = 0; true for **k < k1** or **k > k4**.
- If $k^*v > \omega_{max} + \gamma(T, \mu)k$, then ω-integral = sum rule; true for **k2 < k < k3**.

Stopping Power

$$S_e(v) = \frac{2Z^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon_x(k,\omega)}\right),$$

$$= \frac{2Z^2}{\pi v^2}\left(\int_0^{k_1} dk + \int_{k_1}^{k_2} dk + \int_{k_2}^{k_3} dk + \int_{k_3}^{k_4} dk + \int_{k_4}^{\infty} dk\right)\frac{1}{k}\int_0^{kv} d\omega\omega\mathrm{Im}\left\{\frac{-1}{\epsilon}\right\}$$

Stopping Power

$$S_e(v) = \frac{2Z^2}{\pi v^2}\int_0^\infty \frac{dk}{k}\int_0^{kv} d\omega\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon_x(k,\omega)}\right),$$

$$= \frac{2Z^2}{\pi v^2}\left(\underbrace{\cancel{\int_0^{k_1} dk}}_{=0} + \int_{k_1}^{k_2} dk + \int_{k_2}^{k_3} dk + \int_{k_3}^{k_4} dk + \underbrace{\cancel{\int_{k_4}^{\infty} dk}}_{=0}\right)\frac{1}{k}\int_0^{kv} d\omega\omega\mathrm{Im}\left\{\frac{-1}{\epsilon}\right\}$$

Stopping Power

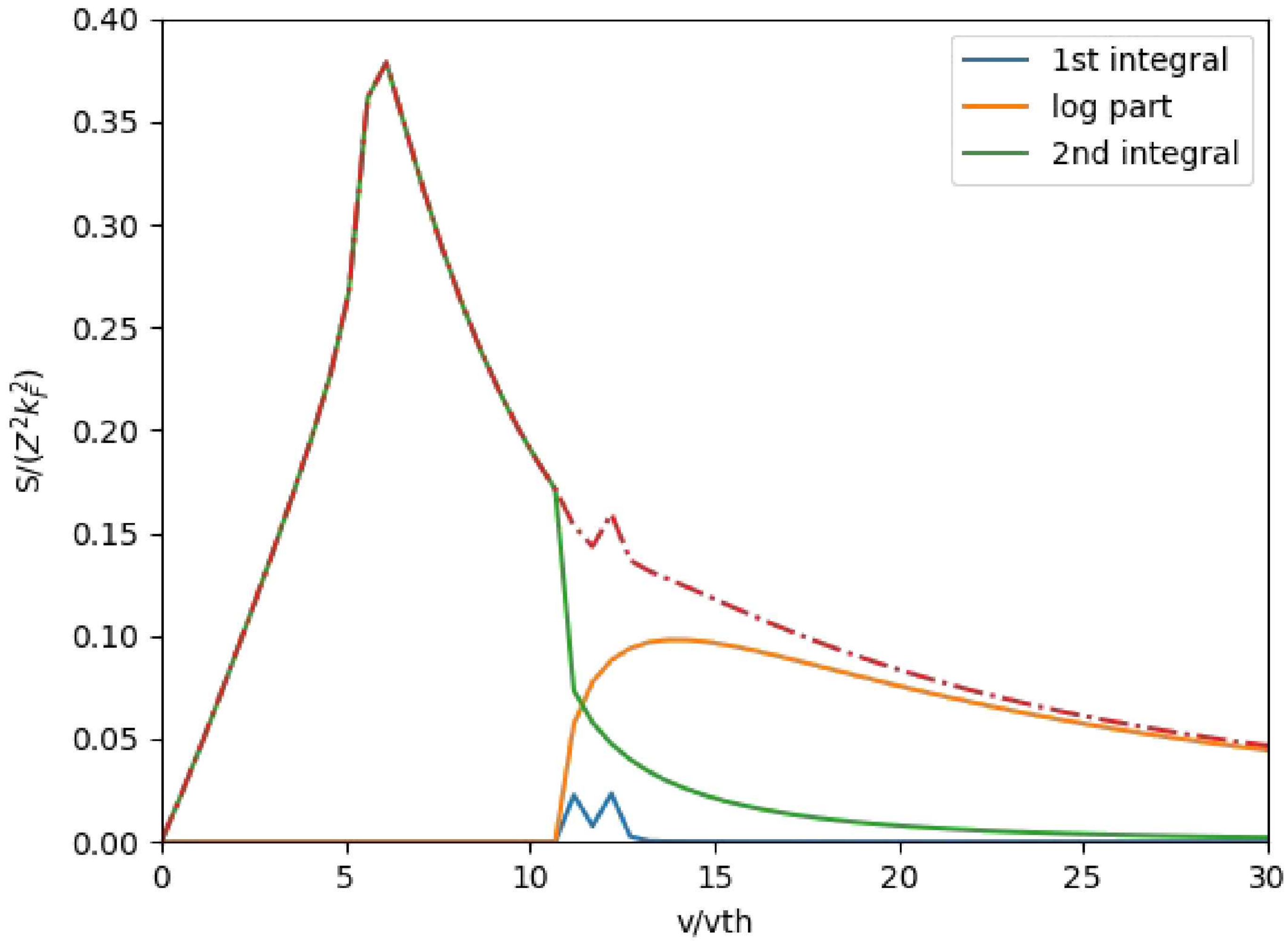
$$S_{\mathrm{e}}(v) = \frac{2Z^2}{\pi v^2}\int_0^{\infty}\frac{dk}{k}\int_0^{kv} d\omega\omega\,\mathrm{Im}\left(\frac{-1}{\epsilon_x(k,\omega)}\right),$$

$$= \frac{2Z^2}{\pi v^2}\left(\cancelto{0}{\int_0^{k_1} dk} + \int_{k_1}^{k_2} dk + \int_{k_2}^{k_3} dk + \int_{k_3}^{k_4} dk + \cancelto{0}{\int_{k_4}^{\infty} dk}\right)\frac{1}{k}\int_0^{kv} d\omega\omega\mathrm{Im}\left\{\frac{-1}{\epsilon}\right\}$$

$$= \frac{2Z^2}{\pi v^2}\left(\int_{k_1}^{k_2} dk\frac{1}{k}\int_0^{kv} d\omega\omega\mathrm{Im}\left\{\frac{-1}{\epsilon}\right\} + \frac{\pi}{2}\omega_p^2\log\left(\frac{k3}{k2}\right) + \int_{k_3}^{k_4} dk\frac{1}{k}\int_0^{kv} d\omega\omega\mathrm{Im}\left\{\frac{-1}{\epsilon}\right\}\right)$$

Stopping Power

T = 1 eV
n_e = 10^23 e/cc
μ = 0.279
(for Al w/ Z*=3)



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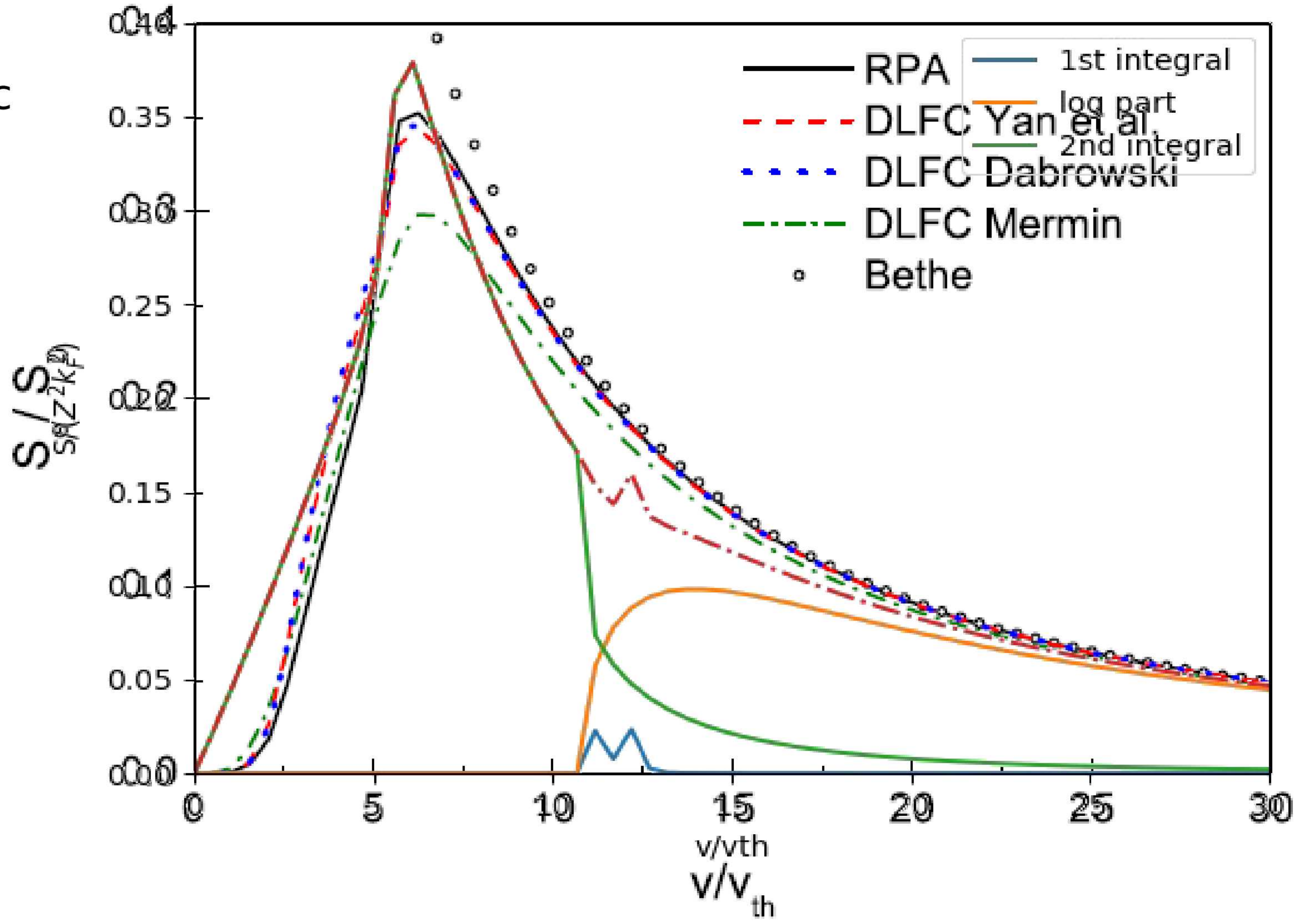

Barriga-Carrasco, PRE, 2009

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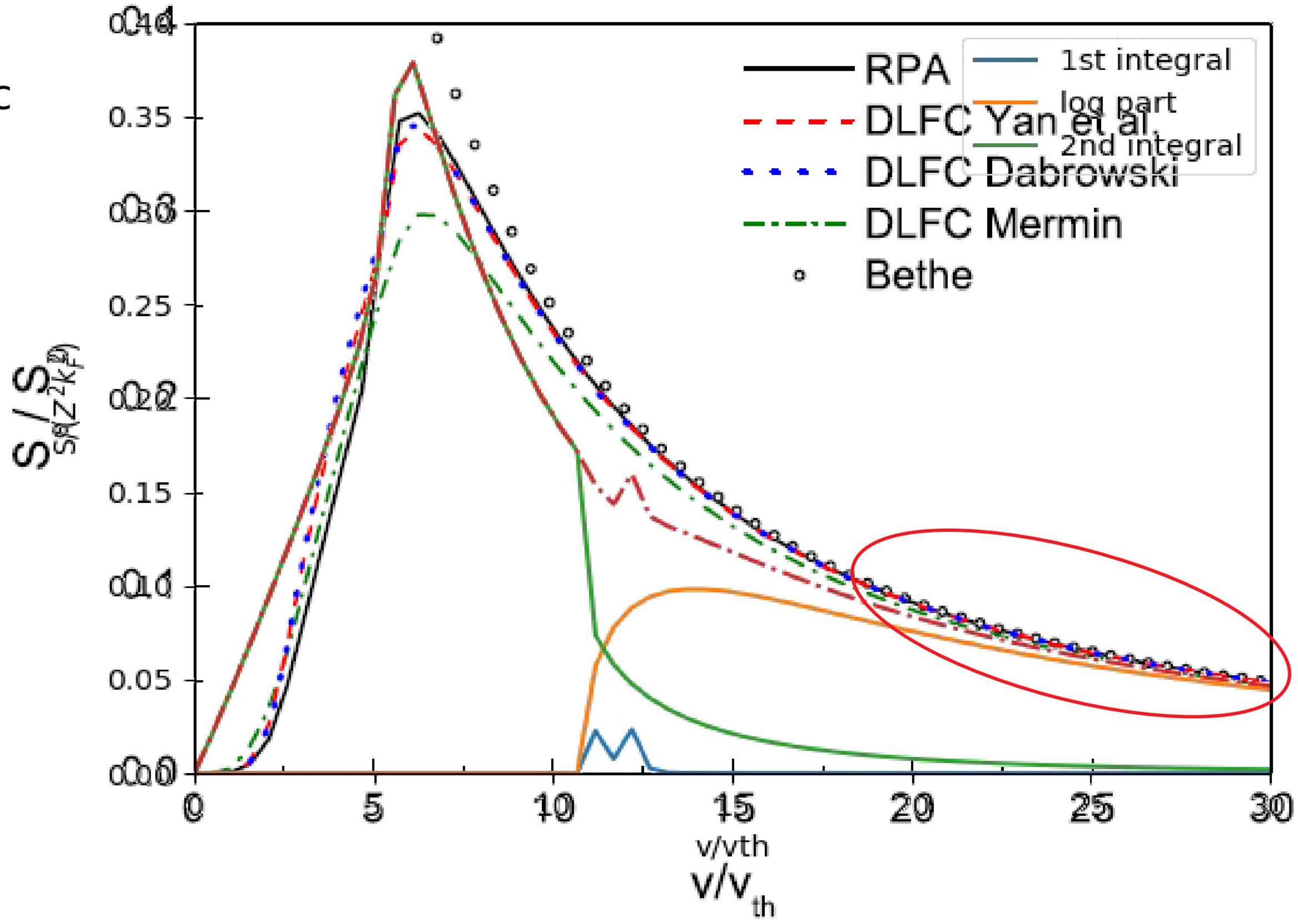

Barriga-Carrasco, PRE, 2009

Future Directions

- Still working on the stopping power ...

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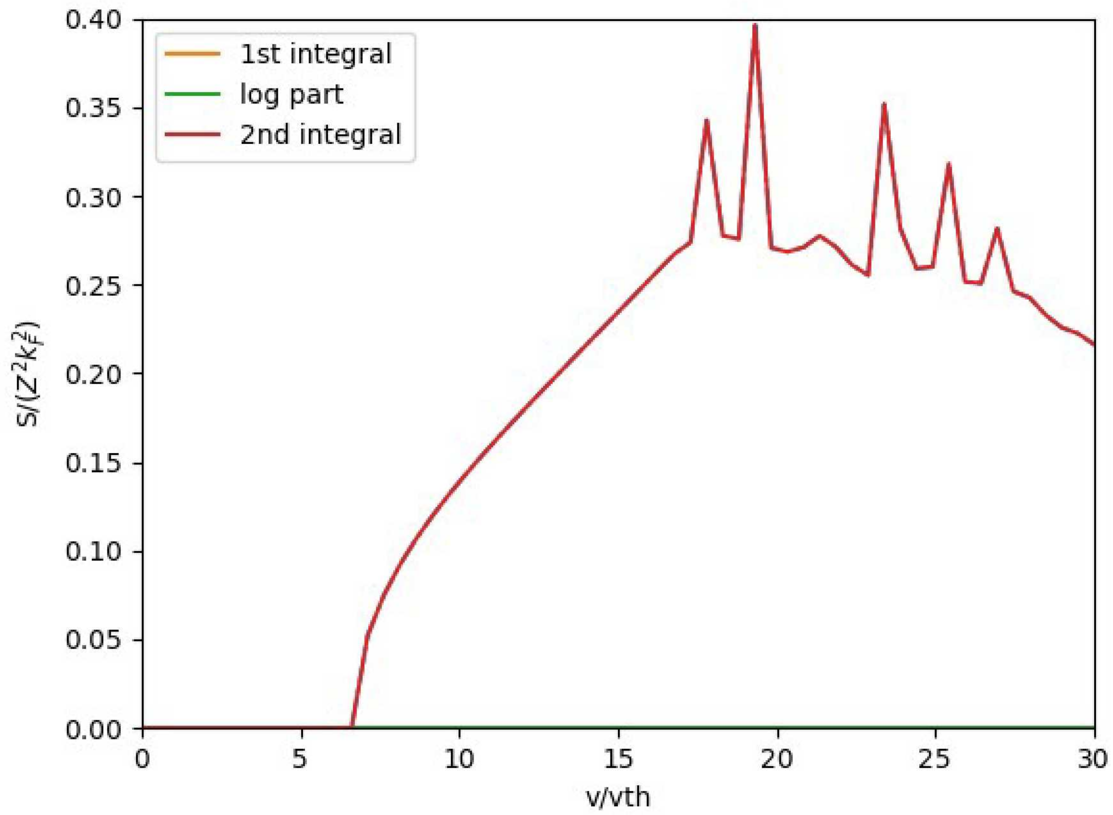
n_e = 10^23 e/cc
μ = 0.288
(for Al w/ Z*=3)



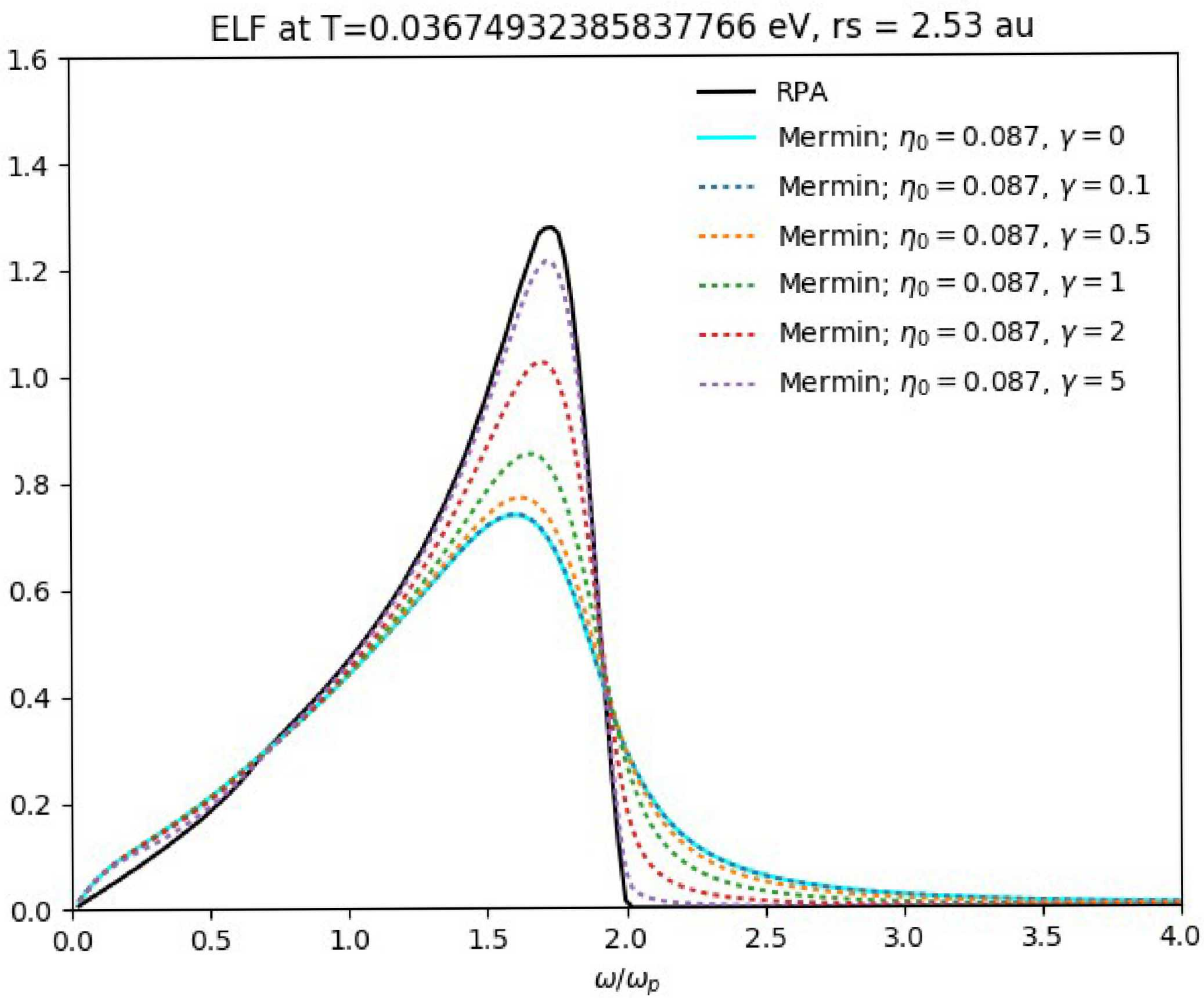
Future Directions

- Going beyond the RPA → include more information of interactions
- Using the Mermin dielectric function

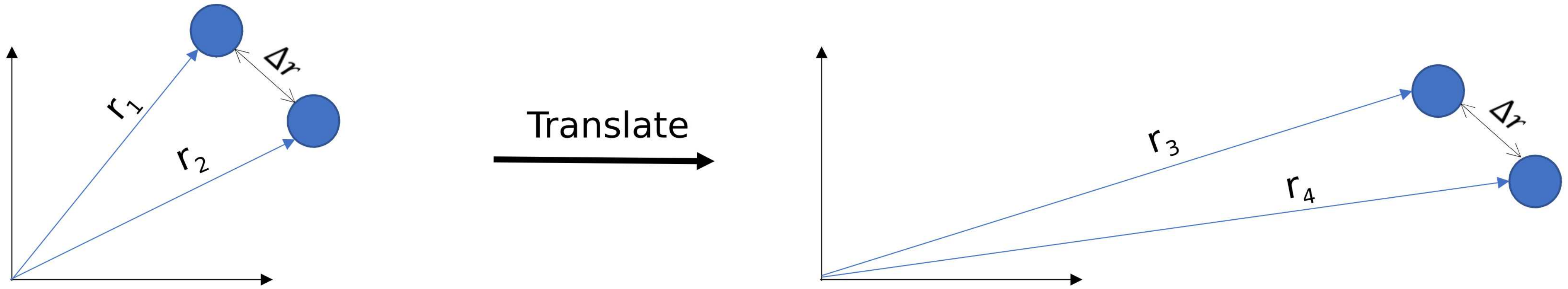
$$\epsilon_M(k,\omega) = 1 + \frac{(\omega + i\nu)[\epsilon(k,\omega + i\nu) - 1]}{\omega + i\nu[\epsilon(k,\omega + i\nu) - 1]/[\epsilon(k,0) - 1]}$$

- ν - collision frequency
- Attila’s code can handle this

Attila's Code with $\nu(\omega) = \frac{\eta_0}{1+(\gamma\omega)^2}$



Translational invariance



- Let *f(x1, x2)* depend on the positions of the two particles.
- Translational invariance: $f(r_1, r_2) = f(r_3, r_4) \; \rightarrow f \equiv f(\Delta r)$