# Kuang's Semi-Classical Formalism for Electron Capture Cross-Sections in Ion-Ion Collisions at ~MeV/amu: Application to ENA Modeling


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**Abstract:** Recent discovery by STEREO A/B of energetic neutral hydrogen is spurring an interest and need for reliable estimates of electron capture cross sections at few MeVs per nucleon as well as for multi-electron ions. Required accuracy in such estimates necessitates detailed and involved quantum-mechanical calculations or expensive numerical simulations. For ENA modeling and similar purposes, a semi-classical approach offers a middle-ground approach. Kuang's semi-classical formalism to calculate electron-capture cross sections for single and multi-electron ions is an elegant and efficient method, but has so far been applied to limited and specific laboratory measurements and at somewhat lower energies. Our goals are to test and extend Kuang's method to all ion-atom and ion-ion collisions relevant to ENA modeling, including multi-electron ions and for K-shell to K-shell transitions


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## Credits and Citations:


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## The Charge-Transfer Process

- A process in which an ion picks up one or more electrons from another atom or ion upon a collision
- In plasma/fusion and space/astrophysical applications, collision energy is not high enough (< 1 MeV) for high-energy (e.g., Born) approximations to apply; realistic estimates must rely on quantum-mechanical calculations
- Process is usually accompanied by others, like impact and radiative ionization and excitation
- Experimental data are quite limited, especially those at energies and systems (multi-electron ions) relevant to ENA modeling (for lower energies, e.g., for plasma/fusion type applications good datasets are available)
- As a result, theoretical approaches tend to vary widely in utility, applicability, efficiency as well as accuracy

## Examples from Space and Astrophysics

- In studies of x-ray emission from comets: x-rays are direct products of charge-transfer reactions between solar-wind ions and cometary neutrals (Dennerl 2010; Hasan et al. 2001)
- Between solar-wind ions and neutrals in planetary atmospheres
- Pick-ions charge-exchanging with neutrals throughout the heliosphere, its termination shock and heliopause
- Energetic neutrals –of solar origin- exchanging with 1 or more electrons with coronal single- and multi-electron ions (which is our focus here)
- Hot-cold gas interfaces, in the interstellar medium, supernovae remnants, stellar winds, superbubbles, etc.
- Low-energy cosmic-ray ions charge-changing with ISM H

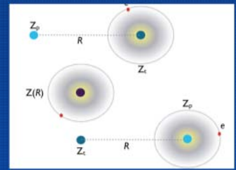
## Theoretical Approaches

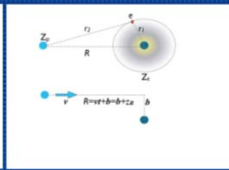
- Classical: like the Monte-Carlo many-body dynamics method (or CTMC), where trajectories for point-like masses are simulated according to Newton (or Hamilton) equations of motion (e.g., Olson & Salop 1977); crude but quite useful
- Fully quantum-mechanical: like the time-dependent close-coupling (CC) method where excited states, angular momentum/spin/isospin, and mixed states are fully described (e.g., Belkic 2009; Pindzola et al. 2007); accurate, but quite involved and time and CPU intensive even for simple collision systems (approximations of which are application dependent!)

***Applicability to space/astrophysics is wide, but appropriate theoretical/computational methodologies (choice) not so!***

## The KSC Semi-Classical Approach

- Method uses a "united-atom" concept to which the exchanged electron is always bound (reduces – asymptotically – to classical limits)



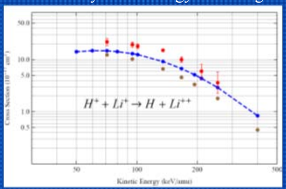

$$
\begin{aligned}
U_j(r_1,R) &= 1/\sqrt{\pi}\, Z(R)^{3/2} \exp\left(-2Z(R)r_1\right)\\
\hat{H}(r_1,R) &= \left(-\frac{1}{2}\nabla^2_{r_1} - \frac{Z}{r_1}\right) + \left(\frac{Z-Z_t}{r_1} - \frac{Z_p}{r_1}\right) + \frac{Z_t Z_p}{R}\\
E_j &= \langle U_j(r_1,R)|\hat{H}|U_j(r_1,R)\rangle\\
&= \frac{1}{2}Z^2 - \left(Z_t Z + \frac{Z_p}{R}\right) + \frac{Z_t Z_p}{R} + \\
&\quad Z_p\left(Z + \frac{1}{R}\right)\exp\left(-2ZR\right)\\
\frac{\partial E_j}{\partial Z} &= 0\\
Z(R) &= Z_t + Z_p\left(1 + 2RZ(R)\right)\exp\left(-2ZR\right)
\end{aligned}
$$

$$
\begin{aligned}
V_j(r_1,t) &= U_j(r_1,R)\exp\left(-iqv\cdot r - \frac{1}{2}iq^2v^2t\right)\\
V_k(r_2,t) &= U_k(r_2,R)\exp\left(-iq'v\cdot r - \frac{1}{2}i(q')^2v^2t\right)\\
\Phi(r_1,t) &= c_j(t)V_j(r_1,t)\exp\left(-iE_t t\right) + \\
&\quad b_k(t)\chi_k(r_2,t)\exp\left(-iE_p t\right)\\
E_p &= -\frac{1}{2}Z_p^2\,;\, E_t = -\frac{1}{2}Z_t^2\,;\, q = M_p/\left(M_p+M_t\right)
\end{aligned}
$$

$$
\begin{aligned}
i\dot{\Phi}(r_1,t) &= \hat{H}\Phi(r_1,t)\\
i\dot{b}_k(t) &= V_{kj}\exp\left(i\epsilon t\right)\\
V_{kj} &= \langle\chi_k|\hat{H} - i\partial/\partial t|V_j\rangle\\
b_k(b) &= \frac{1}{iv}\int_{-\infty}^{+\infty} dz_R\, V_{kj}\exp\left(i\epsilon z_R/v\right)\\
\epsilon &= \frac{1}{2}\left(Z_t^2 - Z_p^2\right)\\
\sigma[1s \to 1s] &= 2\pi\int_0^\infty db\, b|b_k(b)|^2
\end{aligned}
$$

$$
\begin{aligned}
b_k(b) &= \frac{2^3 Z_p^{5/2}}{iv}\int\int dQ_z dz_R\, I(Q_z,R)\times\\
&\quad \exp\left[i\left(\epsilon/v + v/2 - Q_z\right)z_R\right]\\
I(Q_z,R) &= f(D_j(R))\\
D_j(R) &= Z(Z-Z_t) - \frac{Z_p}{R}\left[1 - \left(1 - ZR\right)\times\right.\\
&\quad \left.\exp\left(-2ZR\right)\right]\\
z_R &\to 0:\\
b_k(b) &= \frac{2^4 Z_p^{5/2}}{iv} Z^{3/2}\left[\left(Z - Z_t\right) I_{21}(b) - \right.\\
&\quad \left. Z\, I_{21} - Z\, I_{21} - 2ZD_j(b)\, I_{22}(b)\right]
\end{aligned}
$$

- KSC method is consistent with OBK theory in how the cross sections scale with the collision system's energy and charge



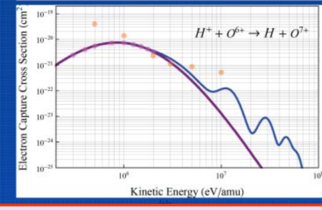

***Calculated 1s-1s transitions using the KSC method (Kuang 1991a, blue symbols); red are measurements of Sewell et al. (1980) for the total cross section, and brown are calculations based on the POHCE (QM) method by Winter (1987)***

## Application to ENA modeling

- Slight modification to the method using an effective charge and ionization potentials (Arnaud & Rothenflung 1985) to model 1s to 1s transitions in proton on multi-electron ions (Kuang 1992):

$$
\begin{aligned}
D_j(R) &= \langle U_j(r_1,R)\left|\frac{Z-Z_t}{r_1} - \frac{Z_p}{r_1}\right|U_j(r_1,R)\rangle\\
E_j &= -\frac{1}{2}Z^2 + D_j \;\&\; Z_t \Leftarrow \sqrt{2\mathcal{E}_{[1s\to 1s]}}:
\end{aligned}
$$

$C^{5+}$: 6.001; $N^{6+}$: 7.002; $O^{7+}$: 8.001; $Ne^{9+}$: 10.005
$C^{4+}$: 5.370; $N^{5+}$: 6.372; $O^{6+}$: 7.373; $Ne^{8+}$: 9.380
$C^{3+}$: 5.021; $N^{4+}$: 6.020; $O^{5+}$: 7.017; $Ne^{7+}$: 9.020
$C^{2+}$: 4.887; $N^{3+}$: 5.884; $O^{4+}$: 6.880; $Ne^{6+}$: 8.881
$C^{1+}$: 1.507; $N^{2+}$: 2.025; $O^{3+}$: 2.537; $Ne^{5+}$: 3.556




***Calculated 1s-1s transitions using the KSC method (magenta curve and light magenta symbols (Kuang 1992) with approximation and without (blue curve); light orange symbols are CTMC estimates used in Mewaldt et al. (2009)***

- Improvement and extension of the KSC method to all ion-ion and ion-atom systems relevant to ENA modeling, including multi-electron systems and K-shell (Kuang 1991b) transitions

$$
\begin{aligned}
b_k(b) &= b_k^{(1)}(b) + b_k^{(2)}(b) + b_k^{(3)}(b) + \cdots\\
b_k^{(1)}(b) &= \frac{1}{iv}\int dz_R\, \exp\left(i\epsilon z_R/v\right)\times\\
&\quad \langle V_k\left|\frac{Z_p}{r_2} - D_j(R)\right|V_j\rangle\\
b_k^{(2)}(b) &= \frac{1}{iv}\int dz_R\, \exp\left(i\epsilon z_R/v\right)\times\\
&\quad \langle V_k\left|\frac{Z-Z_t}{r_1}\right|V_j\rangle\\
b_k^{(3)}(b) &\propto \langle\chi_k|i\partial/\partial t|V_j\rangle\\
&\vdots
\end{aligned}
$$