Ion-Impact Excitation: Scoping Importance in Plasma Regimes Relevant to Fusion and Astrophysics

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Outline

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Introduction

- Presentations at previous ADAS Workshops (Summers 2014, Bluteau 2014, Bluteau 2015) have laid the theoretical ground work for the quick and accurate calculation of fundamental quantities for ion-impact excitation (IIE).
    - 'Quantities' $\equiv$ cross-sections ($\sigma_{i\rightarrow j}$) or collision strengths (Ω_{ij}), rate coefficients ($q_{i\rightarrow j}$) or effective collision strengths (Υ_{ij}), *etc.*
- Although the importance of IIE was motivated *theoretically* in the antecedent presentations, no quantitative proof was provided, and exactly *where* in the parameter space IIE should be considered was not specified.
- In the final analysis, a process is only important if its effects are *measurable* and therefore have magnitudes greater than the experimental uncertainty.
- First step and focus of presentation: model the dominant atomic populations under various plasma conditions and for different systems, both with and without IIE to judge its potential influence.

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Brief Detour: Calculation Updates

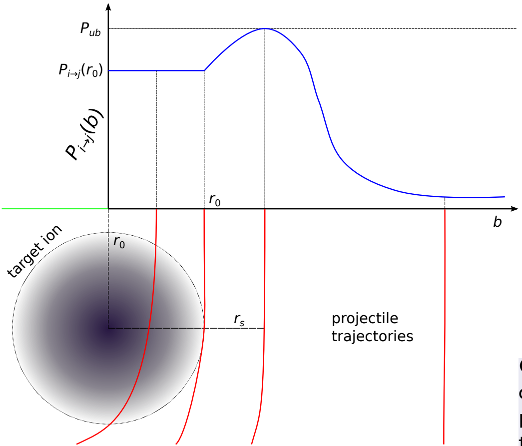
- **Atomic Coulomb excitation**: the projectile follows a classical trajectory determined by scattering in a Coulomb field (Rutherford scattering), and the excitation probability, $P_{i \rightarrow j}$, of the target is obtained through first-order, time dependent perturbation theory, which in turn uses the long-range form of the Coulomb interaction to describe the excitation [Alder et al. (1956)].
  - Also referred to as the Semi-Classical, Impact Parameter (SC IP) approach, or SC-1
  - A similar technique (SC-CC) involves forming a set of coupled differential equations from the truncated Scroëdinger equation while still using the same long-rage approximation for the interaction term and assuming the projectile follows a classical trajectory

a2iratbt

- New offline code in ADAS1#2 (still in beta and not in central ADAS)
- Generates IIE collision data using the SC-1 approach as prescribed in Burgess and Tully (2005)—next slide
- Perl scripts allow for the generation of a new file type, *adf06*, that is analogous to *adf04* but contains blocks of collision data for different projectile cases

Detailed Considerations of $P_{i\to j}$

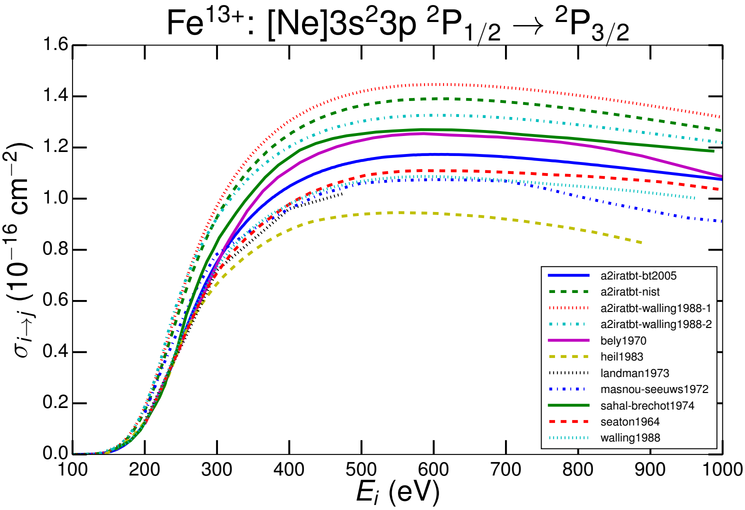
This subject must be revisited because numerous mistakes have been made when calculating $P_{i\to j}$: penetrating collisions, the strong-coupling region, and high energy limits need special consideration.



- Codes due to Bely and Faucher (1970) and Bahcall and Wolf (1968) both mistreat penetrating collisions, leading to the incorrect high energy scaling of the cross-section.
- Both Seaton (1964) and Reid and Schwarz (1963) get this right but do not ensure the correct constant of proportionality of the cross-section fall-off ($\sigma_{ij} \sim C/E, \quad \Omega_{ij} \sim C$).
- Burgess and Tully (2005) summarize the mistakes and present a completely corrected form of the theory, but their resulting code has been lost.

Crucially, most codes we have encountered deal only with protons as ion colliders: proton isotopes and other species will need to be included in fusion scenarios (not a concern for astrophysics).

Fe^{13+} Proton-Impact Cross Section: Literature Comp

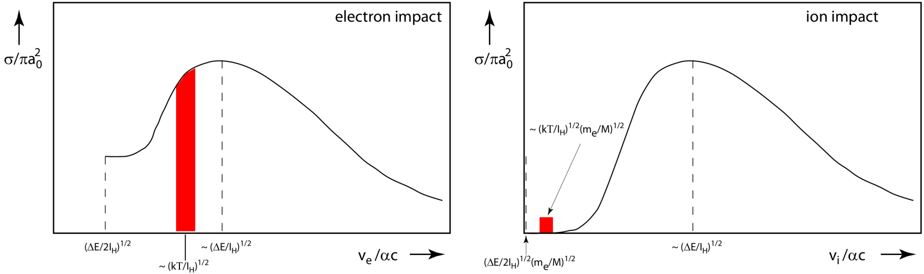


The oft studied 5308 Å "coronal green line": proves that a sensitivity study is required.

Outline

Scoping IIE: "Rules of Thumb" I

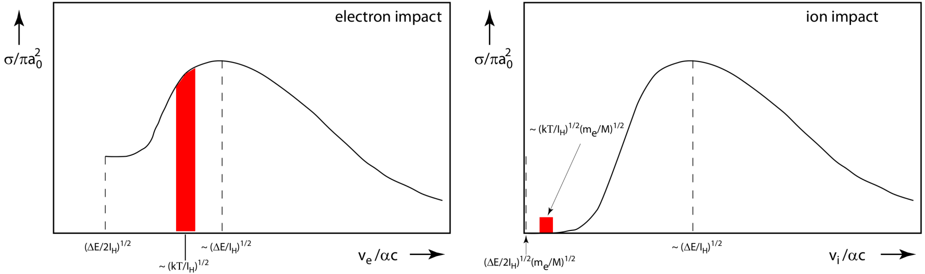
- For an individual transition, the cross sections for both electron- and ion-impact will peak at approximately the same projectile *velocities*, $v_{\rm p}, {\rm p} \in \{{\rm e}, {\rm i}\}$.
- Therefore, in energy space the ion-impact peak will be $\sim M$ times higher since $E_{\rm i} = M \cdot v_{\rm i}/2$, where $M = \frac{m_{\rm t}\, m_{\rm i}}{m_{\rm t} + m_{\rm i}}$ (au)



Working in atomic units (au), $\Delta E/I_{\rm H}$ is the transition energy, $I_{\rm H}$ is the ionization potential of hydrogen in the same units as ΔE, and σ is the cross-section for the arbitrary transition from the target ion level *i* to *j*. The temperature, *T*, of both the colliding ion and electron velocity distributions (red blocks) is assumed to be equal.

Scoping IIE: “Rules of Thumb” II

- For electron-impact in energy space, the excitation cross section typically peaks between 1–10 $\times \Delta E$, and so for ion-impact one would expect the peak to be between M–$10M$ $\times \Delta E$.
- *E.g.* proton impact, $M \sim 2000$ (au), so $E_{\mathrm{peak}} \sim 2000$–$20000 \times \Delta E$
- Thus, if we want the Maxwellian projectile distribution to lie somewhere close to the peak of the cross section (and so yield a large rate), we require $kT_{\mathrm{i}} \gg \Delta E$
- Typically, $1 < kT_{\mathrm{i}}/I_{z+} < 10$ for plasmas in ionization equilibrium, so only “free” parameter is $\Delta E \ll I_{z+}$



Scoping IIE: Preliminary Conclusions

- These "rules of thumb" only apply to individual transitions.
- The ultimate determining factor for whether IIE is significant can only be obtained through population modelling and the applications thereafter.
- Transitions amongst fine structure levels of a metastable term are the classic example where the importance of IIE has been identified: $\Delta E \ll I_{z+}$ except for $z+ \gg 1$.
    - It is this scenario that originally motivated this work on IIE: knowledge of these transitions is required for *ic*-resolved GCR

Outline

Maximum Metastable Population Scans

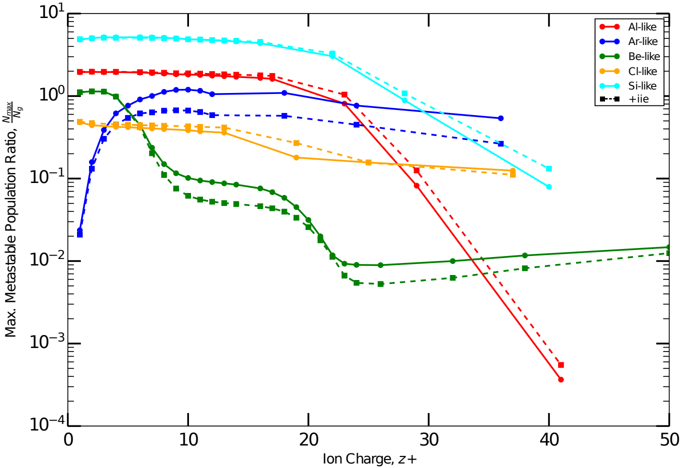


Figure : $N_{\mathrm{e}} = 10^{13}$ cm^{-3}, and $T_{\mathrm{e}} \equiv T_{\mathrm{i}}$ is given by the ionization potential of each species in each isoelectronic sequence. "+iie" indicates the addition of *proton*-impact collisions only in this instance; more projectile species will easily be added in the future once the machinery within ADAS is implemented fully.

Interesting Sequence: Be-like (I)

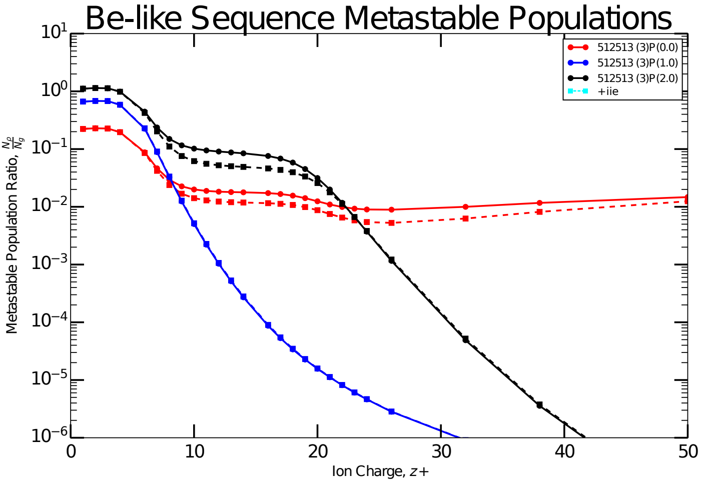
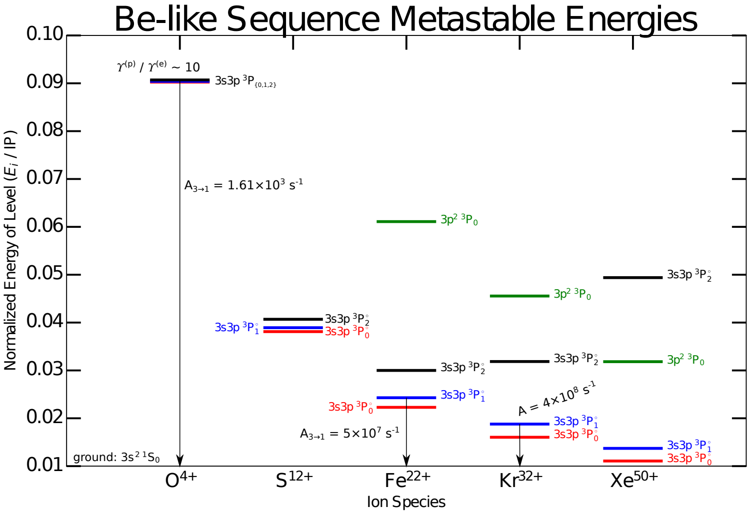
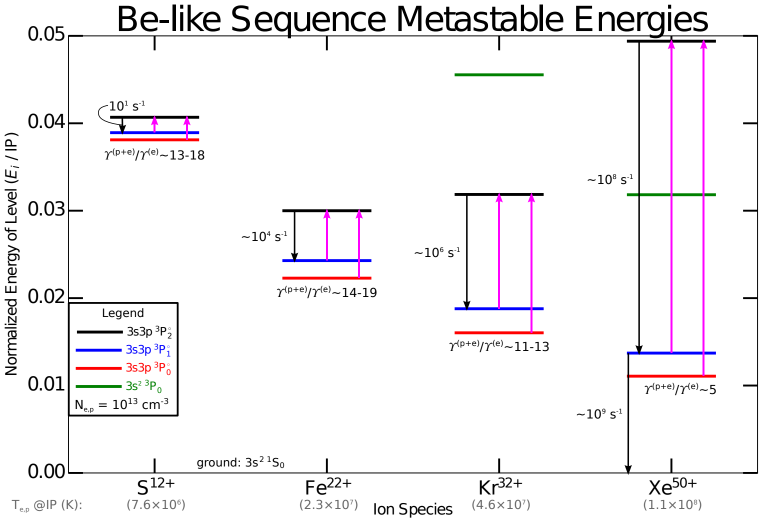


Figure : $N_{\rm e} = 10^{13}$ cm^{-3}, and $T_{\rm e} \equiv T_{\rm i}$ is given by the ionization potential of each species in each isoelectronic sequence. "+iie" indicates the addition of *proton*-impact collisions only.

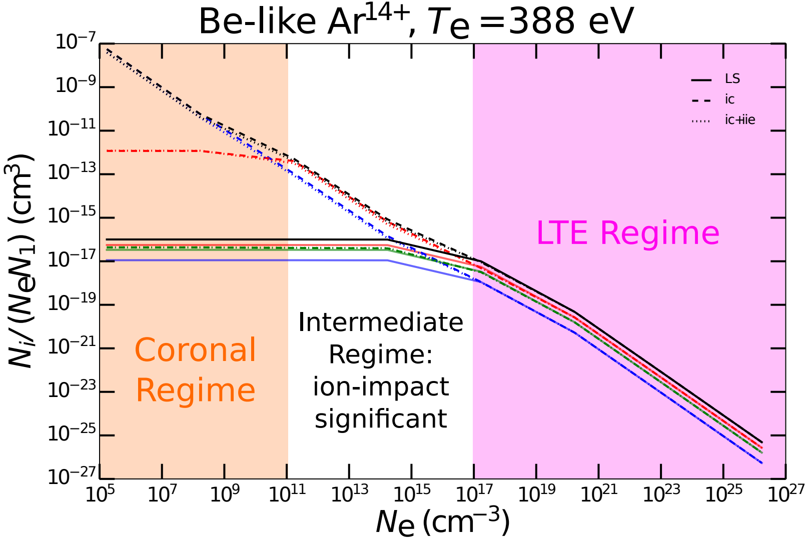
Interesting Sequence: Be-like (II)



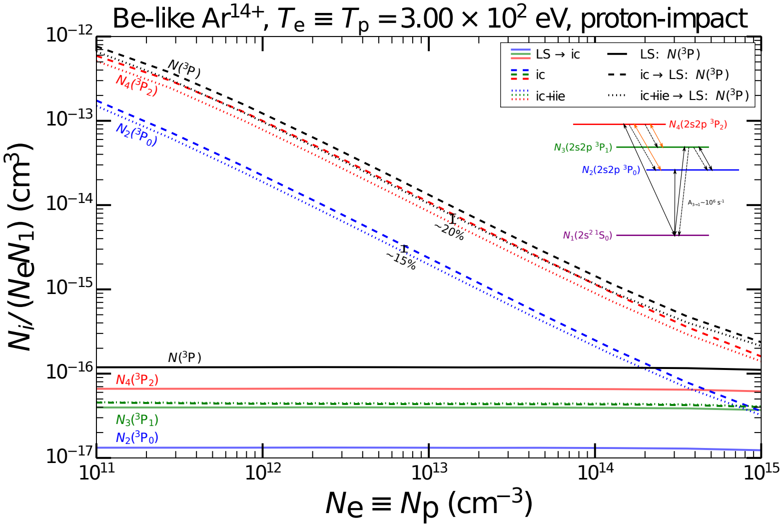
Interesting Sequence: Be-like (III)



Be-like Example Ion: Ar^{14+}



Ar^{14+} in Collisional-Radiative Regime



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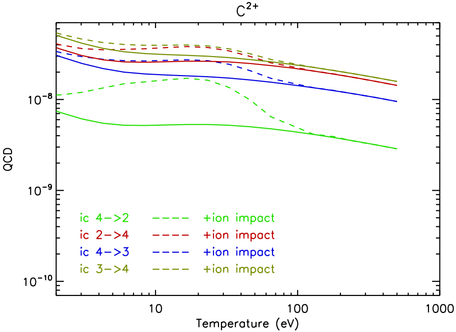
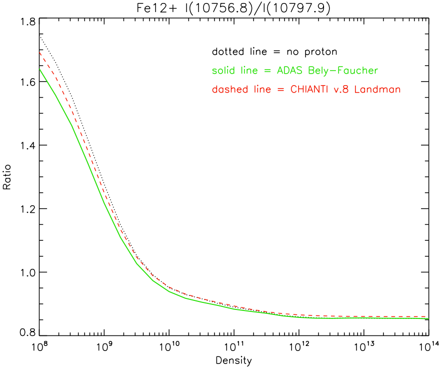
Preliminary Applications (I)



$Q_{\rm CD}$ coefficients are used in GCR atomic population modelling and are of importance when establishing the ionization balance, amongst other things.

Credit: Alessandra Giunta



Line ratios in Fe ions for solar physics are sensitive to proton-impact effects (well known in astrophysics).

Preliminary Applications (II)

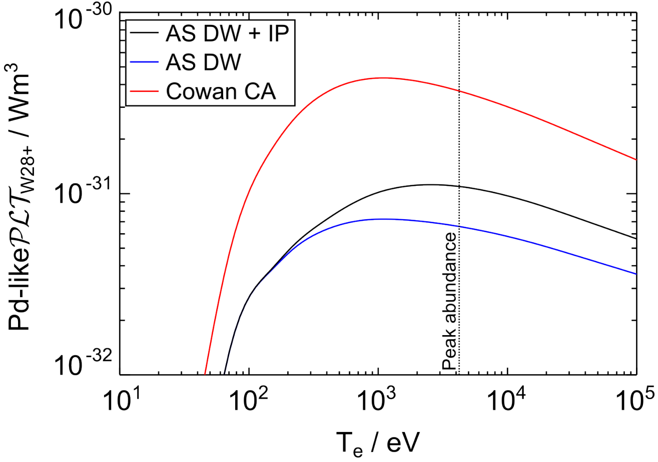


Figure : The ground configuration and term of Pd-like W^{28+} is $[Kr]4d^{10}\ {}^1S_0$, so a closed shell. Shell boundaries are conducive to the formation of many low-lying metastables. Credit: Stuart Henderson

Conclusions and Future Work

- IIE can significantly influence CR population models and their outputs, particularly at shell boundaries where there is a $^1S_0$ ground term and low-lying triplet metastables. It remains to be seen whether this is measurable in practical situations.
- However, it should be emphasised that in the majority of scenarios, this is not the case: EIE is dominant.
- When in doubt: first use the "rules of thumb" to see if IIE collisions have a chance of being significant.
  - This should be done for the transitions within the metastable terms of the system of interest and possibly high-lying *nl* states where ion-impact can contribute to redistribution.
  - Other scenarios are also conducive to IIE: transitions amongst motional Stark states in neutral beams and instances where the ion temperature exceeds the electron temperature.
- If positive, then one can undertake the more arduous task of CR modelling.
- Future: extend consideration of IIE into ionization balance predictions, and follow up on line-ratio influence.

Thanks for listening!

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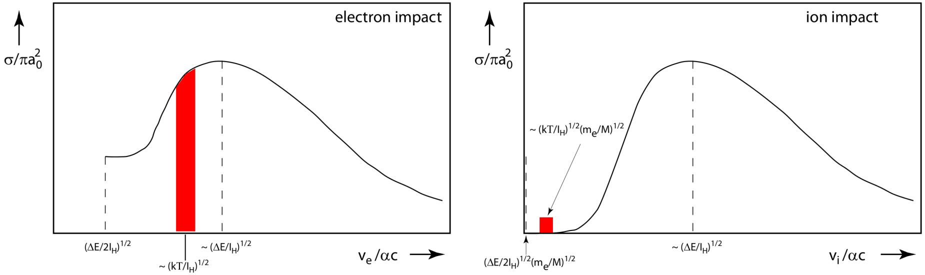
Back-up

Electron-impact vs. Ion-impact

- Discrepancies in the general structure of electron and ion impact cross-sections as well as where the thermal distributions of the colliding species lie explain why ion-impact favours small energy level differences.
- Increased projectile ion speed distributions can also help: at ITER, we will have ion temperatures $T_{\mathrm{i}} \sim 8$ keV, fast fusion alphas $E_{\alpha:\mathrm{D-T}} = 3.5$ MeV, and ionised neutral beam atoms $E_{\mathrm{NB}} \sim 1$ MeV Aymar et al. (2002).



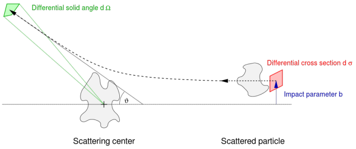
Working in atomic units (au), $\Delta E/I_{\mathrm{H}}$ is the transition energy, I_{H} is the ionization potential of hydrogen in the same units as ΔE, and σ is the cross-section for the arbitrary transition from the target ion level i to j. The temperature, T, of both the colliding ion and electron velocity distributions (red blocks) is assumed to be equal.

Calculation Technique

- The relatively large mass, m_p, of an ion projectile results in an impractically large number of partial waves in the close-coupling region near the target, meaning a *semi-classical* approach is appropriate versus a fully quantum mechanical one.
- *Coulomb excitation* as per Alder et al Alder et al. (1956): the ion projectile follows a classical trajectory determined by scattering in a Coulomb field, and the excitation probability of the target is obtained through first-order, time dependent perturbation theory.
- The Coulomb excitation differential cross-section is thus given by:

$$\mathrm{d}\sigma_{i\to j} = P_{i\to j}(\theta) \boxed{\frac{1}{4\pi}\left(\frac{z_\mathrm{t} z_\mathrm{p}}{E_\mathrm{p}}\right)^2 \csc^4(\theta/2)\mathrm{d}\Omega}, \quad (1)$$

• $P_{i\to j}(\theta)$ is the transition probability for a given trajectory, and the remainder of the theory will address its specification.
• z_t, z_p are the target and projectile charges, respectively.
• E_p is the geometric mean of the projectile kinetic energy: $E_\mathrm{p} = \sqrt{E_{\mathrm{p},i}E_{\mathrm{p},f}}$
• θ is the scattering angle in the cms frame.
• The boxed term is the classical Rutherford differential cross-section.



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The Transition Probability, $P_{i\to j}$

- First-order, time-dependent perturbation theory tells us:

$$P_{i\to j} = \frac{1}{\omega_i}\sum_{M_i M_j}\left|b_{ij}(t=\infty)\right|^2; \quad b_{ij} = \frac{1}{i\hbar}\int_{-\infty}^{\infty}\langle j\left|H(t)\right| i\rangle\, e^{i\omega t}\mathrm{d}t. \qquad (2)$$

- After a great deal of algebra and the use of $\frac{1}{|\mathbf{r}_\mathrm{p}-\mathbf{r}|} \approx \sum_\lambda P_\lambda(\hat{\mathbf{r}}_\mathrm{p}\cdot\hat{\mathbf{r}})r^\lambda/r_\mathrm{p}^{\lambda+1}$, we find for the quadrupole case:

$$P_{i\to j}(E2) = 4m_0 B(E2) z_\mathrm{p}{}^{-2} z_\mathrm{t}^{-4} E_{\mathrm{p},i} E_\mathrm{p}{}^2 \sin^4(\theta/2)\, \frac{\mathrm{d}f_{E2}}{\mathrm{d}\Omega}(\theta,\xi), \qquad (3)$$

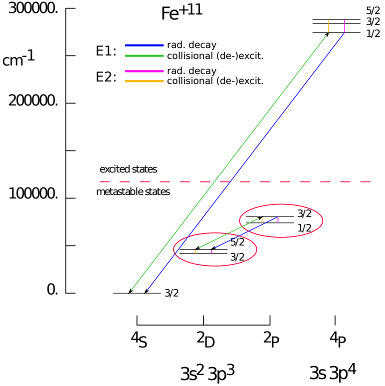
where $B(E2)$ is the reduced, quadrupole atomic transition probability that we obtain from our atomic structure calculations, m_0 is the reduced mass of the projectile and target, and ξ is the dimensionless, symmetrized adiabaticity parameter: $\xi \propto E_\mathrm{p}{}^{-3/2}$.

- $\frac{\mathrm{d}f_{E2}}{\mathrm{d}\Omega}(\theta,\xi)$ is the differential excitation cross-section function made up of classical orbital integrals that fall out of the right hand equation in 2; these integrals need to be computed numerically, and a table of pre-computed values due to Alder et al Alder et al. (1956) has been employed in numerous computer programs — an area for improvement.

Why not use a full quantal treatment for ion-impact excitation (IIE)?

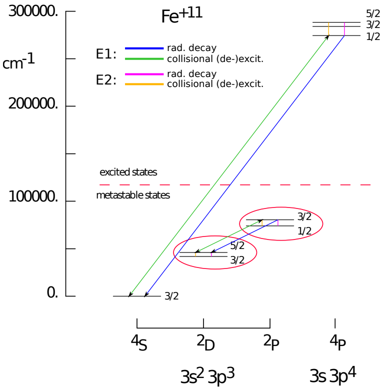
- $m_{\rm i} \gg m_{\rm e} \rightarrow$ highly oscillatory continuum ion wavefunctions
- # of partial waves scales as $\sim \sqrt{m_{\rm i}} \approx 43$
- *simplicity*: the 'thorny issues' of penetrating collisions and high energy behaviour are more easily addressed in the SC IP approach
- *accuracy*: although limited in the literature, comparisons between SC IP and quantal treatments show high level of agreement
- *expediency*: the need for IIE collision data in atomic population modelling is imminent, and in particular different collider mixes for fusion plasmas: impact by d, t, α, etc.

Motivation: *ic*-resolved GCR



- Predicting spectral line intensities, $I(\lambda)$, or fractional abundances, $f_Z(n_{\rm e}, T_{\rm e})$, of impurity species requires some form of atomic population modelling.
- *Generalized collisional-radiative* (GCR) modelling must be used when the lifetimes of groups of low lying states, called metastables, approach plasma timescales: $\tau_m \sim \tau_{T_{\rm e}}, \tau_{N_{\rm e}}$. See Summers et al. (2006).
- For medium weight species and more highly ionised ions, *LS*-coupling is not appropriate because the fine structure separation within a term becomes significant and the relative populations begin to deviate from statistical: *ic* must be used.

Motivation: *ic*-resolved GCR (continued)



- *ic*-resolved GCR will require rate coefficients for transitions between the fine-structure levels of metastable terms in an ion.
- Necessarily, the transitions will be of the **quadrupole (E2)** type: dipole excitation is excluded by parity conservation within a term.
- The relatively small energy level differences and increased ion temperatures in future devices mean ion-impact excitation can become significant.
- But where exactly?