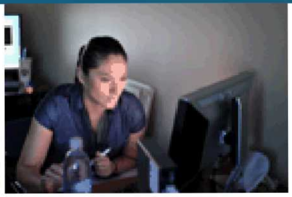
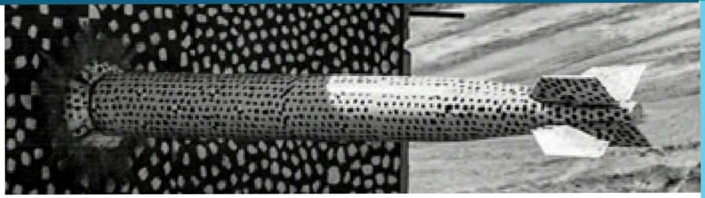
SAND2019-5546C

Leviathan Code Description





Thomas Gomez

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The Calculation

- This is a quantum-mechanical line-shape calculation
  - The wavefunctions of the electrons are solved in the long-range coulomb potential of the atom
    - Meaning that we use Coulomb waves
    - Have option to do a Distorted-wave treatment (in progress)
  - Full Coulomb treatment of the atom-plasma interaction
  - Exchange interactions are included
    - Includes non-orthogonality of perturber and radiator wavefunctions (Seaton 1953)

- This is based on the relaxation theory and uses a second-order expansion of the T-matrix

Relaxation Theory

- Leviathan uses the relaxation-theory results based on what was derived by Gomez et al. (2018)

$$\mathcal{H}(\omega) = \langle T(\omega) \rangle \frac{1}{1 + (\omega - L_0^a)^{-1} \langle T(\omega) \rangle}$$

$$\langle T(\omega) \rangle = Tr \left\{ T(\omega) [\omega - L_0]^{-1} \rho \right\} \rho_a^{-1} (\omega - L_0^a)$$

- Leviathan uses a second-order (binary-collision) expansion so that

$$\mathcal{H}(\omega) \approx n Tr \left\{ L_I^{a,1} f_1 + L_I^{a,1} \frac{1}{\omega - L_0^a - L_0^1} g_{a,1} (\omega - L_0^a) + L_I^{a,1} \frac{1}{\omega - L_0^a - L_0^1} L_I^{a,1} f_1 \right\}$$
$$- n^2 Tr \{ L_I^{a,1} f_1 \} \frac{1}{\omega - L_0^a} \{ L_I^{a,1} f_1 \}$$

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All interactions are Debye Screened

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$$- n^2 Tr\{L_I^{a,1} f_1\} \frac{1}{\omega - L_0^a} \{L_I^{a,1} f_1\}$$

Lowest-Order Fano Factor Correction

The Propagator (the imaginary part)

- The propagator has real and imaginary parts $$\frac{1}{\omega - L_0} \Longrightarrow \frac{\mathrm{PV}}{\omega - L_0} - i\pi\delta(\omega - L_0)$$
- The imaginary part eliminates one of the integrals in the second-order expansion

$$\sum_{Lkk'\mu' l_1 l_2} \int_0^\infty \int_0^\infty dk_1 dk_2 e^{-\beta\frac{1}{2}k_1^2} \left\langle \mu k_1 l_1; L \left\| V^{(k)} \right\| \mu' k_2 l_2; L \right\rangle \left\langle \mu' k_2 l_2; L \left\| V^{(k')} \right\| \mu" k_1 l_1; L \right\rangle$$

$$A^{k}_{l_1,l_2,L} A^{k'}_{l_2,l_1,L} \delta\left(\Delta\omega_{\mu' l} - \frac{1}{2}k_2^2 + \frac{1}{2}k_1^2 \right)$$

$$\sum_{Lkk'\mu' l_1 l_2} \int_0^\infty dk_1 e^{-\beta\frac{1}{2}k_1^2} \left\langle \mu k_1 l_1; L \left\| V^{(k)} \right\| \mu' k_2 l_2; L \right\rangle \left\langle \mu' k_2 l_2; L \left\| V^{(k')} \right\| \mu" k_1 l_1; L \right\rangle A^{k}_{l_1,l_2,L} A^{k'}_{l_2,l_1,L} / k_2$$

$$k_2 = \sqrt{k_1^2 + 2|\Delta\omega_{\mu' l}|};$$

$$\Delta\omega_{\mu' l} > 0$$

$$\sum_{Lkk'\mu' l_1 l_2} \int_0^\infty dk_2 e^{-\beta\frac{1}{2}k_1^2} \left\langle \mu k_1 l_1; L \left\| V^{(k)} \right\| \mu' k_2 l_2; L \right\rangle \left\langle \mu' k_2 l_2; L \left\| V^{(k')} \right\| \mu" k_1 l_1; L \right\rangle A^{k}_{l_1,l_2,L} A^{k'}_{l_2,l_1,L} / k_1$$

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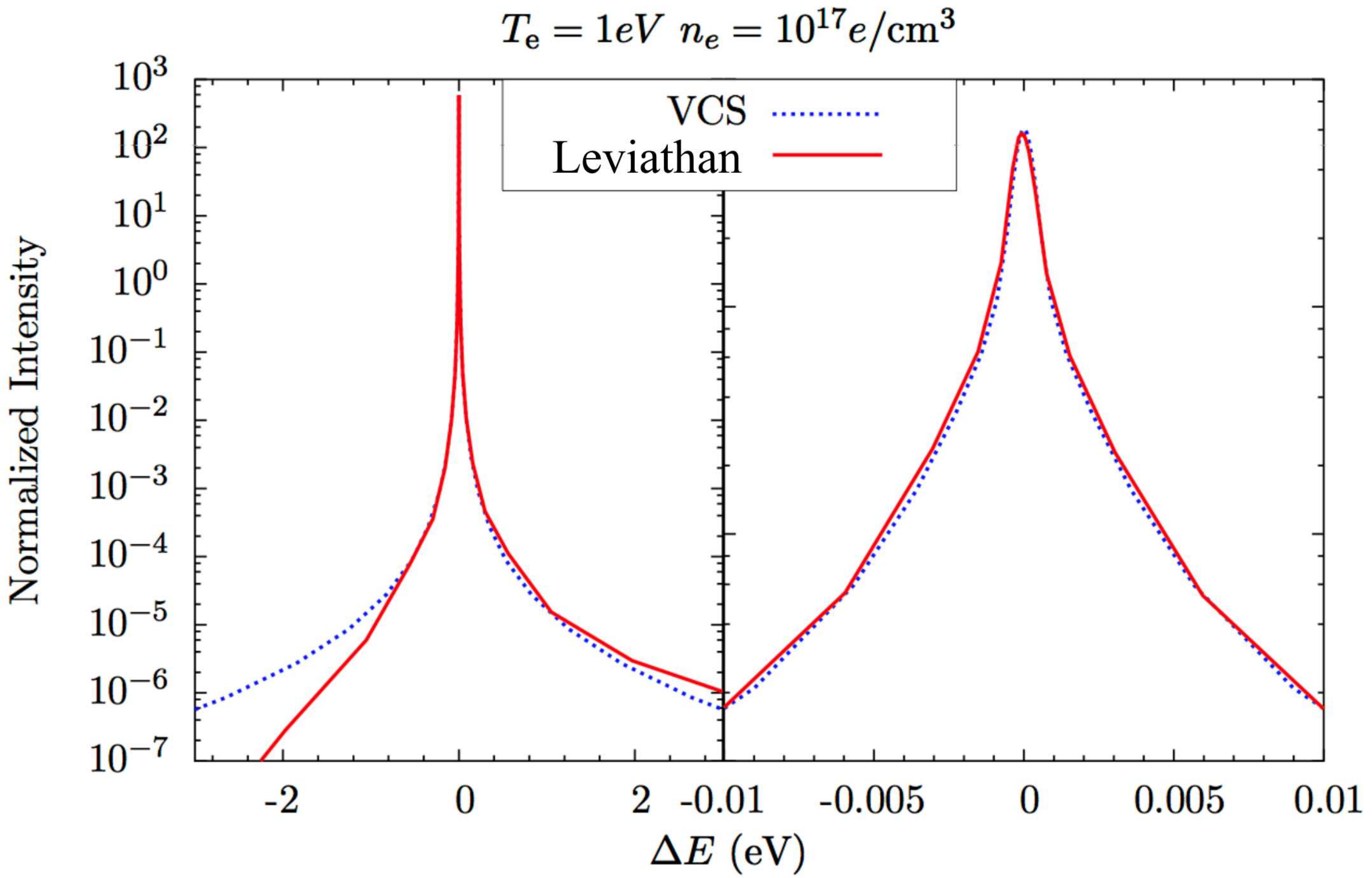
$$\sum_{Lkk'\mu' l_1 l_2} \int_0^\infty \int_0^\infty dk_1 dk$$

$$\sum_{Lkk'\mu' l_1 l_2} \int_0^\infty dk_1 e^{-\beta \frac{1}{2} k_1^2} \left\langle \mu \right.$$



$$\sum_{Lkk'\mu' l_1 l_2} \int_0^\infty dk_2 e^{-\beta \frac{1}{2} k_1^2} \left\langle \mu k_1 l_1; L \left\| V^{(k)} \right\| \mu' k_2 l_2; L \right\rangle \left\langle \mu' k_2 l_2; L \left\| V^{(k')} \right\| \mu" k_1 l_1; L \right\rangle A^{k}_{l_1,l_2,L} A^{k'}_{l_2,l_1,L} / k_1$$

Causes exponential drop off of red wing

$$k_1 = \sqrt{k_2^2 + 2|\Delta\omega_{\mu' l}|};$$

$$\Delta\omega_{\mu' l} < 0$$

The propagator (the real part)

- When we evaluate the principal value, we take the Δk steps that are small enough that V does not vary appreciably over the step

$$\int_0^\infty \int_0^\infty dk_1 dk_2 \left\langle ak_1 \left| V \right| bk_2 \right\rangle \left\langle bk_2 \left| V \right| a'k_1 \right\rangle e^{-\beta \frac{1}{2} k_1^2} \frac{\mathrm{PV}}{\Delta\omega - \frac{1}{2}k_2^2 + \frac{1}{2}k_1^2} \Longrightarrow$$

$$\int_0^\infty \sum_{k_2} dk_1 \left\langle ak_1 \left| V \right| bk_2 \right\rangle \left\langle bk_2 \left| V \right| a'k_1 \right\rangle e^{-\beta \frac{1}{2} k_1^2} \int_{k_2 - \frac{1}{2}\Delta k}^{k_2 + \frac{1}{2}\Delta k} dk_2 \frac{\mathrm{PV}}{\Delta\omega - \frac{1}{2}k_2^2 + \frac{1}{2}k_1^2}$$

- We can evaluate this integral using

$$\int \frac{1}{x^2 - a^2} = \frac{1}{2a} \begin{cases} \ln \frac{a-x}{a+x} & |x| < |a| \\ \ln \frac{x-a}{a+x} & |x| > |a| \end{cases}$$

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$$\int_0^\infty \sum_{k_2} dk_1 \left\langle ak_1 \left| V \right| bk_2 \right\rangle \left\langle bk_2 \left| V \right| a'k_1 \right\rangle e^{-\beta \frac{1}{2} k_1^2} \int_{k_2 - \frac{1}{2}\Delta k}^{k_2 + \frac{1}{2}\Delta k} dk_2 \frac{\mathrm{PV}}{\Delta\omega - \frac{1}{2}k_2^2 + \frac{1}{2}k_1^2}$$

- Then the integral becomes $c = \sqrt{2|\Delta\omega| + k_1^2}$

$$\int_{k2-\frac{1}{2}\Delta k}^{k2+\frac{1}{2}\Delta k} \frac{2}{2\Delta\omega + k_1^2 - k_2^2} dk_2 = \frac{1}{c} \begin{cases} \ln \frac{c-k_2-\frac{1}{2}\Delta k}{c+k_2+\frac{1}{2}\Delta k} - \ln \frac{c-k_2+\frac{1}{2}\Delta k}{c+k_2-\frac{1}{2}\Delta k} & |k_2 + \frac{1}{2}\Delta k| < |c| \\ \ln \frac{k_2+\frac{1}{2}\Delta k-c}{c+k_2+\frac{1}{2}\Delta k} - \ln \frac{k_2-\frac{1}{2}\Delta k-c}{c+k_2-\frac{1}{2}\Delta k} & |k_2 - \frac{1}{2}\Delta k| > |c| \\ \ln \frac{k_2+\frac{1}{2}\Delta k-c}{c+k_2+\frac{1}{2}\Delta k} - \ln \frac{c-k_2+\frac{1}{2}\Delta k}{c+k_2-\frac{1}{2}\Delta k} & |k_2 - \frac{1}{2}\Delta k| < |c| < |k_2 + \frac{1}{2}\Delta k| \end{cases}$$

Evaluating the Angular Integrals

- For each of the matrix elements, we evaluate the angular integrals according to the Cowan prescription
- We have to either de-couple the angular momenta and sum, or use symmetry considerations of the dipole moment—we get the same answer either way
  - For upper-state and lower-state broadening terms, we get a prefactor (and an likewise term for spin)

$$\sum_{M,m_1}(2L+1)\begin{pmatrix} l_a & l_1 & L \\ m_a & m_1 & M \end{pmatrix}^2 = \sum_{L_l}(2L_u+1)(2L_l+1)\begin{Bmatrix} l_a & l_1 & L_u \\ L_l & 1 & l'_a \end{Bmatrix}^2 = \frac{2L+1}{2l_a+1}$$

- The interference term is based on the de-coupling formula in Cowan

$$(-1)^{l_1+l_2}(2L_u+1)(2L_l+1)\begin{Bmatrix} l_u & l_1 & L_u \\ L_l & 1 & l_l \end{Bmatrix}\begin{Bmatrix} l'_u & l_2 & L_u \\ L_l & 1 & l'_l \end{Bmatrix}$$