

The Weekly Progress

Since Nov. 10, 2018

In the autumn semester, hopefully I'll record my progress every Thursday morning

SO FAR

1. Understand why X-ray cause profound effects to ISM
2. Aquire the X-ray spectra emitted the SMBH in the center of Milky Way Galaxy several mys ago
3. Decide to focus on a cold dense cloud 8 kpc from the SMBH, thus fixing the flux
4. Figure out how KROME works, especially its X-ray module (details on <https://github.com/slowdivePTG/X-ray-chemistry/tree/master>)
5. Be able to calculate primary X-ray ionizations according to a X-ray spectra and the cross sections of certain species.

$$\zeta_k^p = \int_{E_{min}}^{E_{max}} \frac{F_X(E)}{E} \sigma_k(E) dE$$

$$F_X(E) : \text{erg} \cdot \text{cm}^{-2} \cdot \text{s}^{-1}$$

6. Learn about the cosmic ray ionization

Nov. 10, 2018

1. Trace the most important reactions using the Jacobian Matrix $pd(i,j)$

$$pd(i,j) = \frac{\partial}{\partial n(j)} \left(\frac{dn(i)}{dt} \right)$$

$$\left(\frac{dn(i)}{dt} \right)_j = n(j) \cdot pd(i,j)$$

2. Test a simple model but consider a mixture of H/He rather than H₂/He. $J_{X21} = 0.1$ for 1 mys then turn off the X-ray radiation. Plot the abundance of CH₄ with time.

For this molecular cloud test we choose the **osu_01_2007** network and the initial conditions proposed by *Wakelam & Herbst (2008)*: a constant temperature of $T = 10$ K, H₂ density of 10^4 cm^{-3} , cosmic rays ionization rate of $1.3 \times 10^{-17} \text{ s}^{-1}$, and a visual extinction of 10. The initial conditions of the species are listed in Table 7 and correspond to the EA2 model of *Wakelam & Herbst (2008)*, an high-metal environment observed in the diffuse cloud ζ Ophiuchi

```
Tgas = 1d1 !gas temperature (K)
xH = 2d4 !Hydrogen density

!user commons for opacity and CR rate
call krome_set_user_av(1d1) !opacity Av (#)E11.3,
```

```

call krome_set_user_crate(1.3d-17) !CR rate (1/s)
call krome_set_user_gas_dust_ratio(7.57d11) !gas/dust

call krome_init()
j21xs = 0d0
call krome_set_J21xray(j21xs)
print *, "J21 Xray = ", j21xs

x(:) = 1.d-20
!initial densities (model EA2 Wakelam+Herbst 2008)
x(KROME_idx_H2) = 0.5d0 * xH !In this case we actually use x(KROME_idx_H) =
0.5d0 * xH, which is not true
x(KROME_idx_He) = 9d-2 * xH
x(KROME_idx_N) = 7.6d-5 * xH
x(KROME_idx_O) = 2.56d-4 * xH
x(KROME_idx_Cj) = 1.2d-4 * xH
x(KROME_idx_Sj) = 1.5d-5 * xH
x(KROME_idx_Sij) = 1.7d-6 * xH
x(KROME_idx_Fej) = 2d-7 * xH
x(KROME_idx_Naj) = 2d-7 * xH
x(KROME_idx_Mgj) = 2.4d-6 * xH
x(KROME_idx_Claj) = 1.8d-7 * xH
x(KROME_idx_Pj) = 1.17d-7 * xH
x(KROME_idx_Fj) = 1.8d-8 * xH

!calculate elctrons (neutral cloud)
x(KROME_idx_e) = krome_get_electrons(x(:))

```

Nov. 15, 2018

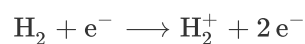
1. (From Prof. Du) The secondary ionization rate of molecular hydrogen can be approximately considered as 2 hydrogen atoms.

Related readings:

X-ray chemistry in the envelopes around young stellar objects, Stäuber 2005

X-Ray-irradiated Molecular Gas. I. Physical Processes and General Results, Maloney 1996

According to Maloney 1996, the main process in the X-ray (secondary) ionization of H_2 is:



We can assume the rate coefficient is twice the ionization rates of H , and thus include it in the network.

INCLUDE means when calculating the secondary ionization rates, we take the abundance of H :

$$n_t(\text{H}) = n(\text{H}) + 2n(\text{H}_2)$$

The modification of Fortran code in `krome_subs.f90` is shown here

```
!H2 -> H2+ + E
```

```

k(38) = rateEvaluateOnce(38)

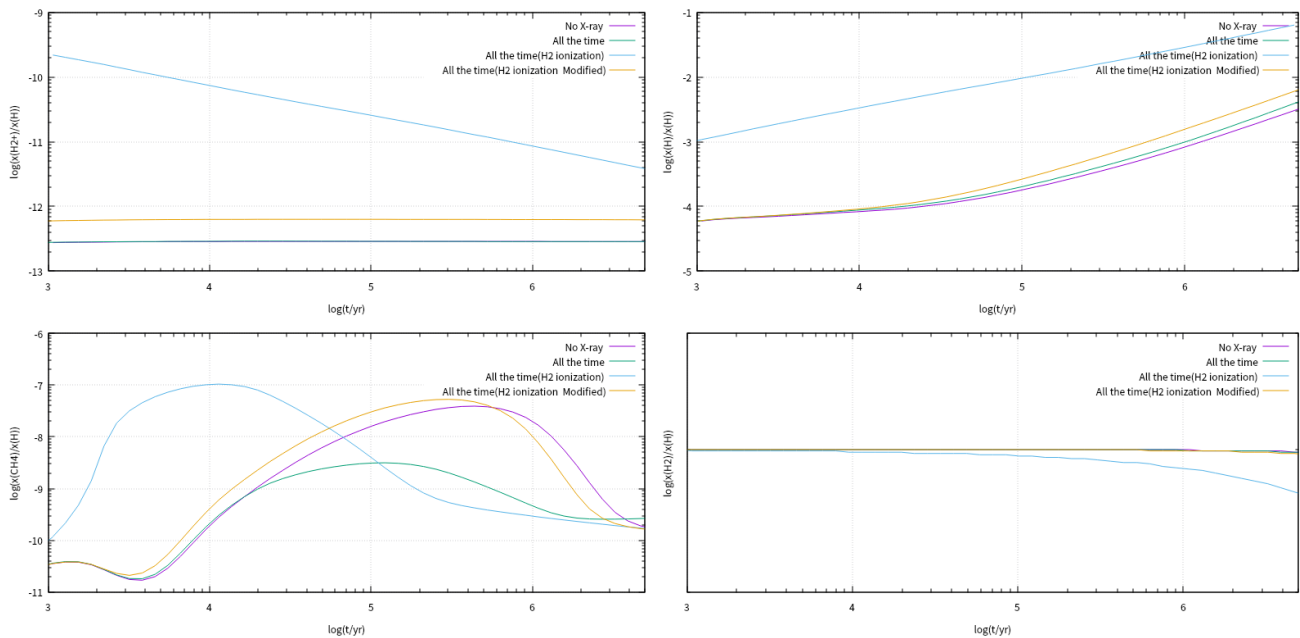
!H -> H+ + E
k(4430) = small + ((ratexH &
  * (1d0+phiH) + n(idx_He)&
  / (n(idx_H)+2*n(idx_H2)+1d-40) * ratexHe * phiH)&
  * J21xray)

k(38) = k(38) + 2*k(4430)

!HE -> HE+ + E
k(4431) = small + ((ratexHe &
  * (1d0+phiHe) + (n(idx_H)+2*n(idx_H2))&
  / (n(idx_He)+1d-40) * ratexH * phiHe)&
  * J21xray)

```

Some results are:



Obviously the ionization of H₂ becomes more significant, and the profile of CH₄ changes a lot. If we don't take $n_t(\text{H})$ the effect is even more profound.

- (NOT AT PRESENT) For heavier atoms or other molecules, we can apply the approximation with the energy E fixed, neglecting the dependence of the cross sections on energy:

$$\zeta_i = \zeta_{\text{H}_2} \frac{\sigma_i(E)}{\sigma_{\text{H}_2}(E)}$$

2. Species observants most interested in:

经常观测的分子包括CO、 HCO^+ 、 N_2H^+ 、HCN、各种碳氢化合物 C_2H 、 C_3H_3 等等。可以关注一下代表了电离度的电子丰度 x_e ，以及 H_3^+ 、 C^+ 、 OH^+ 、 H_2O^+ 等离子的丰度；OH、CH、 NH_3 、 H_2O 等也可以看看。还可以看更复杂一些的 CH_3CN 、 CH_3OH 等

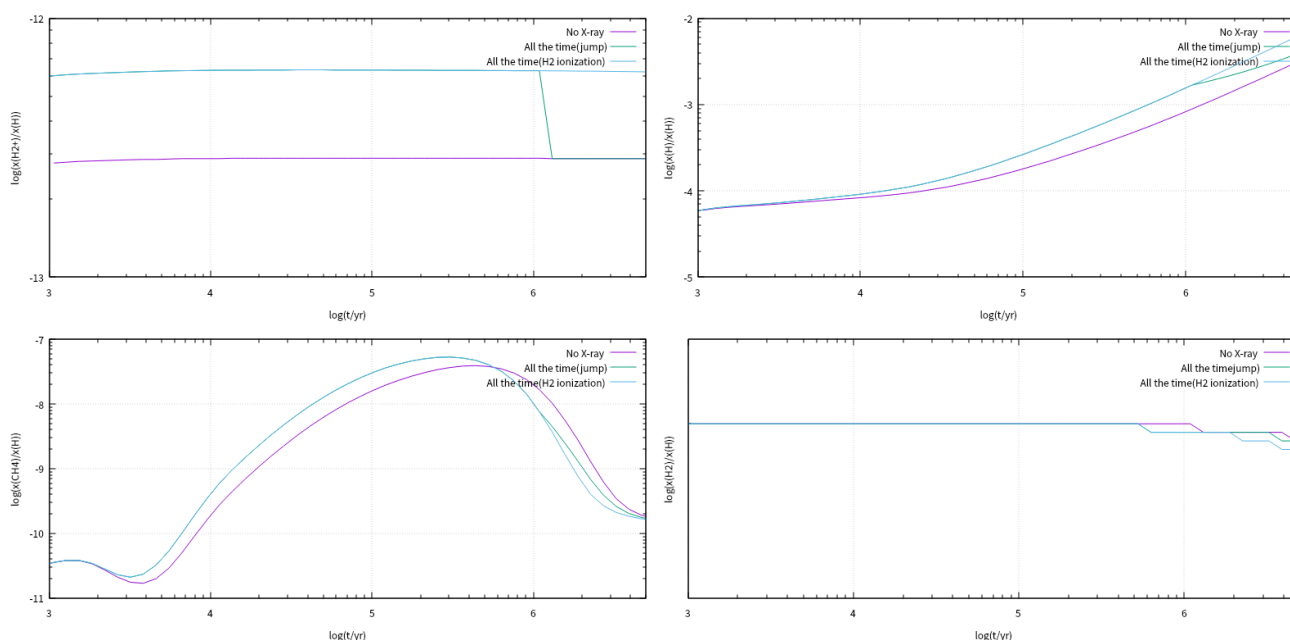
x_e is important because it decides the chemical composition and whether the heating process is sufficient

3. The simple H/He model used before:

- Abundance of CH_4 too low
- Not enough time to form H_2
- Does not include H_2 formation on **grains**

Therefore it is not reasonable enough, and I shall focus on the new H_2/He model to see what will happen if I turn off the X-ray after 1 mys.

Without H_2 formation on **grains**, there seems no jump in the abundance of CH_4 , which is shown in the plot.



Nov. 22, 2018

1. More details on secondary ionization

The secondary ionization rate for H (Stäuber 2005, Maloney 1996,):

$$\zeta_H^{(2)} = \int_{E_{min}}^{E_{max}} \frac{F(E)}{E} N_{sec}(E, x_e) \sigma(E) dE$$

$$N_{sec}(E, x_e) = \frac{E - E_{th}}{W(E)} \approx \frac{E}{W(E)}$$

$N_{sec}(E)$ is the number of secondary **ionizations** per unit energy produced by primary photoelectrons
 $W(E)$ is the mean energy expended to produce an ion pair through rapid electron process

A BIG MISTAKE HERE LAST WEEK!

$N_{sec}(E)$ is not the number of secondary electrons but the number of ion pairs produced by a secondary electron. **WE DON'T COUNT ELECTRONS HERE!**

More comments on the formula

- $W(E)$ is nearly independent of E if $E > 200$ eV, which is easy to satisfy in our case
- $N_{sec}(E, x_e)$ is dependent on x_e . When $x_e > 1\%$, the energy in photoelectrons will be mainly lost to Coulomb Interaction with ambient thermal electrons. In our case, $n_e/n_H < 10^{-4}$. For weakly ionized gases, $\approx 40\%$ of the primary electron energy will be used for ionization (Krolik 1983, Shull 1985), then for a secondary electron with energy 1 keV, the number of H it can ionize is:

$$N = \frac{0.40 \times 1 \text{ keV}}{13.6 \text{ eV}} \approx 30$$

More precise calculation (Glassgold & Langer 1973, Dalgarno 1999, Glassgold 2012) shows that in $H_2 + He$ neutral gas, 47% of energy goes to ionization, 47% in H_2 and He excitation, the rest goes for heating. $N_{sec}(E) \approx 27$ and thus we can take $W(E) \approx 37$ eV.

The formula I actually use

$$\zeta_{tot}^i = \zeta_p^i + \sum_{j=H,He} \frac{n_j}{n_i} \zeta_p^j \langle \phi^i \rangle$$

- The numbers of secondary ionization of H and He per primary ionization are taken from Shull 1985

$$\phi^H(E, x_e) = \left(\frac{E}{13.6 \text{ eV}} - 1 \right) 0.3908 (1 - x_e^{0.4092})^{1.7592}$$

$$\phi^{He}(E, x_e) = \left(\frac{E}{24.6 \text{ eV}} - 1 \right) 0.0554 (1 - x_e^{0.4014})^{1.660}$$

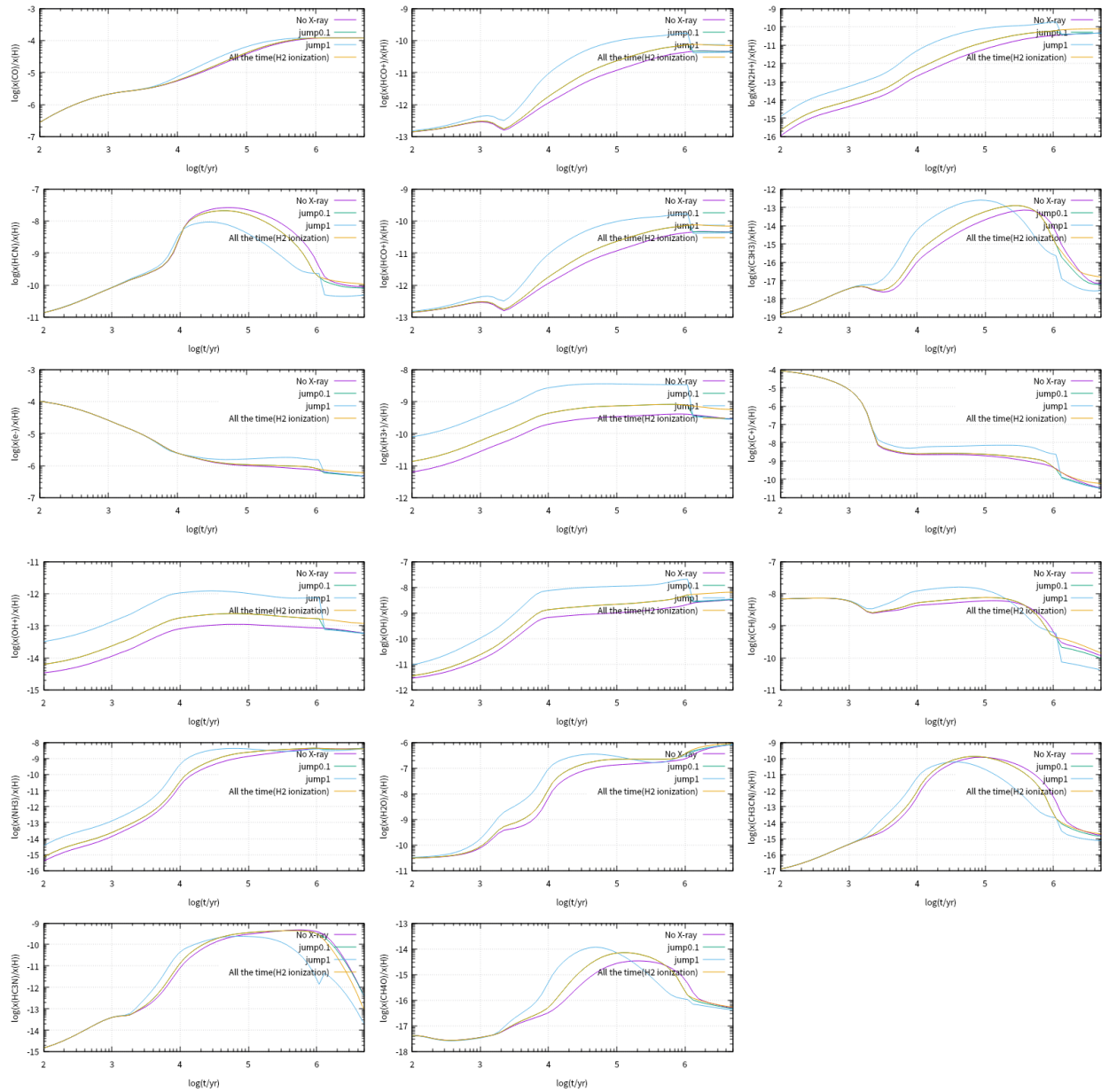
- Can be rewritten like this:

$$\zeta_{tot}^H = \zeta_p^H (1 + \langle \phi^H \rangle) + \zeta_p^{He} \frac{n_{He}}{n_H} \langle \phi^H \rangle$$

$$\zeta_{tot}^{He} = \zeta_p^{He} (1 + \langle \phi^{He} \rangle) + \zeta_p^H \frac{n_H}{n_{He}} \langle \phi^{He} \rangle$$

which average ϕ over the X-ray spectrum $F(E)$

2. Test all the species listed last week



Nov. 29, 2018

1. Recalculate the ionization rate using the primal formula

$$\zeta_{tot}^H = \zeta_p^H + \frac{n_{He}}{n_H} \int_{E_{min}}^{E_{max}} \frac{F(E)}{E} e^{-\tau(E)} \phi^H \sigma_{He}(E) dE + \int_{E_{min}}^{E_{max}} \frac{F(E)}{E} e^{-\tau(E)} \phi^H \sigma_H(E) dE$$

rather than the simplified one

$$\zeta_{tot}^H = \zeta_p^H (1 + \langle \phi^H \rangle) + \zeta_p^{He} \frac{n_{He}}{n_H} \langle \phi^H \rangle$$

and compare the results.

When we set $n_H = 2 \times 10^4 \text{ cm}^{-3}$, $n_{He} = 2 \times 10^3 \text{ cm}^{-3}$, $J_{X21} = 0.1$, $T = 160 \text{ K}$, we get

$$\begin{aligned}\zeta_{\text{H}} &= 4.09 \times 10^{-18} \text{ s}^{-1}, & \zeta_{\text{He}} &= 3.61 \times 10^{-18} \text{ s}^{-1} & (\text{Primal}) \\ \zeta'_{\text{H}} &= 7.23 \times 10^{-18} \text{ s}^{-1}, & \zeta'_{\text{He}} &= 6.07 \times 10^{-18} \text{ s}^{-1} & (\text{Simplified}) \\ \frac{\zeta_{\text{H}}}{\zeta'_{\text{H}}} &\approx \frac{\zeta_{\text{He}}}{\zeta'_{\text{He}}} \approx 0.56\end{aligned}$$

Since we take $E_{\min} = 2 \text{ keV}$, $E_{\max} = 10 \text{ keV}$, and in our case, $F(E) \propto E^{-1.5}$, $\sigma(E) \propto E^{-3}$, $\phi(E, x_e) \propto E$, $e^{-\tau(E)} \sim 1$, we have

$$\zeta^{(2)} = \int_{E_{\min}}^{E_{\max}} \frac{F(E)}{E} \phi(E) \sigma(E) dE = F_0 \phi_0 \sigma_0 \cdot \int_2^{10} E^{-4.5} dE = \frac{2^{-3.5} - 10^{-3.5}}{3.5} F_0 \phi_0 \sigma_0 \approx 0.025 F_0 \phi_0 \sigma_0$$

and

$$\begin{aligned}\int_{E_{\min}}^{E_{\max}} \frac{F(E)}{E} \sigma(E) dE &= F_0 \sigma_0 \int_2^{10} E^{-5.5} dE \approx 0.0098 F_0 \sigma_0 \\ \int_{E_{\min}}^{E_{\max}} F(E) \phi(E) dE &= F_0 \phi_0 \int_2^{10} E^{-0.5} dE \approx 3.50 F_0 \phi_0 \\ \int_{E_{\min}}^{E_{\max}} F(E) dE &= F_0 \int_2^{10} E^{-1.5} dE \approx 0.078 F_0 \\ \Rightarrow \zeta^{(2)'} &\approx \frac{0.0098 F_0 \sigma_0 \cdot 3.50 F_0 \phi_0}{0.078 F_0} \approx 0.044 F_0 \phi_0 \sigma_0 \approx 0.57 \zeta^{(2)}\end{aligned}$$

2. Why does KROME use a simplified formula to calculate the total ionization rate?

- $\zeta_p^{\text{H}}, \zeta_p^{\text{He}}$ are stored in data-files `rateH.dat` and `rateHe.dat` (column density v.s. primary ionization rate)
- To calculate $\zeta^{(2)}$ the program needs to read $x_e, n_{\text{H}}, n_{\text{He}}$ for each calculation
- By using the simplified formula, we may avoid integration

Here is part of the codes (`krome_subs.f90`):

```
T = Tgas
Trad = 2d4
ncolH = num2col(n(idx_H),n(:))
ncolHe = num2col(n(idx_He),n(:)) !number density to column density
logHe = log10(ncolHe) !take log
logH = log10(ncolH)
xe = min(n(idx_e) / (get_Hnuclei(n(:)) + 1d-40), 1d0)
user_xray_H = fit_anysub2D(user_xray_H_anysubx(:), &
    user_xray_H_anysuby(:), &
    user_xray_H_anysubz(:, :), &
    user_xray_H_anysubxmul, &
    user_xray_H_anysubymul, &
    logH, logHe-logH)
!linear interpolation to find the proper rate for the column density
phiH = .3908d0*(1e0-xe**.4092)**1.7592 * 327.832286034056d0 ! avoid
integration
ratexH = 1d1**user_xray_H
```

```

user_xray_He = fit_anytab2D(user_xray_He_anytabx(:), &
    user_xray_He_anytaby(:), &
    user_xray_He_anytabz(:, :), &
    user_xray_He_anytabxmul, &
    user_xray_He_anytabymul, &
    logH, logHe-logH)
phiHe = .0554d0*(1d0-xe**.4614)**1.666 * 180.793458763612d0
ratexHe = 1d1**user_xray_He

k(:) = small !initialize coefficients

!H -> H+ + E
k(1) = small + ((ratexH &
    * (1d0+phiH) + n(idx_He) &
    / (n(idx_H)+1d-40) * ratexHe * phiH) &
    * J21xray)

!HE -> HE+ + E
k(2) = small + ((ratexHe &
    * (1d0+phiHe) + n(idx_H) &
    / (n(idx_He)+1d-40) * ratexH * phiHe) &
    * J21xray)

print ' (a10,E15.8) ', "XrateH:", log10(k(1))
print ' (a10,E15.8) ', "XrateHe:", log10(k(2))
coe(:) = k(:) !set coefficients to return variable

```

Dec. 5, 2018

1. Try to repeat some results in former papers...but pretty difficult to do

- Krolik 1983 did not consider the X-ray ionization of H_2

Dec. 12 review: Actually, H_2 ionization is considered with an approximate model (Brown and Gould's 1970)

- Those who have considered the x-ray ionization of H_2 usually have too complex physical problems and models, which means they are not easy to fully understand and repeat within hours
- The model we consider is simple and does not include heating/cooling process and totally ignore UV-photon process

2. Add molecular hydrogen formation process to the network (from react_primordial, primordial rates from several authors mostly based on Abel et al. 1997 + Grassi et al. 2014)

Dec. 12, 2018

1. Reread and try to repeat the results in Krolik 1983.

[A Review on Krolik 1983](#)

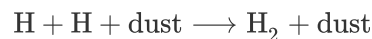
- Modify the codes

- Initial abundances
 - Longer time period (steady-state solutions) $\Delta t = 10^8$ yrs
(Strange tendency appears when $\Delta t > 10^8$ yrs, abundances of some species changes rapidly)
 - Set two branches for H_2 ionization & dissociation
 - Add H_2 formation process on grains
 - Step 1. Still use the power law spectrum,
 - It is the total ionization rate rather than the detail of the spectrum that is the most important to the chemistry
2. A new paper on the enhanced molecular ionization in the central molecular zone of our Galaxy
[Molecular Ionization Rates and Ultracompact Dark Matter Minihalos, Silk, J. 2018, PRL](#)

Dec. 17, 2018

1. Grain Process

- It's important to find out how H_2 molecules form on the grain surface as well as how KROME deal with the process



- Theoretically, KROME uses

$$\frac{dn_{\text{H}_2}}{dt} = \frac{\pi}{2} n_{\text{H}} v_g \sum_{j \in [\text{C}, \text{Si}]} \sum_i n_{ij} a_{ij}^2 \epsilon_j(T, T_i) \alpha(T, T_i)$$

where v_g is the gas thermal velocity, a_{ij} is the size of the grain, T_i is the dust temperature, ϵ_j depends on the type of the dust and α is the sticking coefficient

- The rate is defined in the file `krome_dust.f90`

```
function krome_H2_dust(nndust, Tgas, Tdust, nH, H2_eps_f, myvgas)
  !H2 formed on dust (1/cm3/s)
  use krome_constants
  use krome_commons
  real*8 :: H2_dust, krome_H2_dust, Tgas, Tdust(:)
  real*8 :: myvgas, H2_eps, nndust(:), nH, H2_eps_f
  integer :: i

  H2_dust = 0.d0
  do i = 1, size(Tdust)
    H2_eps = H2_eps_f(Tgas, Tdust(i))
    H2_dust = H2_dust + 0.5d0 * nH * myvgas * nndust(i) &
      * krome_dust_asize2(i) &
      * pi * H2_eps * stick(Tgas, Tdust(i))
  end do

  krome_H2_dust = H2_dust
```

```
end function krome_H2_dust
```

as well as related functions. Again in `krome_ode.f90` this rate is added to the total rate of H_2 formation. The process is shown in `kromeobj.py` where

```
#add H2 formation on dust
if(self.useDustH2const):
    if("H"==specs[idnw].name): x += " - 2d0*nH2dust"
    if("H2"==specs[idnw].name): x += " + nH2dust"
```

It seems that the bug comes from the `nH2dust` , of which the output is `NAN`

2.