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.

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

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

6. Learn about the cosmic ray ionization

Nov. 10, 2018

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

$$pd(i,j) = \frac{\partial}{\partial n(j)} \left(\frac{\mathrm{d}n(i)}{\mathrm{d}t} \right)$$

$$\left(\frac{\mathrm{d}n(i)}{\mathrm{d}t} \right)_j = n(j) \cdot pd(i,j)$$

2. Test a simple model but consider a mixture of H/He rather than H_2/He. $J_{X21} = 0.1$ for 1 mys then turn off the X-ray radiation. Plot the abundance of CH_4 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, H_2 density of 10^4 cm^{-3}, cosmic rays ionization rate of 1.3×10^{-17} 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,
```

```fortran
    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_Clj) = 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:

$$H_2 + e^- \longrightarrow H_2^+ + 2\,e^-$$
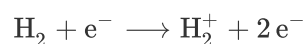
We can assume the rate coefficient is twice the ionization rates of H, and thus include it in the network.

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

$$n_t(H) = n(H) + 2n(H_2)$$

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

```fortran
    !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)
```
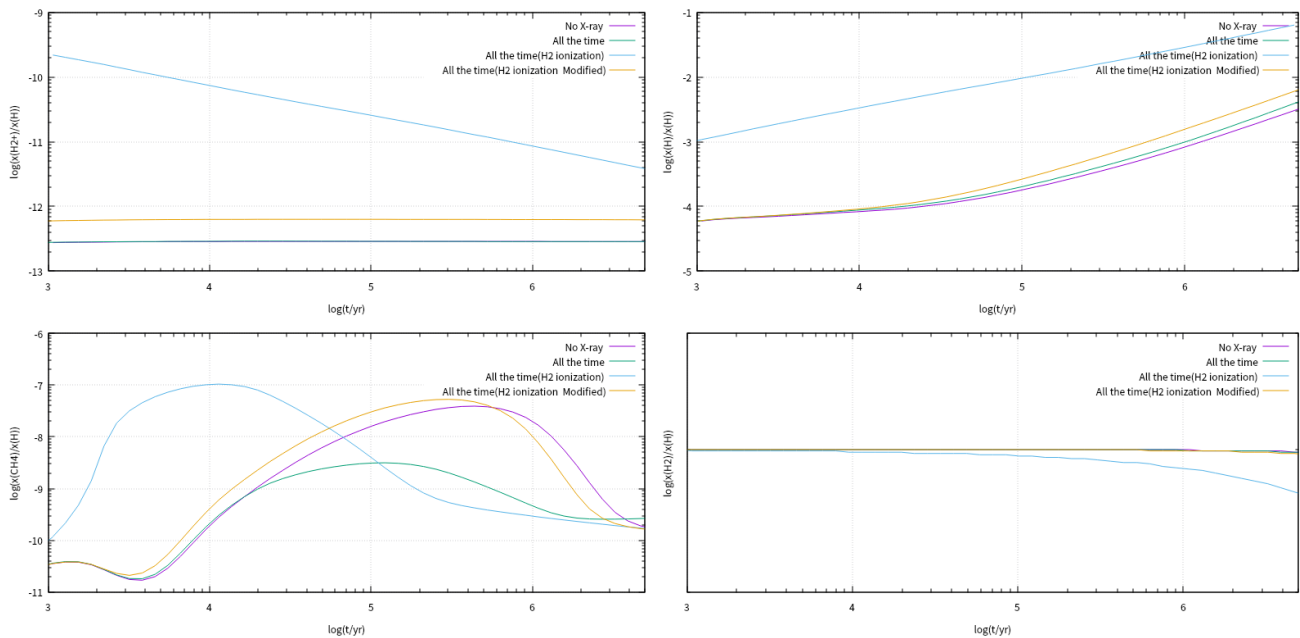
Some results are:

Obviously the ionization of H_2 becomes more significant, and the profile of CH_4 changes a lot. If we don't take $n_t(H)$ 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:

$$\zeta_i = \zeta_{H_2} \frac{\sigma_i(E)}{\sigma_{H_2}(E)}$$

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.
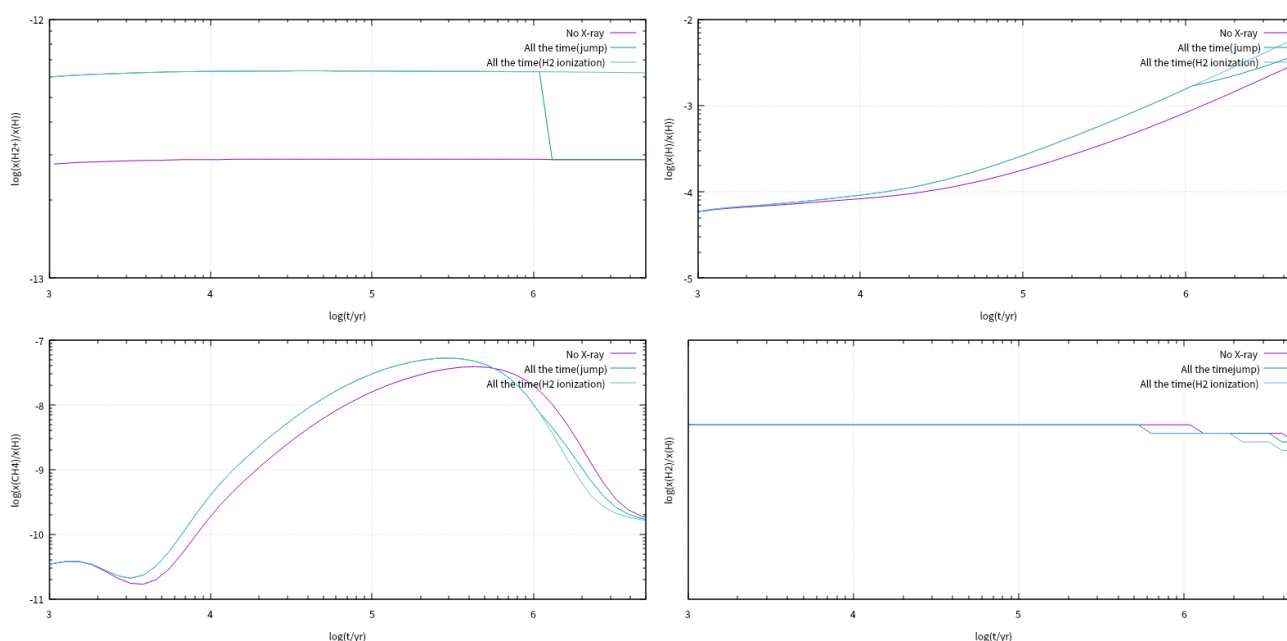
Nov. 22, 2018

1. More details on secondary ionization

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

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

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

$N_{sec}(E)$ 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 $E > 200\ \text{eV}$, which is easy to satisfied 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, $n_e/n_{\mathrm{H}} < 10^{-4}$. 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 $1\ \text{keV}$, 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 $\mathrm{H_2 + He}$ neutral gas, 47% of energy goes to ionization, 47% in $\mathrm{H_2}$ and He excitation, the rest goes for heating. $N_{sec}(E) \approx 27$ and thus we can take $W(E) \approx 37\ \text{eV}$.

The formula I actually use

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

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

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

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

- Can be rewritten like this:

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

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

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

2. Test all the species listed last week
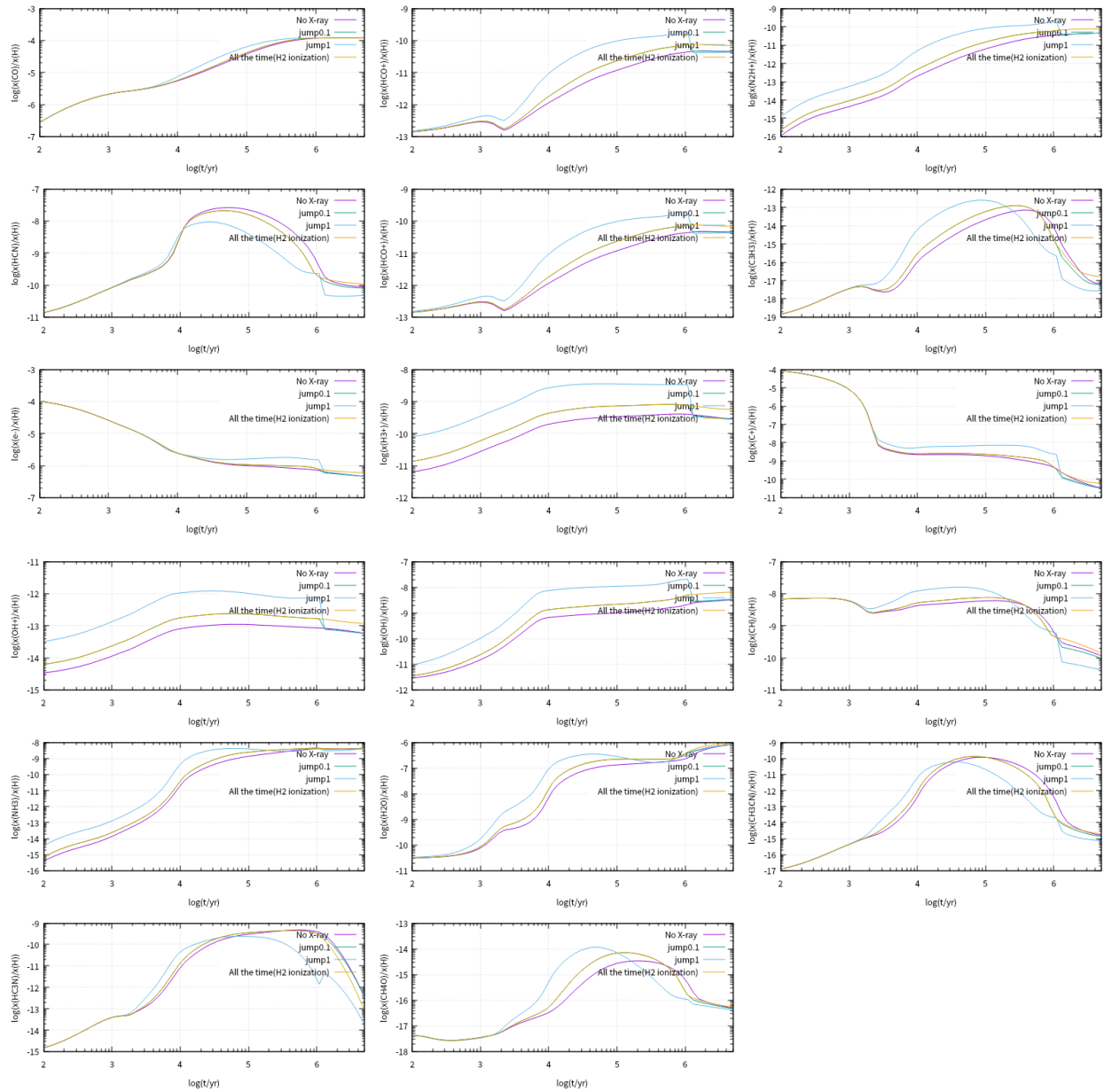
Nov. 29, 2018

1. Recalculate the ionization rate using the primal formula

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

rather than the simplified one

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

and compare the results.

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

$$\zeta_{\text{H}} = 4.09 \times 10^{-18} \text{ s}^{-1}, \quad \zeta_{\text{He}} = 3.61 \times 10^{-18} \text{ s}^{-1} \quad \text{(Primal)}$$

$$\zeta'_{\text{H}} = 7.23 \times 10^{-18} \text{ s}^{-1}, \quad \zeta'_{\text{He}} = 6.07 \times 10^{-18} \text{ s}^{-1} \quad \text{(Simplified)}$$

$$\frac{\zeta_{\text{H}}}{\zeta'_{\text{H}}} \approx \frac{\zeta_{\text{He}}}{\zeta'_{\text{He}}} \approx 0.56$$

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

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

and

$$\int_{E_{min}}^{E_{max}} \frac{F(E)}{E} \sigma(E)\mathrm{d}E = F_0 \sigma_0 \int_2^{10} E^{-5.5}\mathrm{d}E \approx 0.0098 F_0 \sigma_0$$

$$\int_{E_{min}}^{E_{max}} F(E)\phi(E)\mathrm{d}E = F_0 \phi_0 \int_2^{10} E^{-0.5}\mathrm{d}E \approx 3.50 F_0 \phi_0$$

$$\int_{E_{min}}^{E_{max}} F(E)\mathrm{d}E = F_0 \int_2^{10} E^{-1.5}\mathrm{d}E \approx 0.078 F_0$$

$$\Rightarrow \zeta^{(2)'} \approx \frac{0.0098 F_0 \sigma_0 \cdot 3.50 F_0 \phi_0}{0.078 F_0} \approx 0.044 F_0 \phi_0 \sigma_0 \approx 0.57 \zeta^{(2)}$$

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_anytab2D(user_xray_H_anytabx(:), &
    user_xray_H_anytaby(:), &
    user_xray_H_anytabz(:,:), &
    user_xray_H_anytabxmul, &
    user_xray_H_anytabymul, &
    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 !inizialize 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

$$H + H + dust \longrightarrow H_2 + dust$$
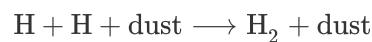
   - Theoretically, KROME uses

$$\frac{dn_{H_2}}{dt} = \frac{\pi}{2} n_H v_g \sum_{j \in [C, Si]} \sum_{i} n_{ij} a_{ij}^2 \epsilon_j (T, T_i) \alpha (T, T_i)$$

   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

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

2. Compare with the results without the H_2 formation on grains