Database for Imaging and Transport with Energetic Neutral Atoms (ENAs)

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Energetic neutral atoms (ENAs) are significantly more energetic than local thermal environment:
- Planetary atmosphere $E \sim 0.01$ eV
- Local interstellar cloud $E \sim 0.1$ eV
- Local interstellar bubble $E \sim 100$ eV

ENAs result from charge exchange (CX) collisions between hot ions and neutral gases.

Produced in any environment with hot plasma and cold gas:
- Solar wind (SW) ions
- Magnetospheric ions

Earth ENAs
(Brandt et al., 2005)

Mars ENAs
(Brinkfeldt, et al., 2005)

Titan ENAs
(Brandt et al., 2005)
Introduction

- ENAs offer a way to image space plasmas
  - No interaction with magnetic fields
  - Plasma velocity during creation is maintained through ENAs
- ENAs may be a large source of energy deposition in astrophysical environments
- Precipitation of ENAs in planetary atmospheres induce atomic escape fluxes

Parameters needed for accurate modeling
- Energy transfer/relaxation rates
- Collision induced emissions and reactions
- Production rates of secondary hot atoms (SHAs)
- Transport/thermalization rates
- Energy balance in astrophysical systems

Accurate quantum mechanical (QM) cross sections needed to study interaction between ENAs and astrophysical environments
Atomic Collisions: Database

- Database for atomic/molecular collisions in astrophysical environments
  - Energy relaxation governed by collisional dynamics
  - Require energy-angular dependent cross sections
- Collision energy 0.01 eV-10 keV
  - Inelastic channels not considered in current energy interval
- Current QM elastic atom-atom cross sections
  - H+H
  - He+H
  - He+He
  - He+O

Asymptotic wavefunction

$$\psi(r \to \infty) \sim e^{ikz} + f(\theta) \frac{e^{ikr}}{r}$$

Scattering Amplitude

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)e^{i\delta_l} \sin \delta_l P_l(\cos \theta)$$

DCS

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$
QM cross sections compared with available laboratory data

Semi-classical Eikonal method also compared with QM results

\[ \delta(\rho) = \frac{-1}{2\hbar v} \int_{-\infty}^{\infty} U \left( \sqrt{\rho^2 + z^2} \right) dz \]

\[ f(\theta) = -ik \int_{0}^{\infty} \left[ e^{2i\delta(\rho)} - 1 \right] J_0(k\theta\rho) \rho \, d\rho \]
Atomic Collisions: Total Cross Sections

- **Total elastic cross section** \( \sigma_{EL}(E) \)
  - Cross sections available for several small energy intervals
  - No cross sections available over entire interval meV - keV
  \[
  \sigma_{EL}(E) = \int |f(\theta, E)|^2 \, d\Omega
  \]

- **Total diffusion cross section** \( \sigma_{DF}(E) \)
  - Useful for energy-momentum transfer without solving Boltzmann equation
  \[
  \sigma_{DF}(E) = \int |f(\theta, E)|^2 (1 - \cos \theta) \, d\Omega
  \]
Atomic Collisions: Probability Densities

**Probability Density**

\[ \rho(E, \theta) = \frac{2\pi \sin \theta}{\sigma(E)} |f(E, \theta)|^2 \]

**Normalized**

\[ \int_0^\pi \rho(E, \theta) \, d\theta = 1 \]

**Cumulative Probability**

\[ P(E, \theta) = \int_0^\theta \rho(E, \theta') \, d\theta' \]

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He+He

- **Scattering Angle (deg)**: 0.018, 0.050, 0.120
- **Lab Scattering Angle**: 0.018, 0.050, 0.120
- **Collision Energy (eV)**: 0, 50, 100
- **Probability Distribution**

He+H

- **Collision Energy (eV)**: 0, 50, 100
- **Scattering Angle (deg)**: 0.018, 0.050, 0.120

He+O

- **Collision Energy (eV)**: 0, 50, 100
- **Scattering Angle (deg)**: 0.018, 0.050, 0.120

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**He+H collisions**

Extremely forward peaked!

Several collisions to thermalize

Very little momentum transferred per collision
Atomic Collisions: Thermalization

Average Energy Loss Per Collision [eV]

\[ <\delta E> = E \frac{2m_pm_t}{(m_p + m_t)^2} \left( \frac{\sigma_{DF}(E)}{\sigma_{EL}(E)} \right) \]

Number of Collisions

\[ N(E_i, E_f) = \int_{E_f}^{E_i} \frac{dE}{<\delta E>} \]
Many atmospheres have significant molecular constituents.

Accurate QM atom-molecule cross sections extremely difficult to calculate:

- Complex potential surfaces
- Lots of scattering channels

Empirical scaling methods may be used for unknown atom-atom, atom-molecule collisions.

Krasnopolonsky, 2002.
Reduced energy coordinates
\[ \rho = \theta \sin \theta |f(E, \theta)|^2 \quad \tau = E\theta \]

Reduced velocity coordinates
\[ \rho = \theta \sin \theta |f(E, \theta)|^2 \quad \tau = \frac{E\theta}{\mu} \]

Universal amplitude fit
\[ |f(E, \theta)|^2 = \frac{\exp \left[ A (\log \tau)^2 + B \log \tau + C \right]}{\theta \sin \theta} \]
\[ A = -0.13 \quad B = 1.0 \quad C = 2.7 \]
Atom-molecule cross sections require a scaling of \( \rho \) to match atom-atom cross sections and the universal amplitude curve

\[
\rho(E, \theta) \rightarrow \frac{\rho(E, \theta)}{\lambda} \quad \text{where} \quad \lambda = 1.4
\]
Simple models used
- No magnetic SW
- No SW ion energy loss

\[ N_{sw} \rightarrow \text{Ion density at } R_0 \]
\[ u_{sw} \rightarrow \text{SW velocity at } R_0 \]
\[ \sigma^{cx} \rightarrow \text{CX cross section} \]
\[ n \rightarrow \text{neutral density} \]

Solar wind flux density

\[ J_{sw}(R) = N_{sw} u_{sw} \frac{R_0^2}{R^2} \exp \left( -\sum_i \int_R^\infty \sigma_i^{cx} n_i(R') \, dR' \right) \]

ENA production rate

\[ q(R) = J_{sw}(R) \sum_i \sigma_i^{cx} n_i(R) \]

Interstellar Medium

Target gas: H and He
Homogeneous distribution

Martian Atmosphere

Target gas: H, He, O, and CO_2
Non-homogeneous distribution
Monte Carlo transport

- **Transport:** Martian Atmosphere
- **Monte Carlo transport**
- **ENA Created**
- **SHA Created**
- **ENA Escape**
- **Thermalize**

**Thermalization height**

- $10^6$ particle ensemble
- $10^3 - 10^5$ collisions to thermalize
- $\sim 200$ SHAs created per ENA
Local bubble
- \( T = 10^6 \text{ K} \) (86 eV)
- Low density, \( \sim 95\% \) ionized

Local clouds
- \( T = 6000 \text{ K} \) (0.5 eV)
- High density, \( \sim 25\% \) ionized

ENAs may have large displacements during thermalization

Helium ENAs thermalize faster than hydrogen ENAs
- More energy transferred per collision
ENAs offer a way to image remote space plasmas

Accurate modeling of interactions between ENAs and astrophysical environments requires angular-energy dependent cross sections

Database of QM atomic collisions
- H+H
- He+H
- He+He
- He+O
- Collision energies 0.01 eV - 10 keV

Empirical model for unknown atom-molecule collision developed

Newly computed database used in transport of ENAs in interstellar medium and Martian atmosphere
- Forward peaked QM cross sections require several collisions and large displacements before thermalization