VdW for circular Rydberg atoms

April 17, 2015

```
In [1]: %pylab inline
        path = 'C:\\Users\\r14\\Documents\\GitHub\\test\\python' #should be change to the propriate fol
        if path not in sys.path:
            sys.path.append(path)
        from imp import reload
```

```
Populating the interactive namespace from numpy and matplotlib
```

Define atom pair to calculate $C6$. Here is $|60C60C\rangle$ pair. Due to degeneration in the absence of external fields, the coupling can be propagated very long to lower l states, which explosed the basis. This was verified by enlarging the cut off of l and each time the value changed dramatically. So let's keep a constant magnetic field of ~ 10 G.

```
In [9]: # Define levels builtins to globalize the parameters
        import builtins
        builtins.n1 = 60
        builtins.l1 = n1-1
        builtins.m1 = l1

        builtins.n2 = 60
        builtins.l2 = n2-1
        builtins.m2 = l2

        builtins.Bfield = 10.e-4 # Magnetic field from experiment 1 Teslta = 10*4 Gauss
        builtins.theta = 0*pi/2 # angle between magnetic field (quantization axis) and atom pair
```

Set some criterion for the program but mainly not in use now

```
In [10]: # Setup criterion
         delta_n_max = 6
         l_max = 2
         Choice = 1e7# cut off energy for 1st order term, in Hz
         builtins.R_test = 1e-6
         Choice2 = 10* Choice

         builtins.Choice_F = 1e-1 # cut off for Stark shift
```

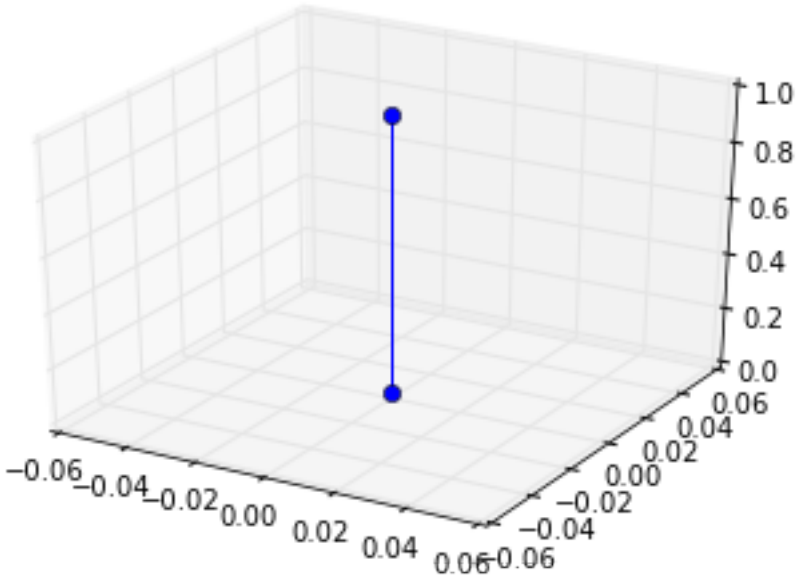
0.1 No electric field

Define electric field and set up configuration and launch the calculation from VdW file

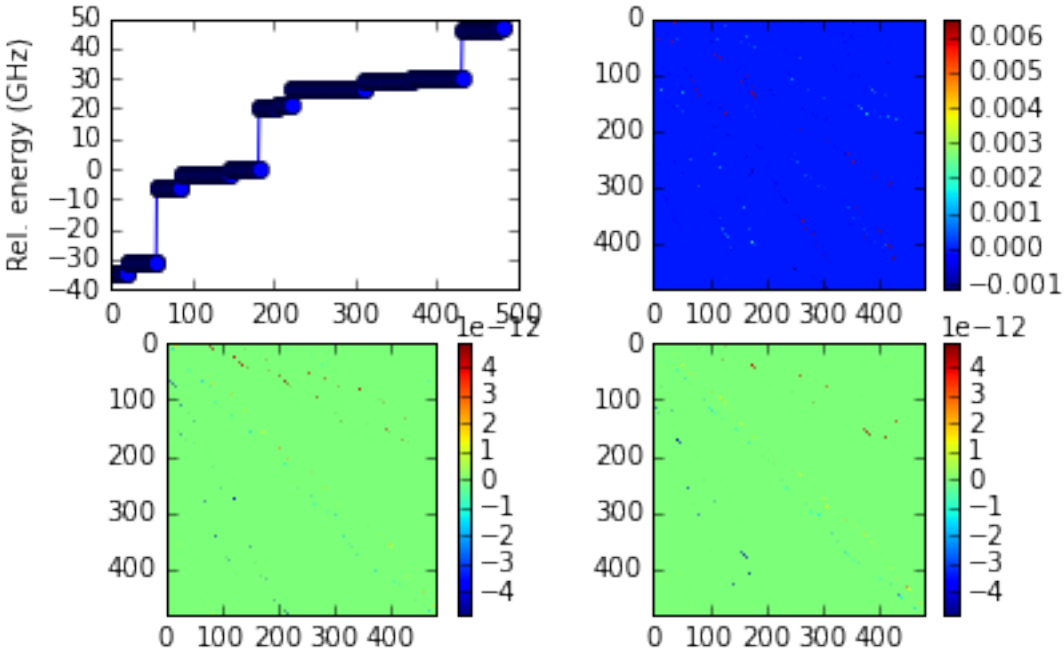
```
In [11]: builtins.Ffield = 0*1e-1 # V/cm
         builtins.theta_F = 0.001*pi/2 # angle between F field and magnetic field
         builtins.phi_F = 0.001*pi/2 # angle between F_field and magnetic field , atom pair plan
         if __name__ == '__main__':
```

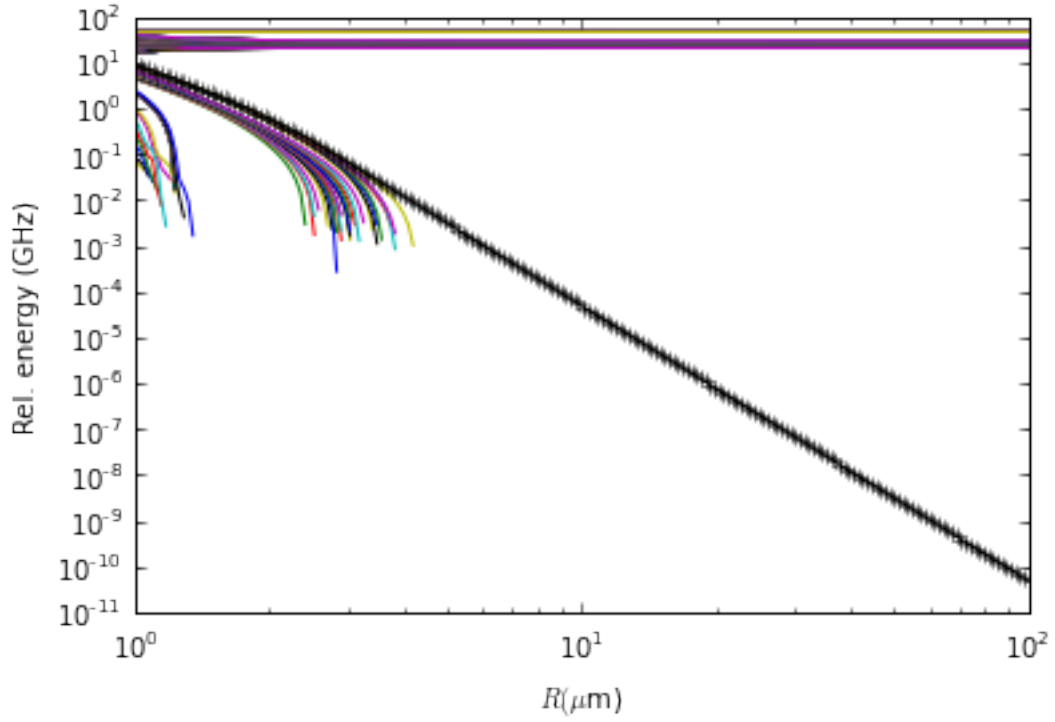
```
            if 'cal_VdW' not in locals():
                import cal_VdW
            else:
                reload(cal_VdW)
```

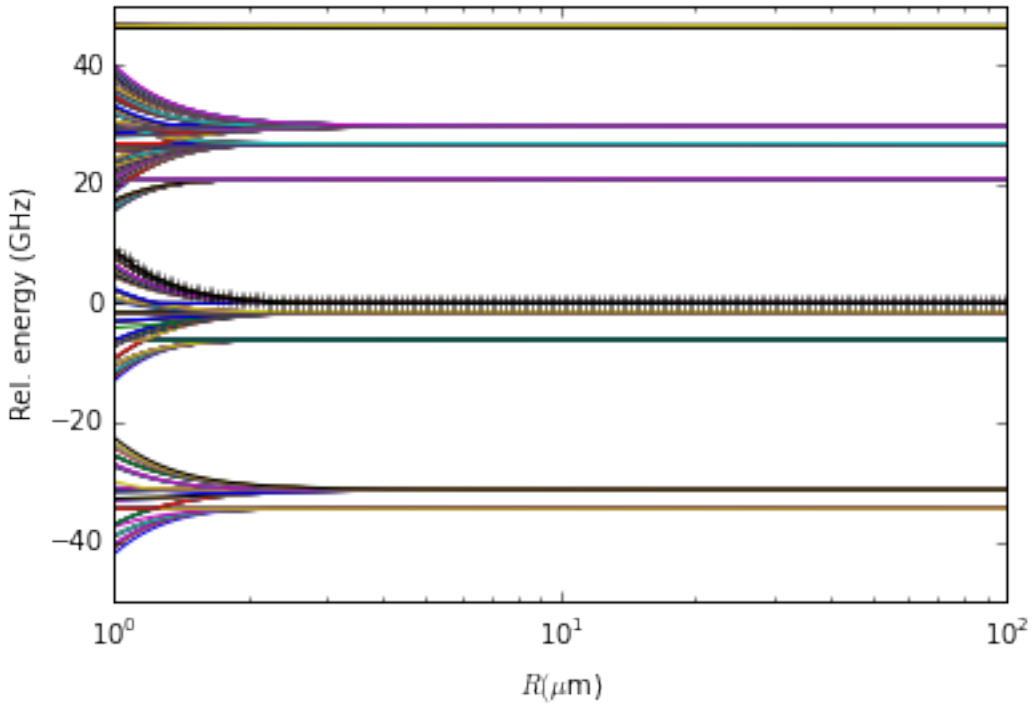
```
atom 60, 59, 59 and atom 60, 59, 59
theta = 0.0 deg
B_field = 10.0 G
F_field = 0.0 V/cm
theta_F = 0.09 deg
phi_F = 0.09 deg
```

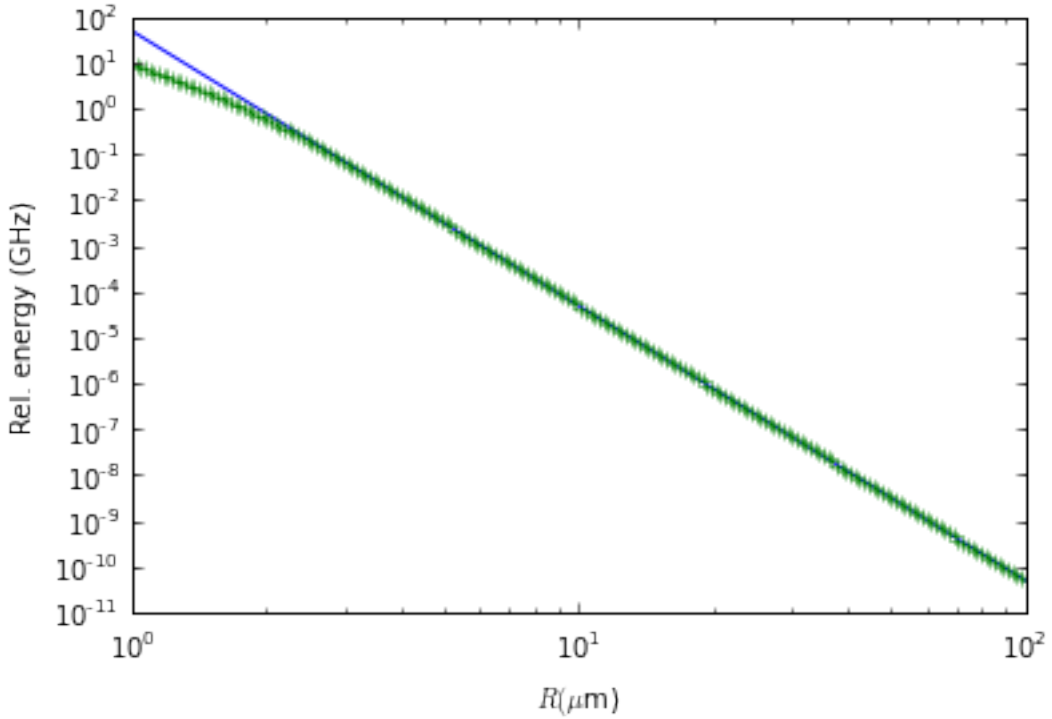


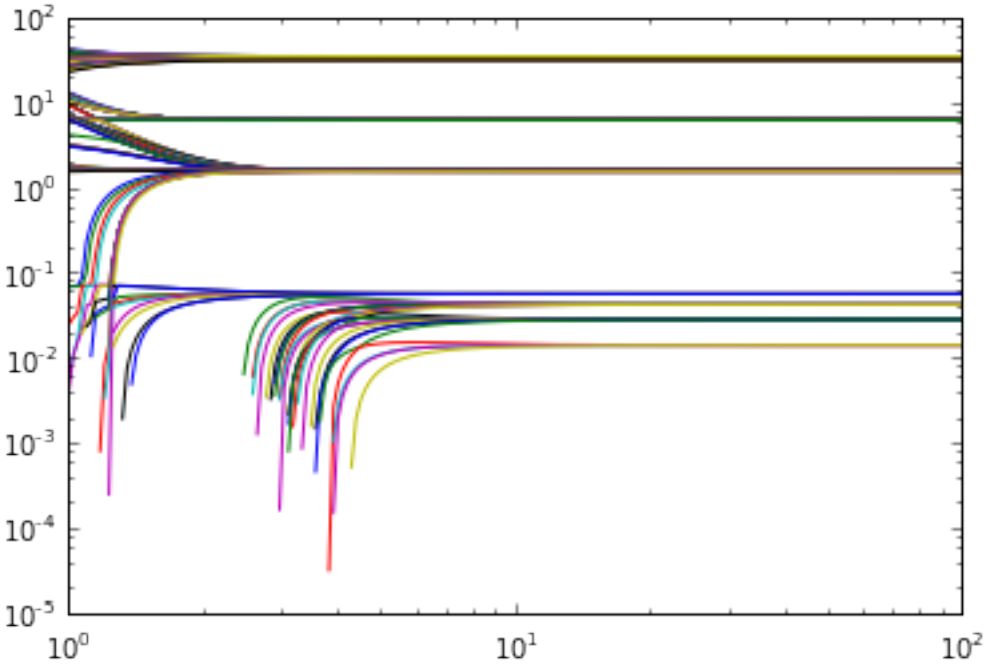

```
Matrix size: 482
C6 = [ 49.58656712   3.        ] GHz.um^6
R_1 MHz = 5.941133984965034 um
```

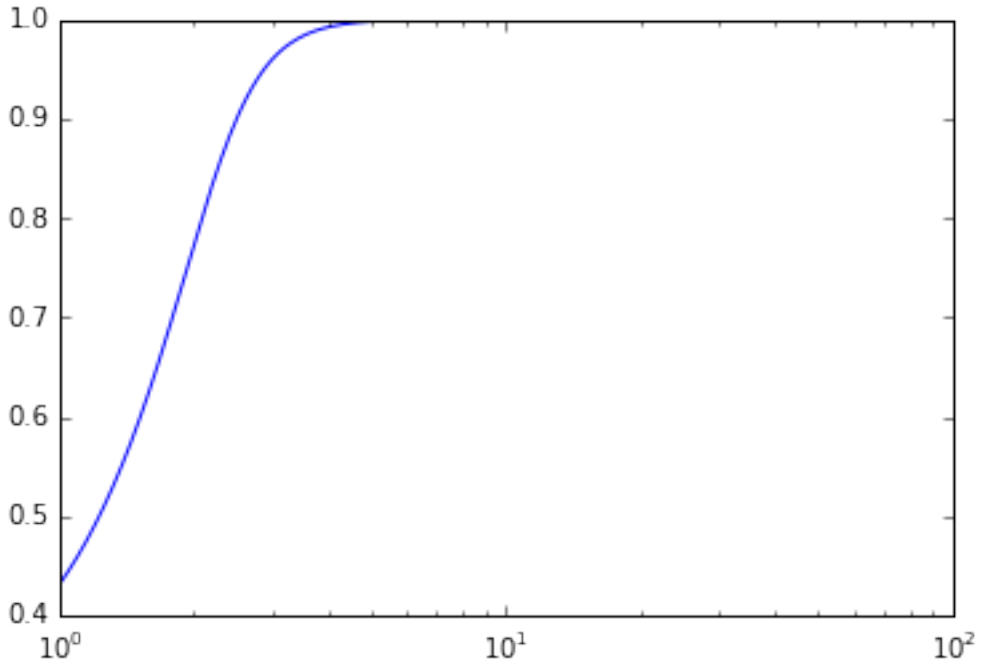

Rel. energy (GHz)
1e−12
1e−12


Rel. energy (GHz)
$R(\mu\mathrm{m})$


40
20
0
−20
−40
Rel. energy (GHz)
10^0
10^1
10^2
$R(\mu\mathrm{m})$


10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
Rel. energy (GHz)
10^0
10^1
10^2
$R(\mu\mathrm{m})$



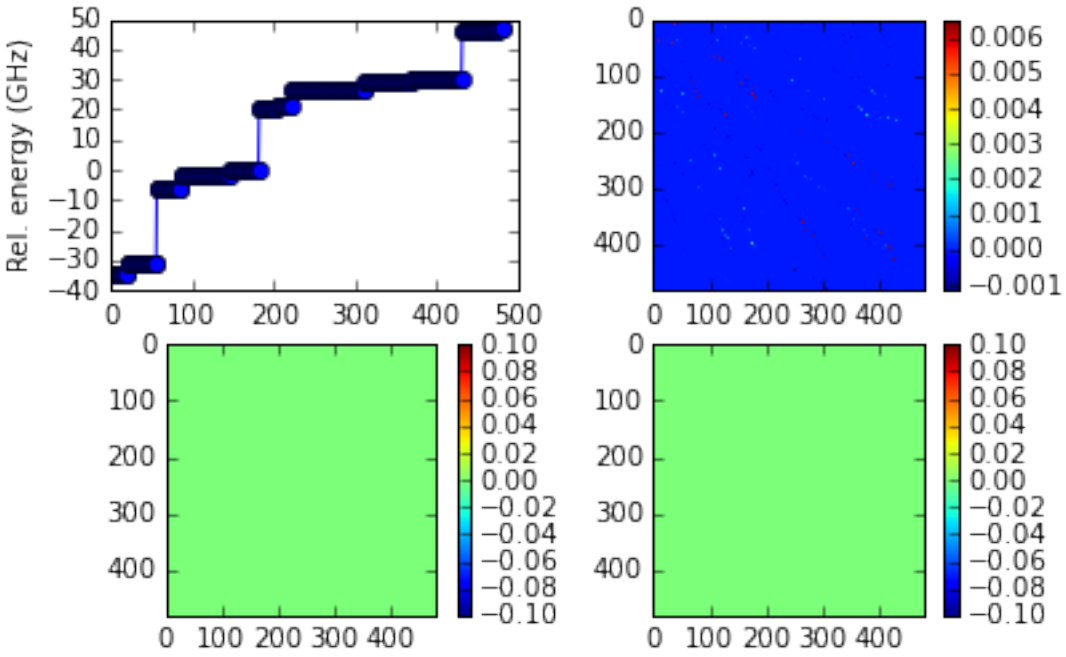


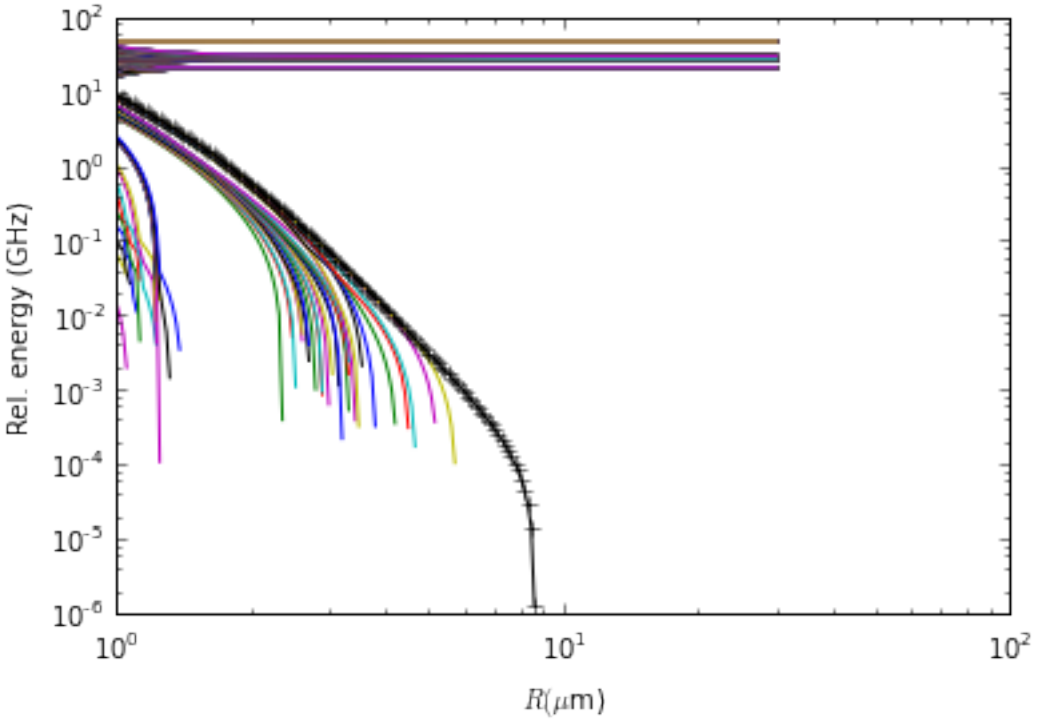
A Van der Waals potential fits well with the result up to 3 μm where the levels mixed (dipole interactions comparable to Zeeman shifts) in which the $|60C60C\rangle$ couple quasi resonance with $|60E60E\rangle$ which leads to $1/R^3$ interaction. Last figure show the contribution from $|60C60C\rangle$ where from $\sim 5\mu$m, it is nolonger pure $C_6 = 49.55$ GHz.μm^6

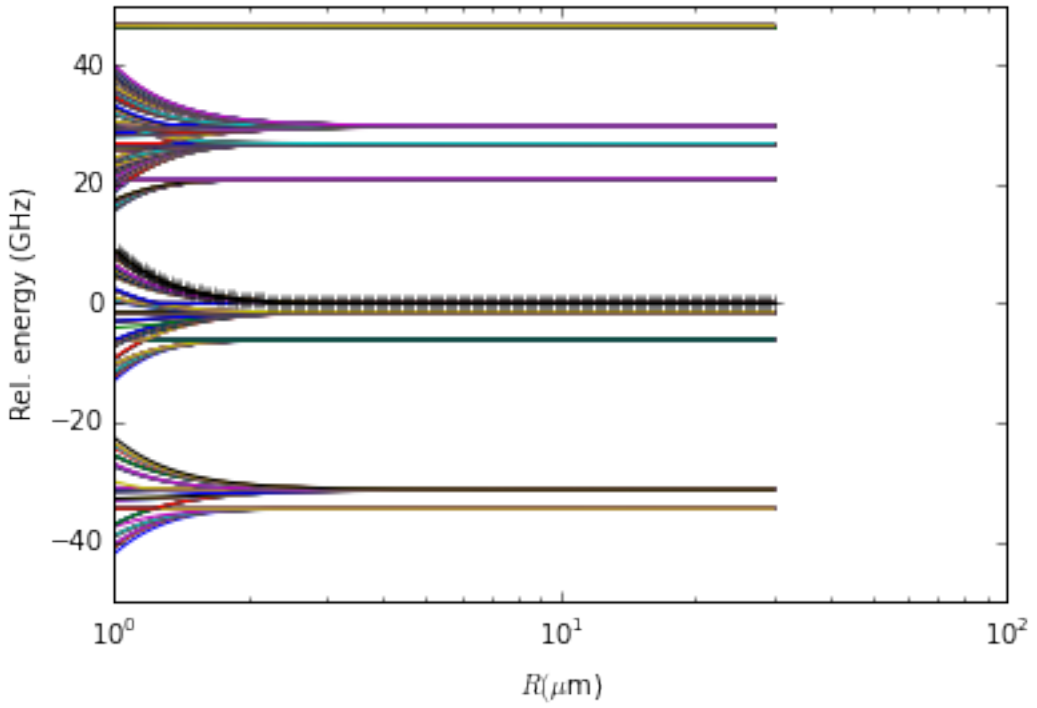
0.2 Electric field, aligned with magnetic field, atom pair aligned to magnetic field

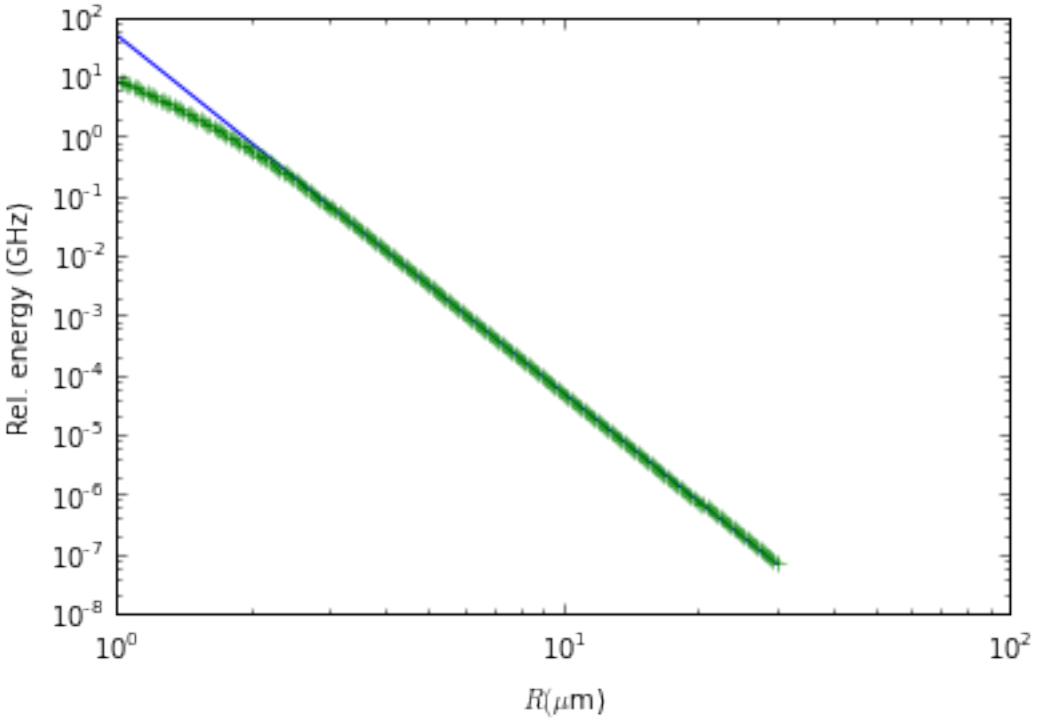
```
In [23]: builtins.Ffield = 1.e-1 # V/cm
         builtins.theta_F = 0.*pi/2 # angle between F field and magnetic field
         builtins.phi_F = 0.*pi/2 # angle between F_field and magnetic field , atom pair plan
         if __name__ == '__main__':
             if 'cal_VdW' not in locals():
                 import cal_VdW
             else:
                 reload(cal_VdW)
```

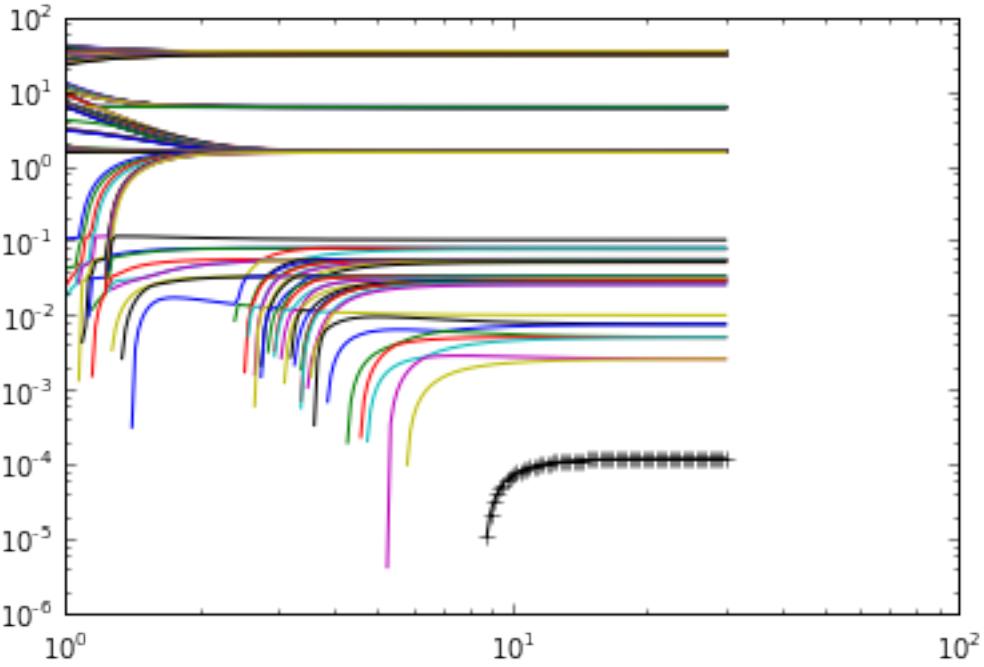
```
atom 60, 59, 59 and atom 60, 59, 59
theta = 0.0 deg
B_field = 10.0 G
F_field = 0.1 V/cm
theta_F = 0.0 deg
phi_F = 0.0 deg
10.0
Matrix size: 482
C6 = [ 49.5523487] GHz.um^6
R_1 MHz = 6.017077242542638 um
```

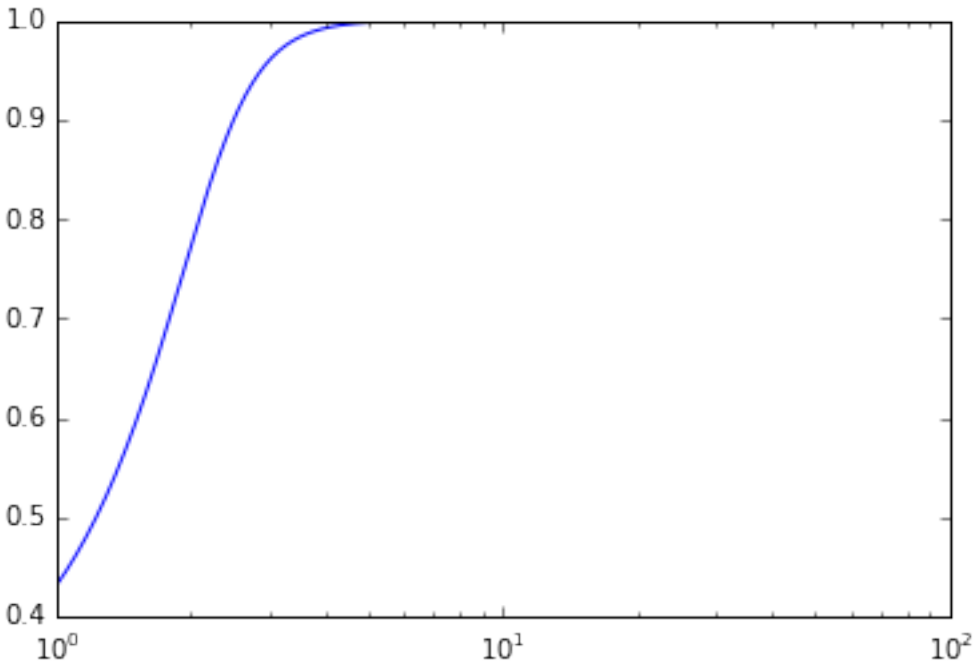



Rel. energy (GHz)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
40
20
0
−20
−40
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
$R(\mu\mathrm{m})$





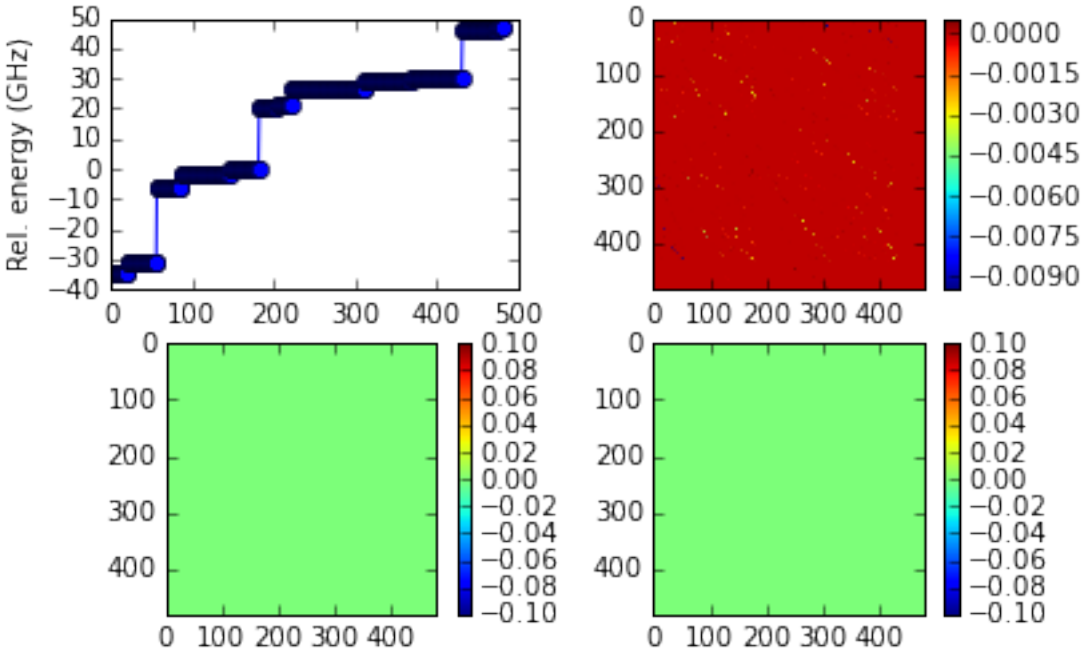
$C_6 = 49.55$ GHzμm^6

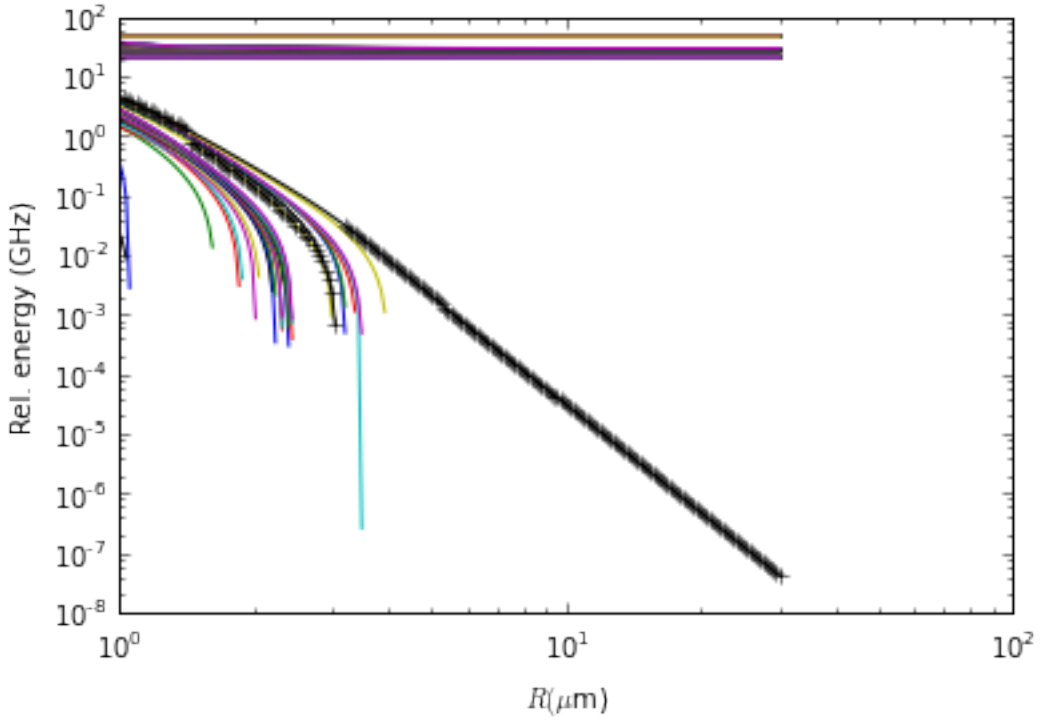
More less the same with the above result, which is easily understood from the configuration. More than that the propagation of coupling has very small effect as the Hamiltonian only couple pair states which conserve $M = m1 + m2$. Now let's tilt the atomic pair to perpendicular to the field.

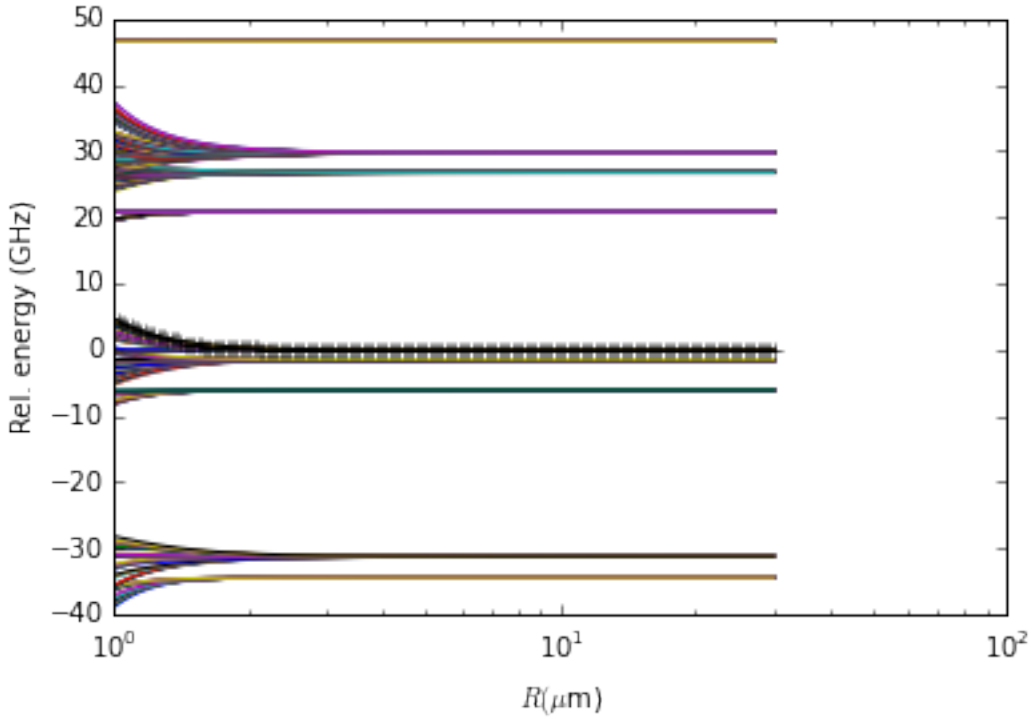
0.3 No electric field

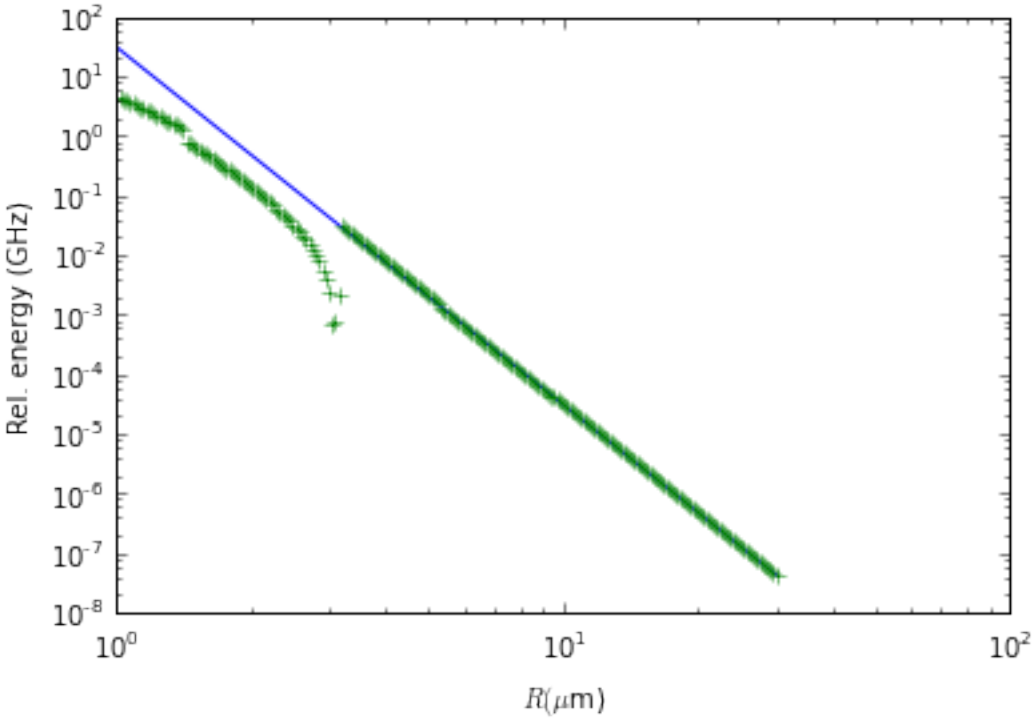
```
In [20]: builtins.theta = pi/2 # angle between magnetic field (quantization axis) and atom pair
         builtins.Ffield = 0*1.e-1 # V/cm
         builtins.theta_F = 0.*pi/2 # angle between F field and magnetic field
         builtins.phi_F = 0.*pi/2 # angle between F_field and magnetic field , atom pair plan
         if __name__ == '__main__':
             if 'cal_VdW' not in locals():
                 import cal_VdW
             else:
                 reload(cal_VdW)
```

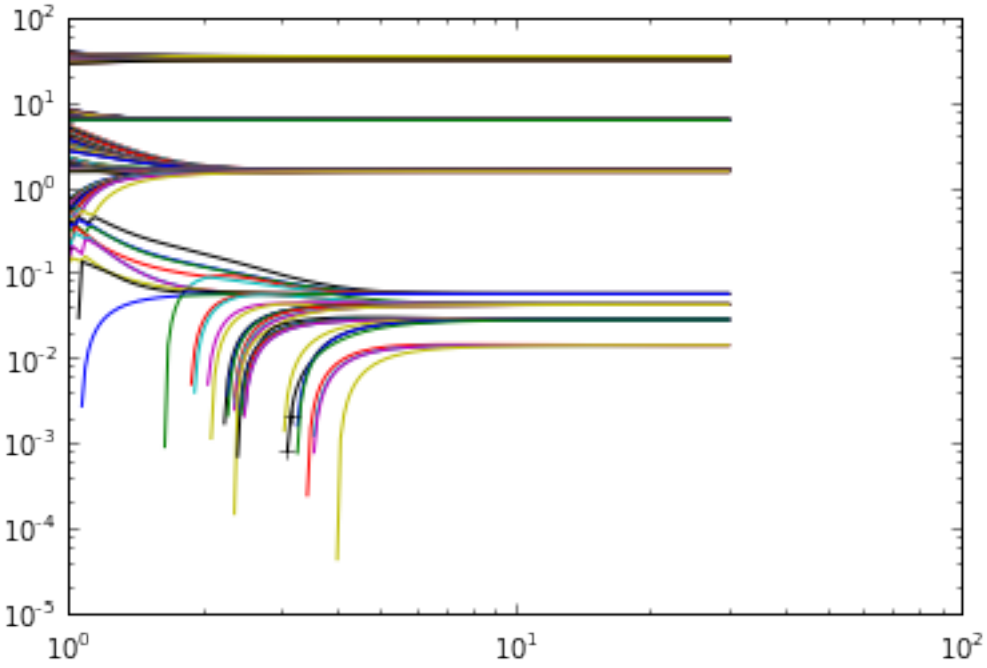
```
atom 60, 59, 59 and atom 60, 59, 59
theta = 90.0 deg
B_field = 10.0 G
F_field = 0.0 V/cm
theta_F = 0.0 deg
phi_F = 0.0 deg
0.0
Matrix size: 482
C6 = [ 30.76966515] GHz.um^6
R_1 MHz = 5.524232992586637 um
```

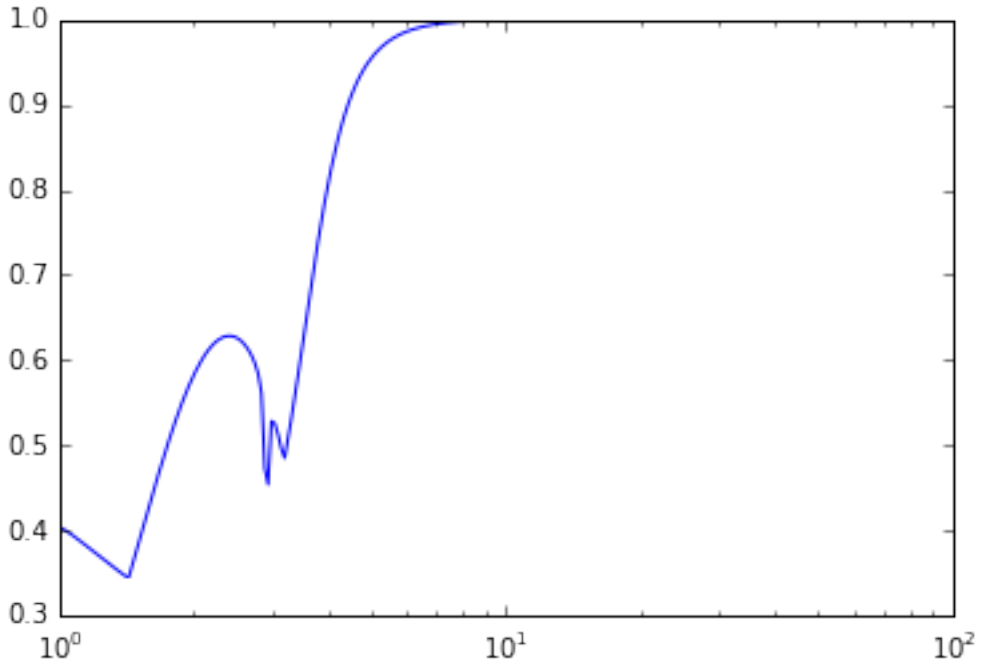

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0 100 200 300 400 500
0
100
200
300
400
0.0000
−0.0015
−0.0030
−0.0045
−0.0060
−0.0075
−0.0090
0.10
0.08
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
−0.08
−0.10


Rel. energy (GHz)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
10^0
10^1
10^2
$R(\mu\mathrm{m})$


Rel. energy (GHz)
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^0
10^1
10^2
$R(\mu\mathrm{m})$





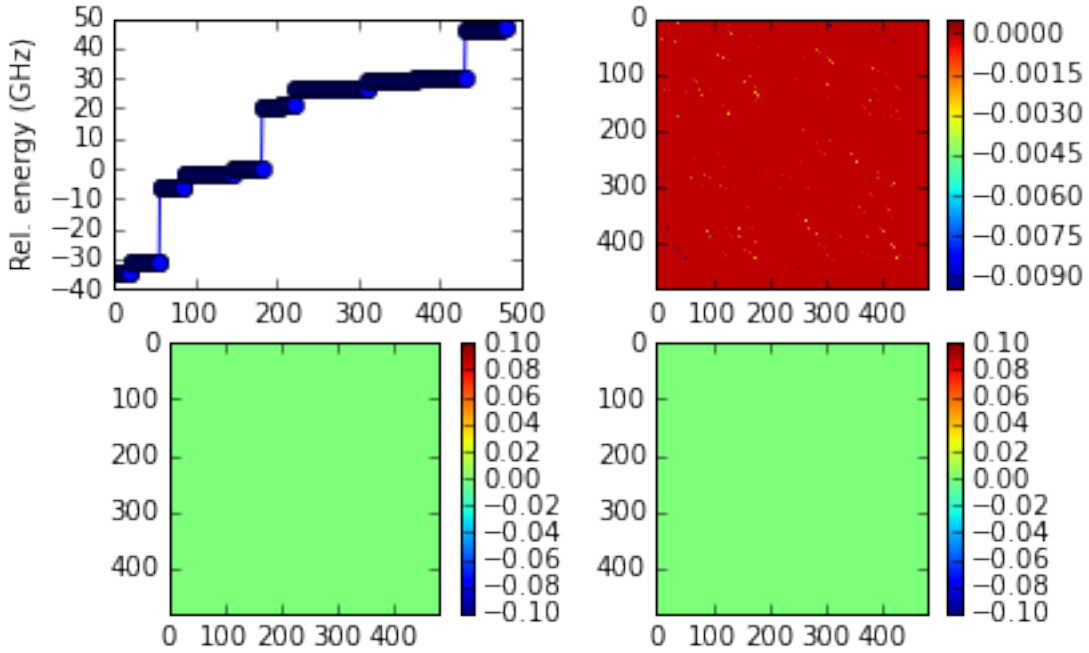
The coupling is more complicated as much more levels contribute. The effect of degeneration is much more crutial. Van der Waals still fits as magnetic field lift up the degeneracies.

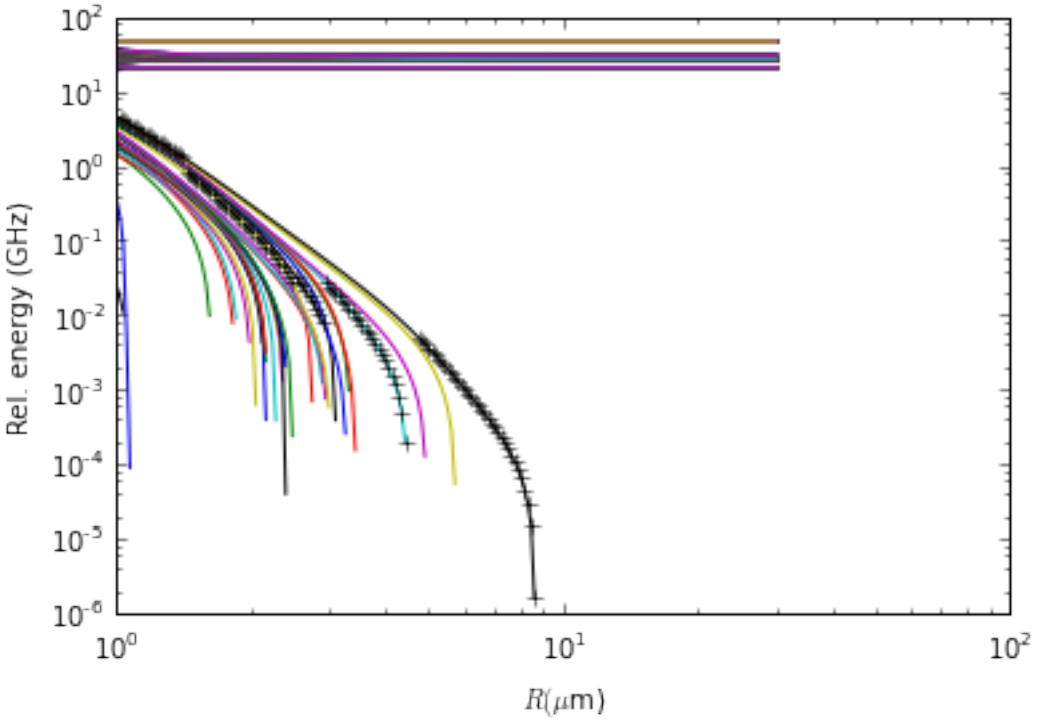
$C_6 = 30.77$ GHz.μm^6. The anti crossing is at about 3μm.

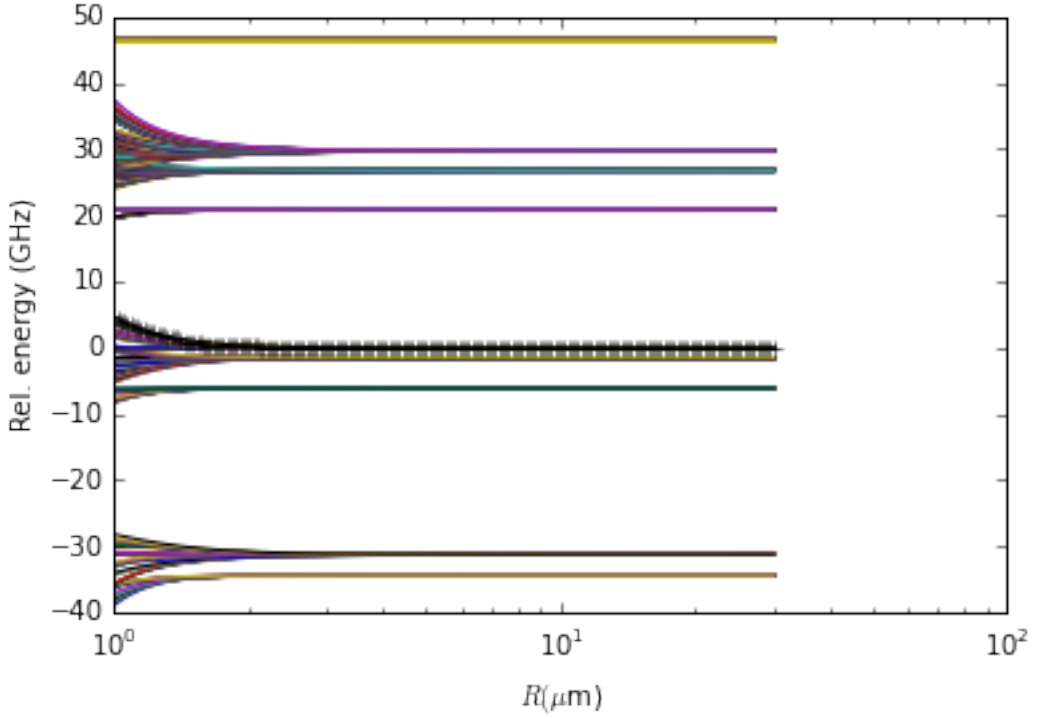
0.4 Weak electric field

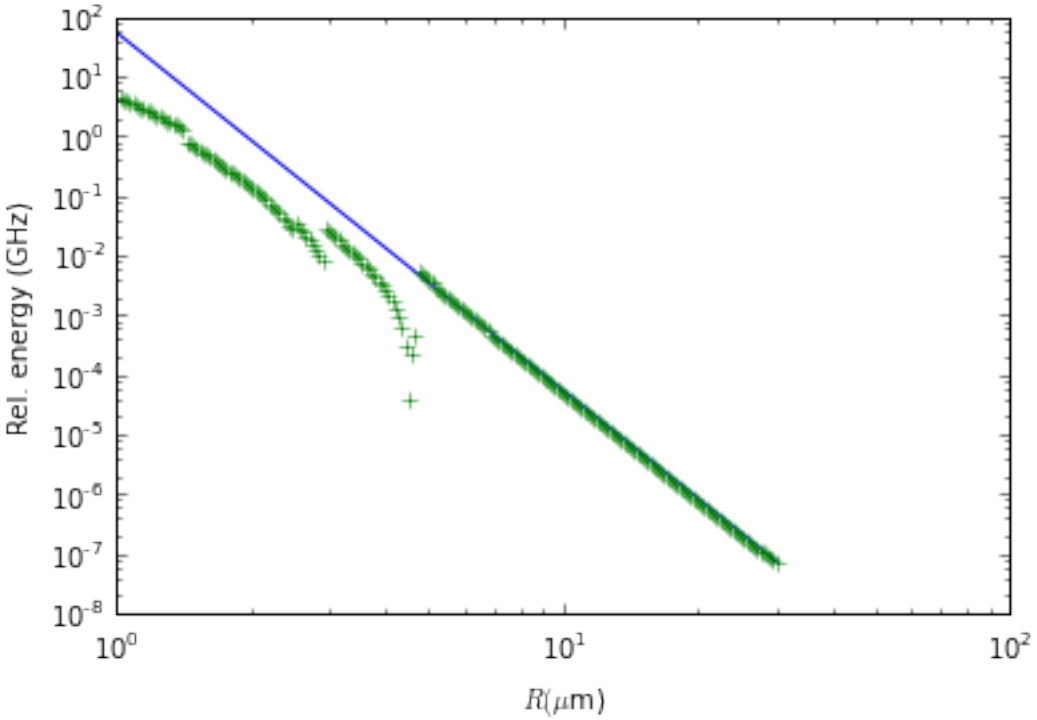
```
In [25]: builtins.theta = pi/2 # angle between magnetic field (quantization axis) and atom pair
         builtins.Ffield = 1.e-1 # V/cm
         builtins.theta_F = 0.*pi/2 # angle between F field and magnetic field
         builtins.phi_F = 0.*pi/2 # angle between F_field and magnetic field , atom pair plan
         if __name__ == '__main__':
             if 'cal_VdW' not in locals():
                 import cal_VdW
             else:
                 reload(cal_VdW)
```

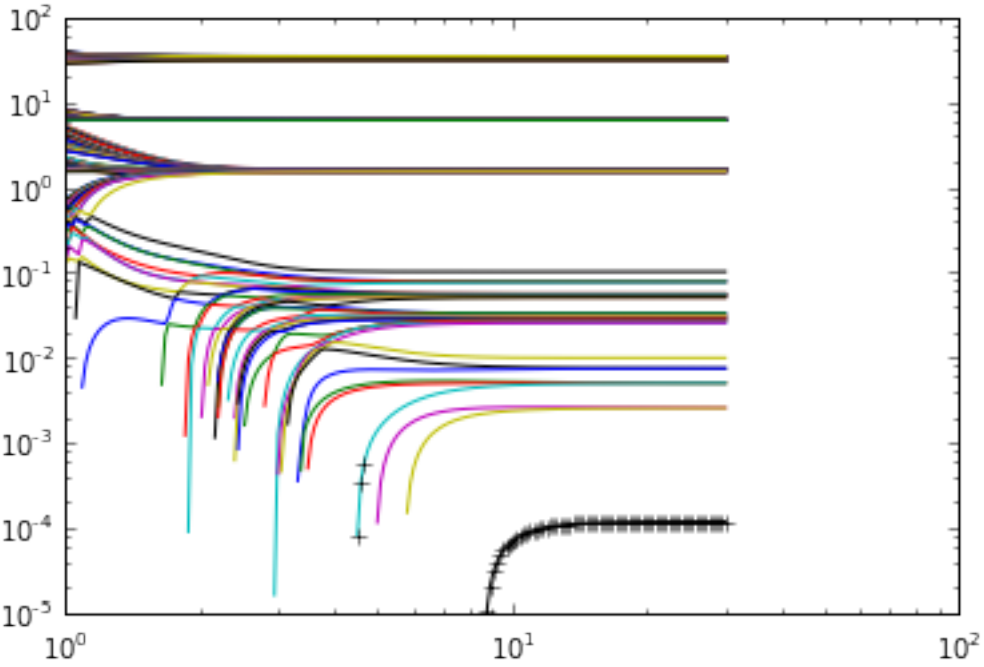
```
atom 60, 59, 59 and atom 60, 59, 59
theta = 90.0 deg
B_field = 10.0 G
F_field = 0.1 V/cm
theta_F = 0.0 deg
phi_F = 0.0 deg
10.0
Matrix size: 482
C6 = [ 54.42595878] GHz.um^6
R_1 MHz = 6.120801657107568 um
```

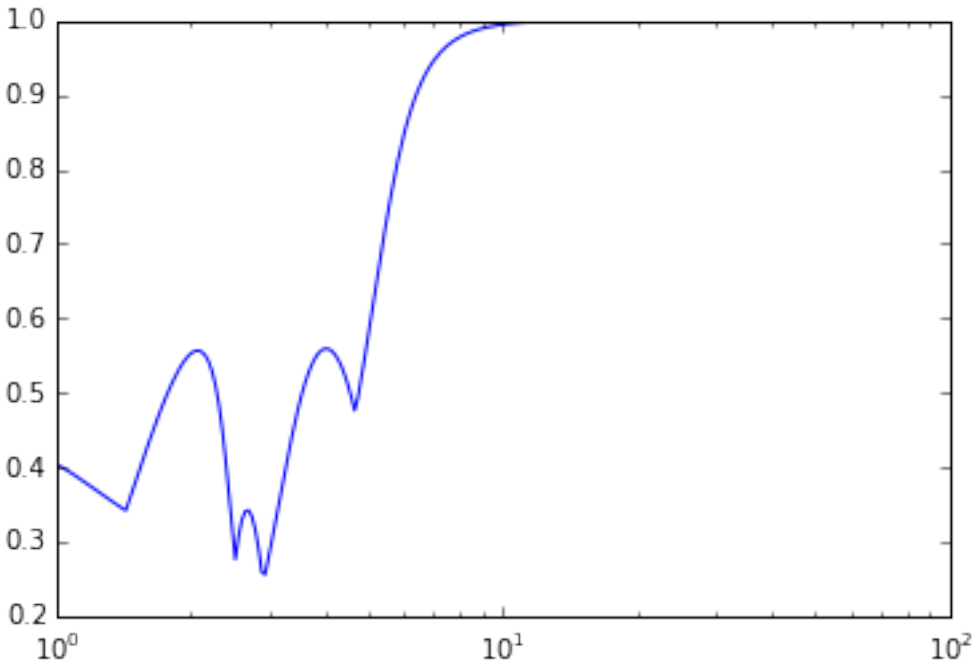



Rel. energy (GHz)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
$R(\mu m)$





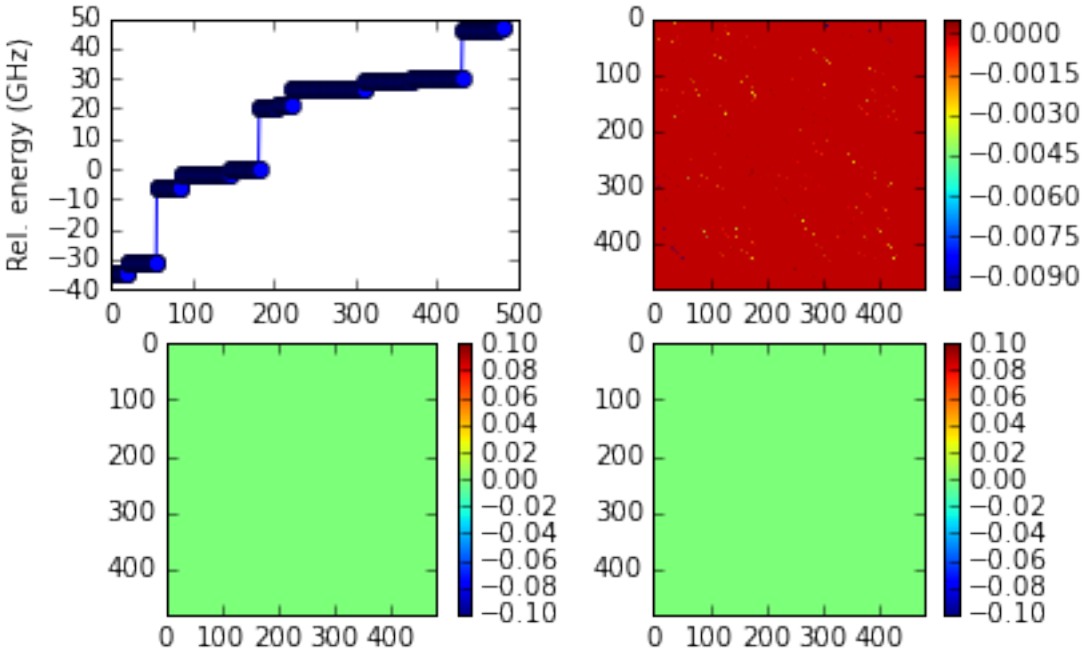
The crossing point is moved to larger distances as the Stark effect starts to take over the Zeeman splitting.

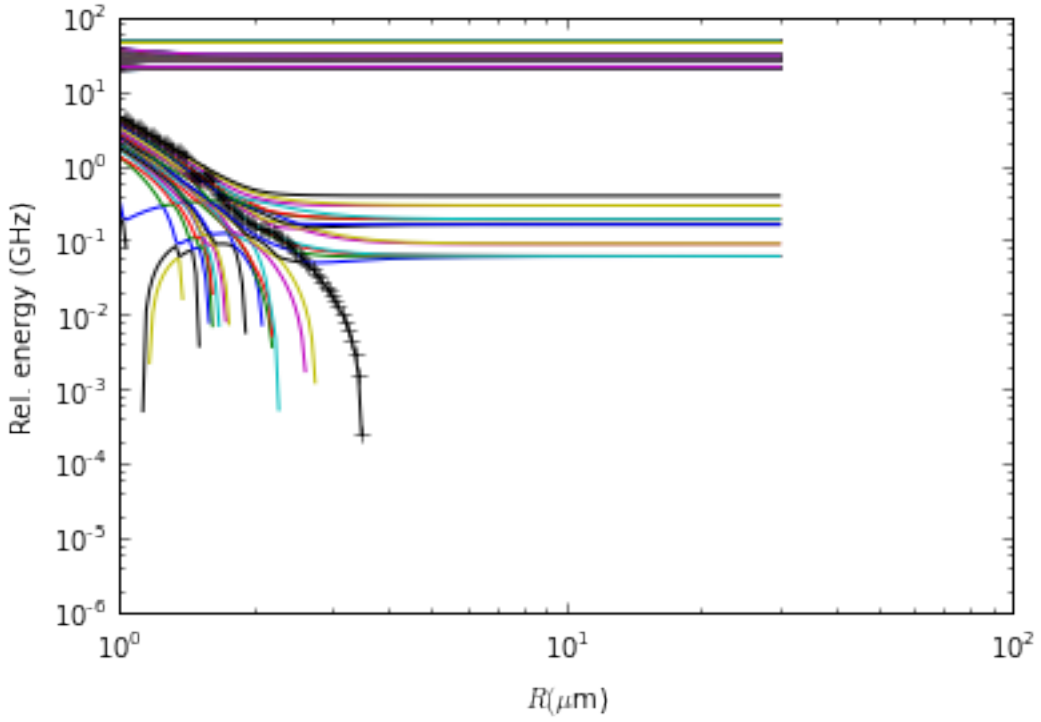
$C_6 = 54.4$ GHz.μm^6 up to $\sim 5\mu$m. To $\sim 10\mu$m the pair is still more less pure circular. Increase l terms yields $C_6 = 53.25$ GHz.μm^6. If we put in a little bit stronger field, levels are mixed up and the mess happens (verified for 200 mV/cm)

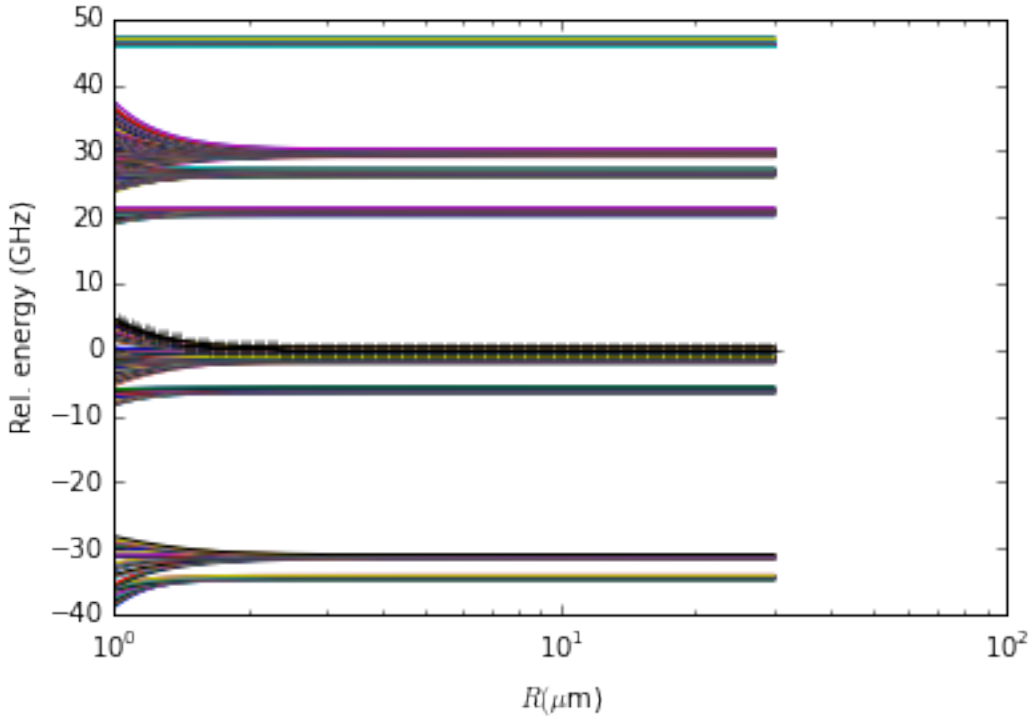
0.5 Strong electric field

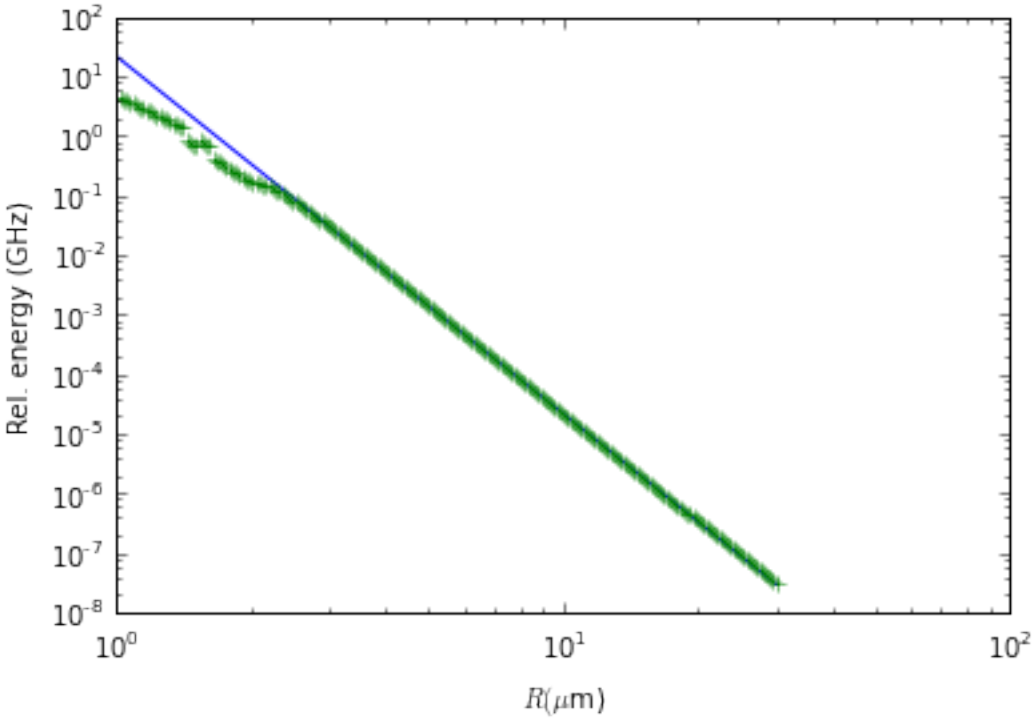
```
In [26]: builtins.theta = pi/2 # angle between magnetic field (quantization axis) and atom pair
         builtins.Ffield = 1.e-0 # V/cm
         builtins.theta_F = 0.*pi/2 # angle between F field and magnetic field
         builtins.phi_F = 0.*pi/2 # angle between F_field and magnetic field , atom pair plan
         if __name__ == '__main__':
             if 'cal_VdW' not in locals():
                 import cal_VdW
             else:
                 reload(cal_VdW)
```

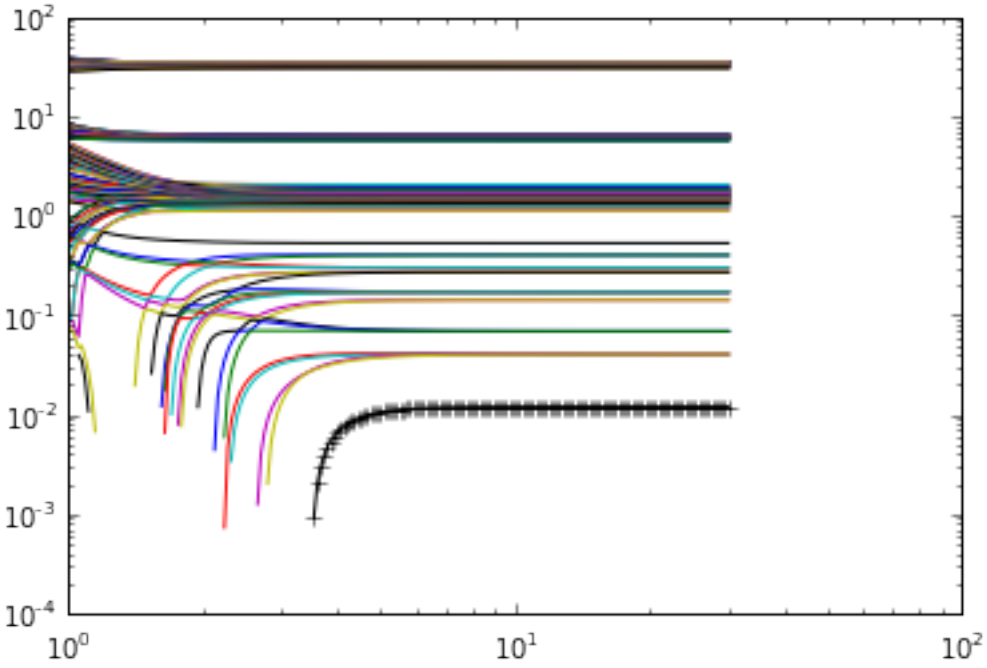
```
atom 60, 59, 59 and atom 60, 59, 59
theta = 90.0 deg
B_field = 10.0 G
F_field = 1.0 V/cm
theta_F = 0.0 deg
phi_F = 0.0 deg
100.0
Matrix size: 482
C6 = [ 21.50986621] GHz.um^6
R_1 MHz = 5.248120856885088 um
```

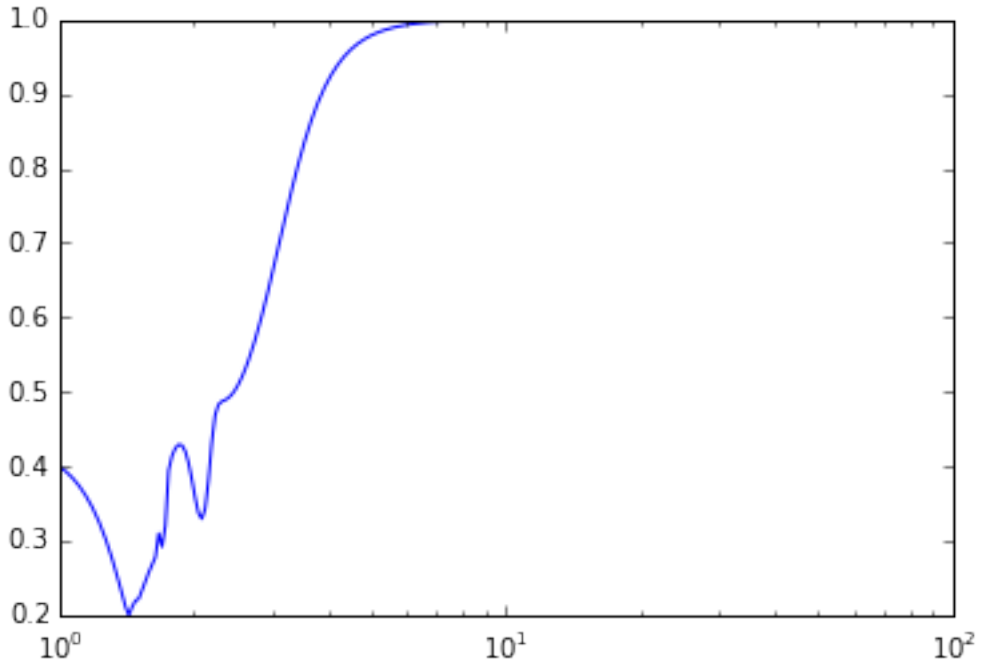

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0 100 200 300 400 500
0
100
200
300
400
0.0000
−0.0015
−0.0030
−0.0045
−0.0060
−0.0075
−0.0090
0.10
0.08
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
−0.08
−0.10


Rel. energy (GHz)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
10^0
10^1
10^2
$R(\mu m)$


Rel. energy (GHz)
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^0
10^1
10^2
$R(\mu m)$





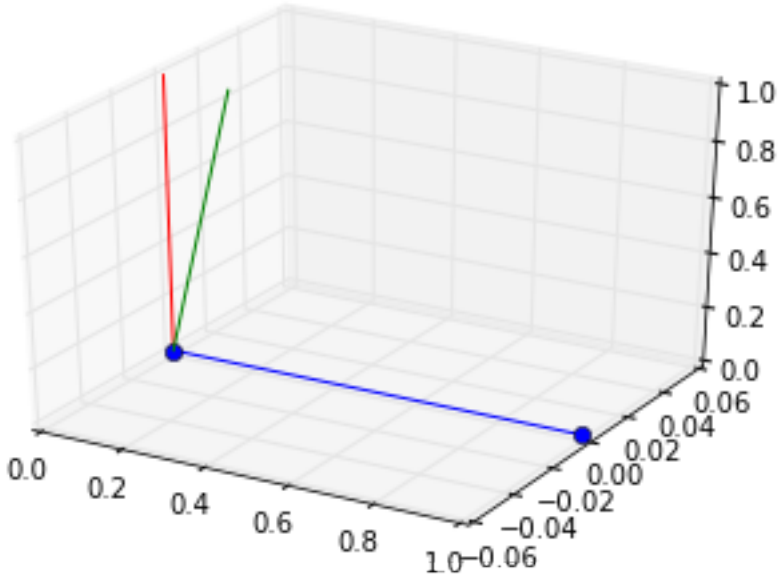
In fact the levels are mixed up in a complicated way. The $|60C60C\rangle$ is no longer on the top, isolated from the other eliptical states. We have to introduce more terms into our basis. The result here is **not trustable**.

0.6 Effect of electric field alignment

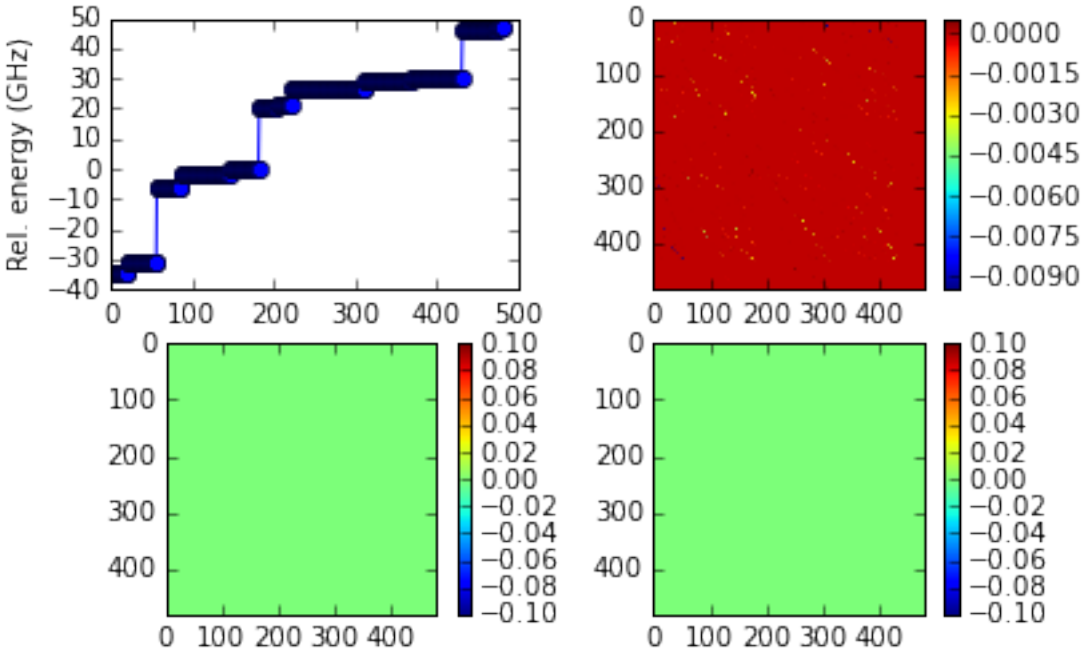
0.6.1 In plan of B field and atomic pair

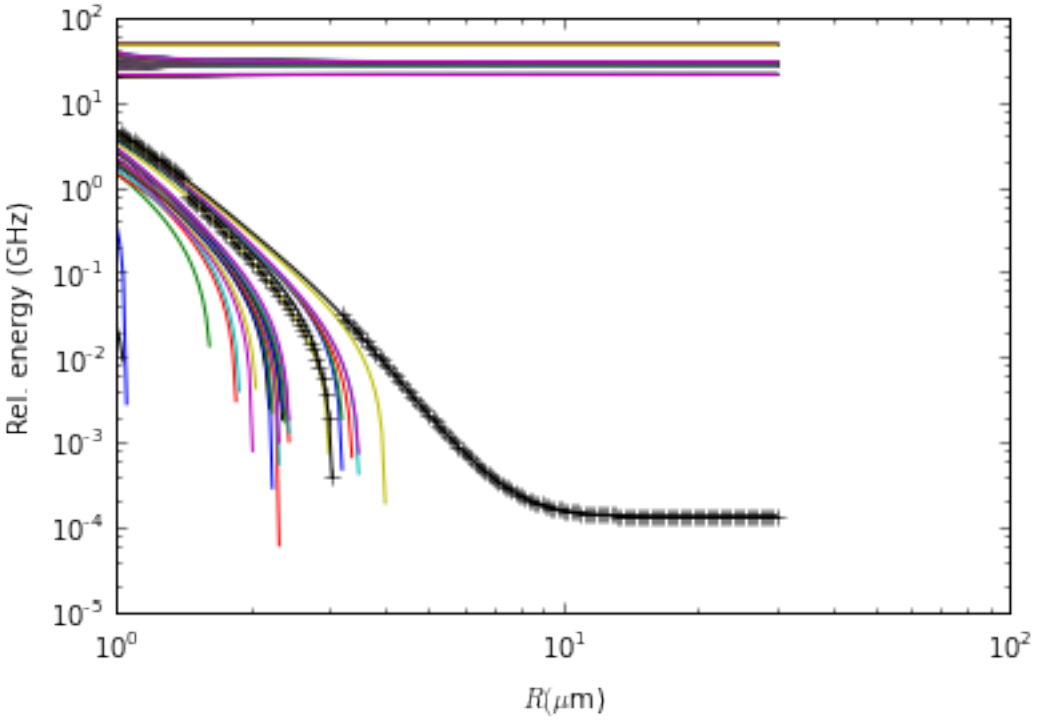
```
In [14]: builtins.theta = pi/2 # angle between magnetic field (quantization axis) and atom pair
         builtins.Ffield = 1.e-2 # V/cm
         builtins.theta_F = 0.1*pi/2 # angle between F field and magnetic field
         builtins.phi_F = 0.*pi/2 # angle between F_field and magnetic field , atom pair plan
         if __name__ == '__main__':
             if 'cal_VdW' not in locals():
                 import cal_VdW
             else:
                 reload(cal_VdW)
```

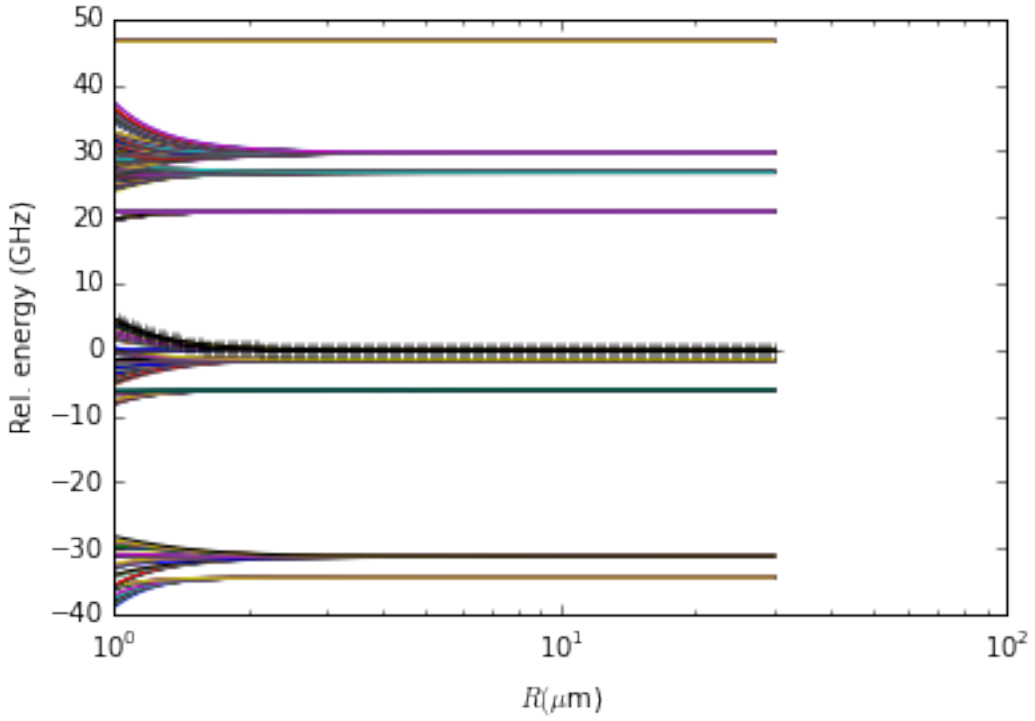
```
atom 60, 59, 59 and atom 60, 59, 59
theta = 90.0 deg
B_field = 10.0 G
F_field = 0.01 V/cm
theta_F = 9.0 deg
phi_F = 0.0 deg
```

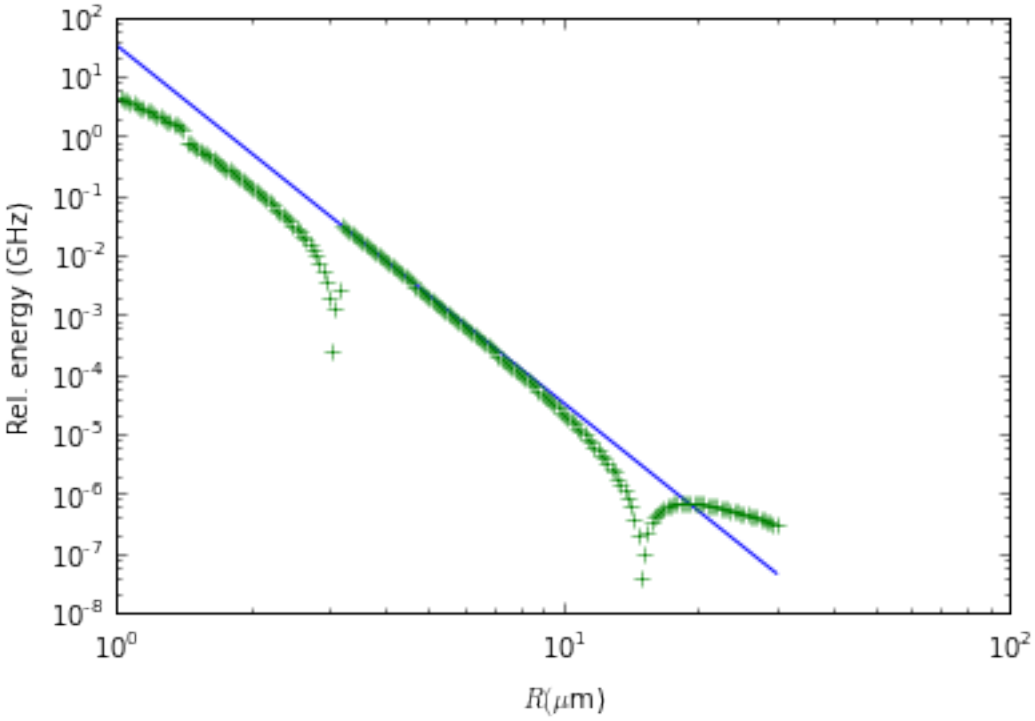


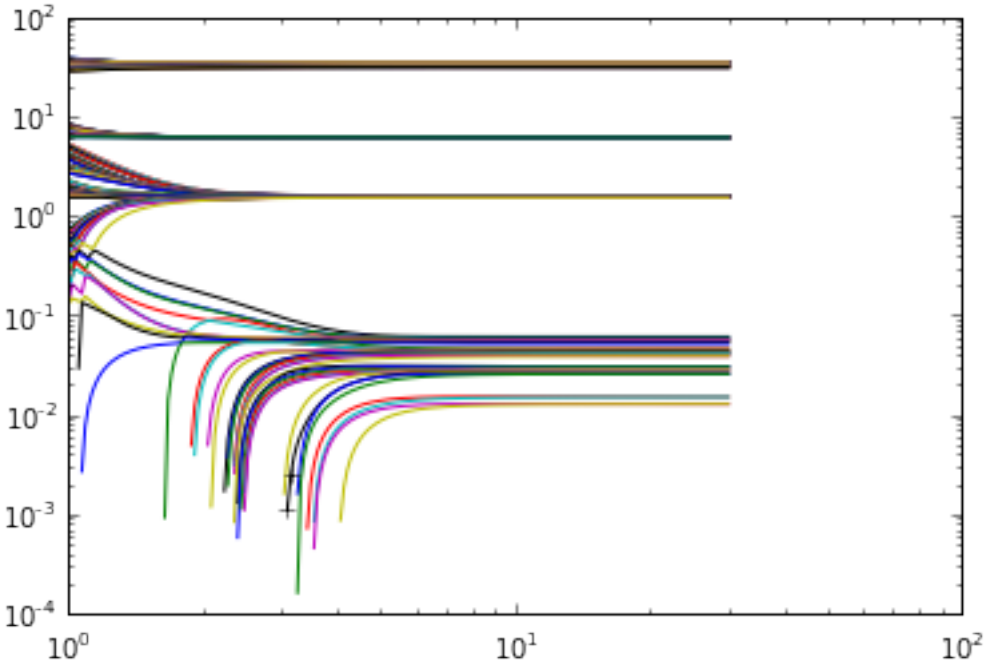

```
Matrix size: 482
C6 = [ 33.07014508   6.        ] GHz.um^6
R_1 MHz = 5.524232992586637 um

C:\Users\r14\Documents\GitHub\test\python\cal_VdW.py:268: ComplexWarning: Casting complex values to real
  out_egr[i] , out_vector[i] = np.linalg.eigh(EI + 1e18*V_VdW* coef/(elm**3) + coef_F*(V_Stark1 + V_Stark
```

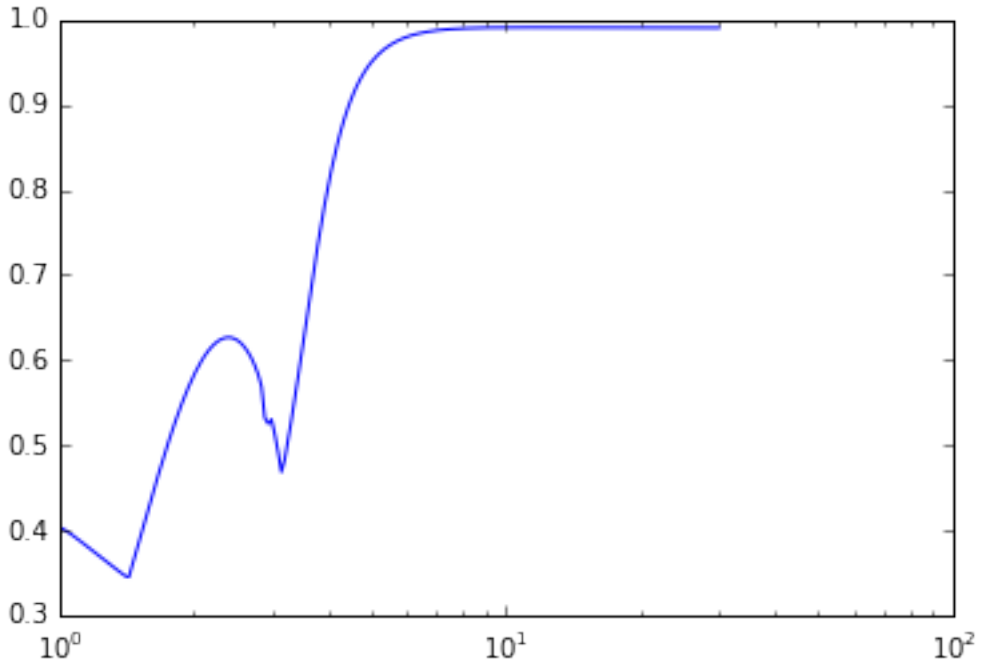

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0 100 200 300 400 500
0 100 200 300 400
0.0000
−0.0015
−0.0030
−0.0045
−0.0060
−0.0075
−0.0090
0.10
0.08
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
−0.08
−0.10


Rel. energy (GHz)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
10^0
10^1
10^2
$R(\mu\mathrm{m})$


Rel. energy (GHz)
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^0
10^1
10^2
$R(\mu\mathrm{m})$



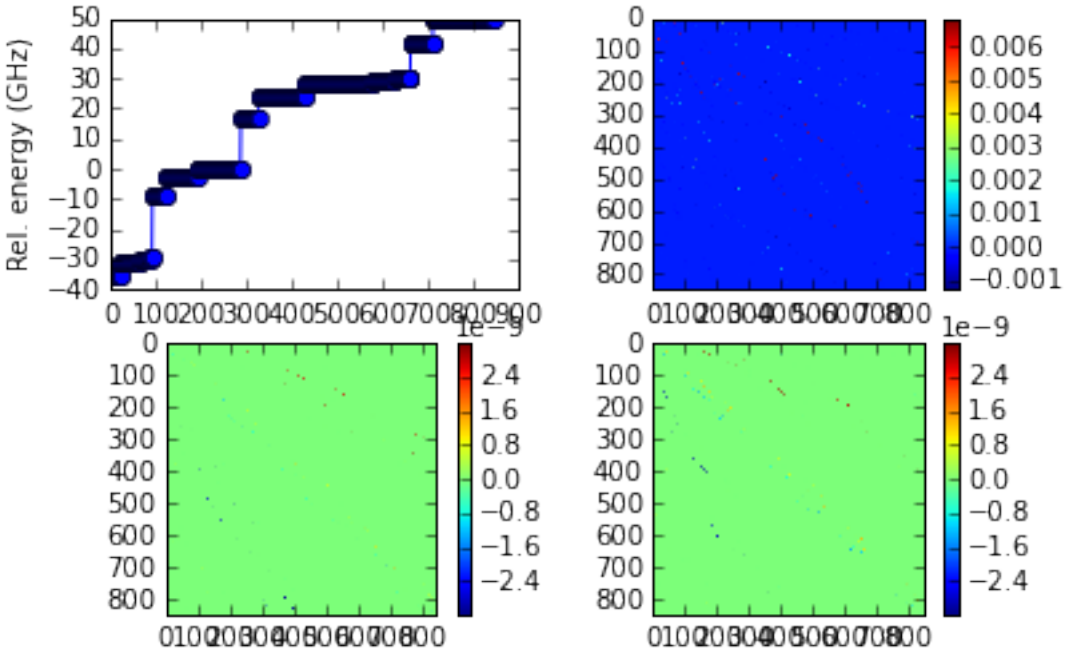


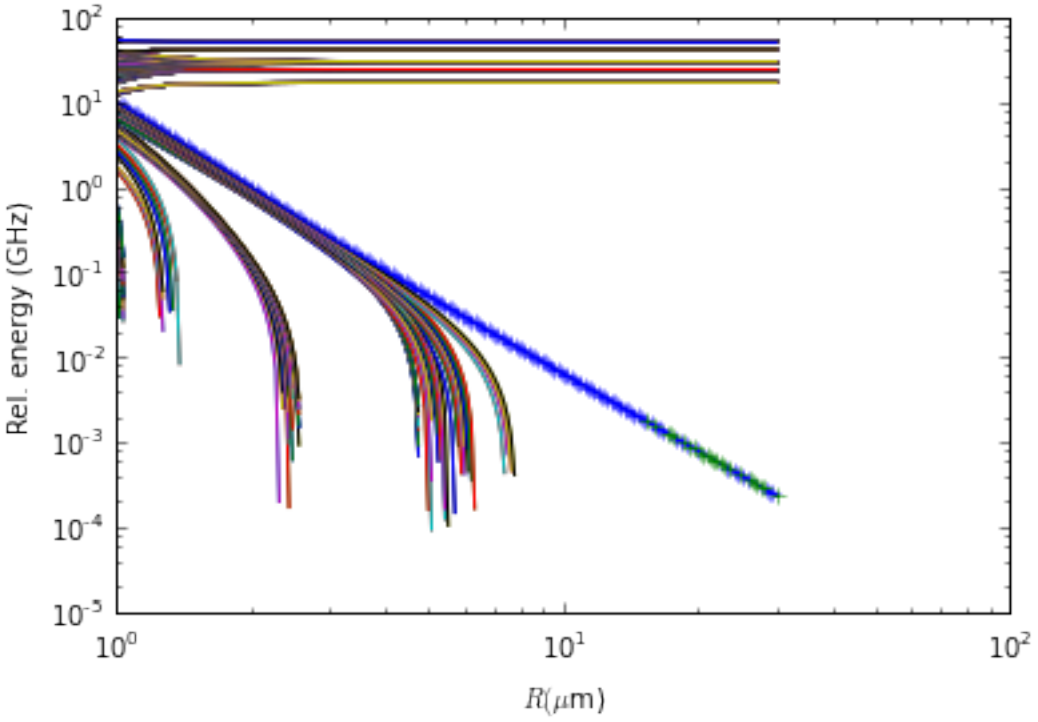
$C_6 \sim 33$ GHz.μm^6 which is close to the VdW shift due to the z component of the field. Larger than 10μm, the pair energy is lightly attractive. This may be caused coupling with higher order due to complicated Stark effect created by x component of the electric field.

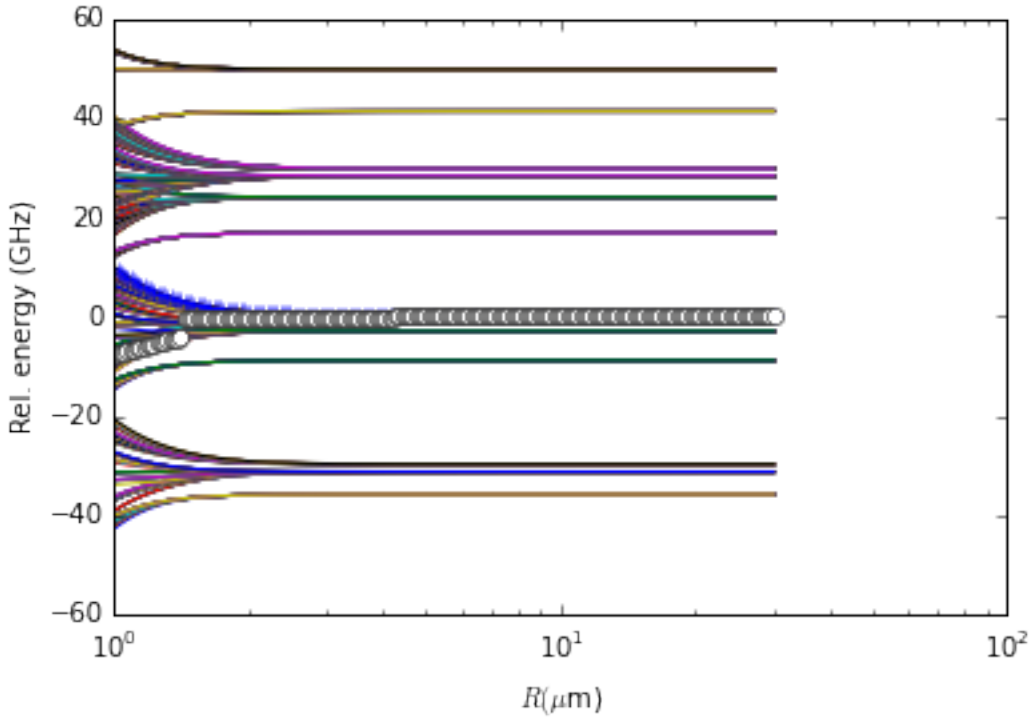
0.7 $|60C61C\rangle$ no electric field, parallel pair of atoms

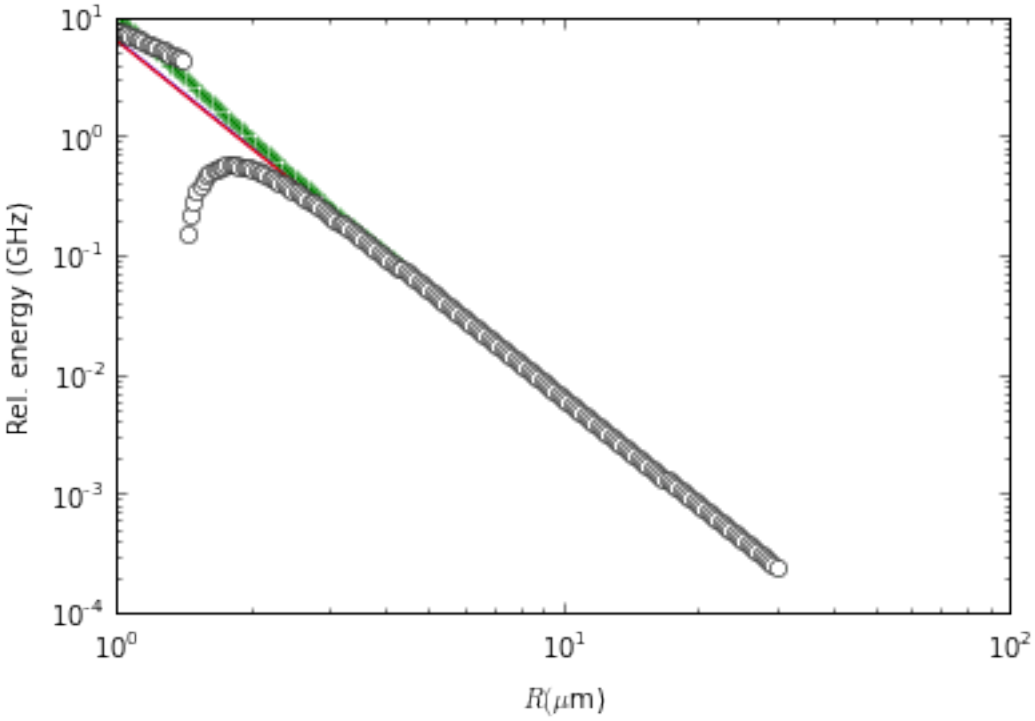
In [8]:
```
# Define levels builtins to globalize the parameters
import builtins
builtins.n1 = 60
builtins.l1 = n1-1
builtins.m1 = l1

builtins.n2 = 61
builtins.l2 = n2-1
builtins.m2 = l2

builtins.Bfield = 10.e-4 # Magnetic field from experiment 1 Teslta = 10*4 Gauss
builtins.theta = 0*pi/2 # angle between magnetic field (quantization axis) and atom pair

# Setup criterion
delta_n_max = 6
l_max = 2
Choice = 1e7# cut off energy for 1st order term, in Hz
builtins.R_test = 1e-6
Choice2 = 10* Choice

builtins.Choice_F = 1e-1 # cut off for Stark shift

builtins.Ffield = 0*1e-1 # V/cm
builtins.theta_F = 0.001*pi/2 # angle between F field and magnetic field
builtins.phi_F = 0.001*pi/2 # angle between F_field and magnetic field , atom pair plan
if __name__ == '__main__':
    if 'cal_VdW' not in locals():
        import cal_VdW
    else:
        reload(cal_VdW)
```

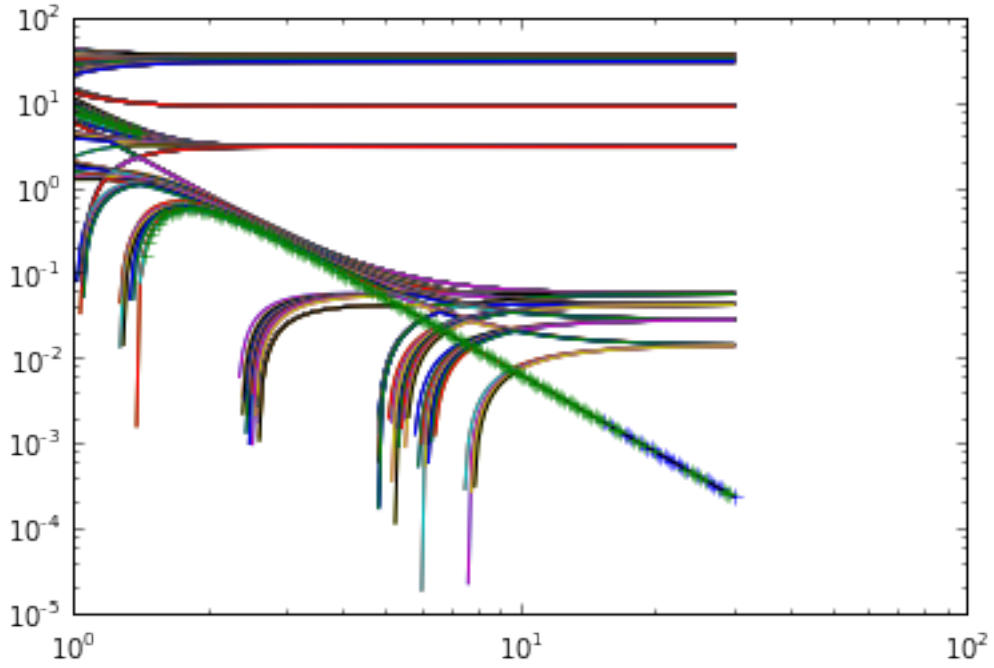
```
atom 60, 59, 59 and atom 61, 60, 60
theta = 0.0 deg
B_field = 10.0 G
F_field = 0.0 V/cm
theta_F = 0.09 deg
phi_F = 0.09 deg
0.0
Matrix size: 847
C6 = [ 6.41010324  3.        ] GHz.um^6
R_1 MHz = 18.27521009584531 um
[ 6.31527539  3.        ]
```

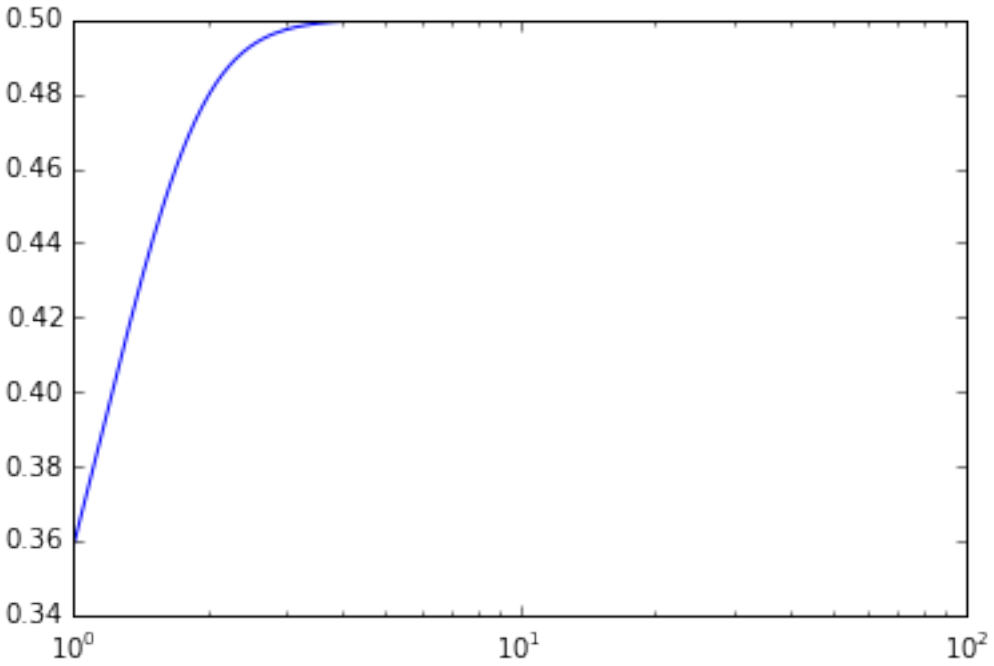

Rel. energy (GHz)
1e−9
1e−9


Rel. energy (GHz)
$R(\mu\mathrm{m})$


60
40
20
0
−20
−40
−60
Rel. energy (GHz)
10^0
10^1
10^2
$R(\mu\mathrm{m})$


10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
Rel. energy (GHz)
10^0
10^1
10^2
$R(\mu\mathrm{m})$



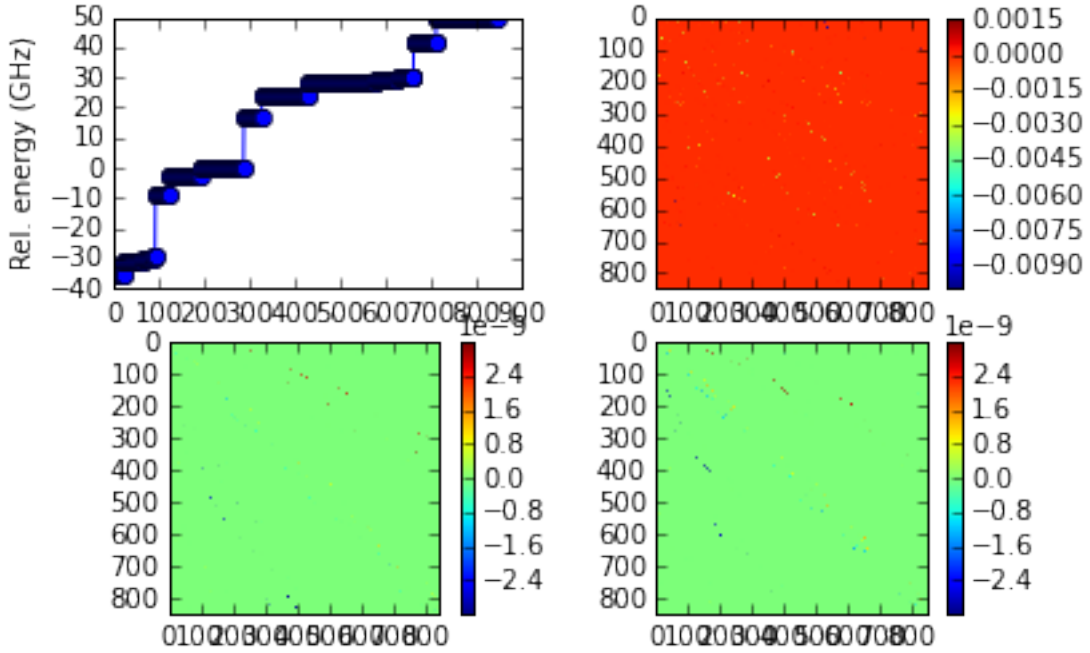


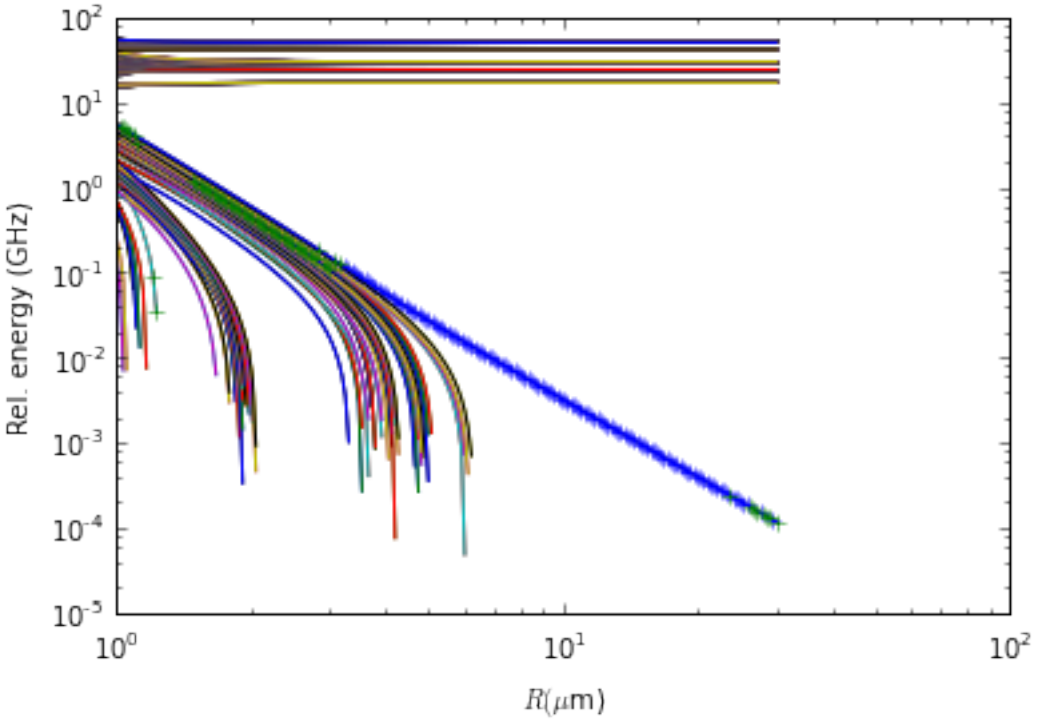
$|60C61C\rangle$ and $61C60C\rangle$ are resonantly coupled $\longrightarrow 1/R^3$ behaviour.
\$C_3A =6.41, C_3S =6.32 \$ GHzμm^3

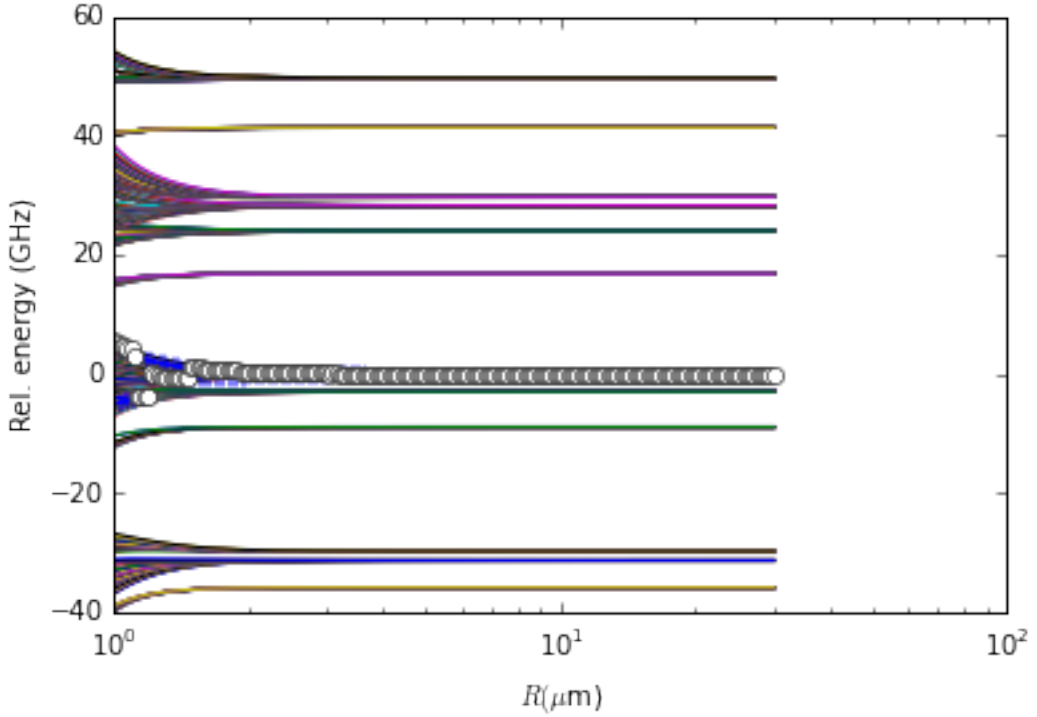
0.7.1 pair of atoms perpendicular to the B field

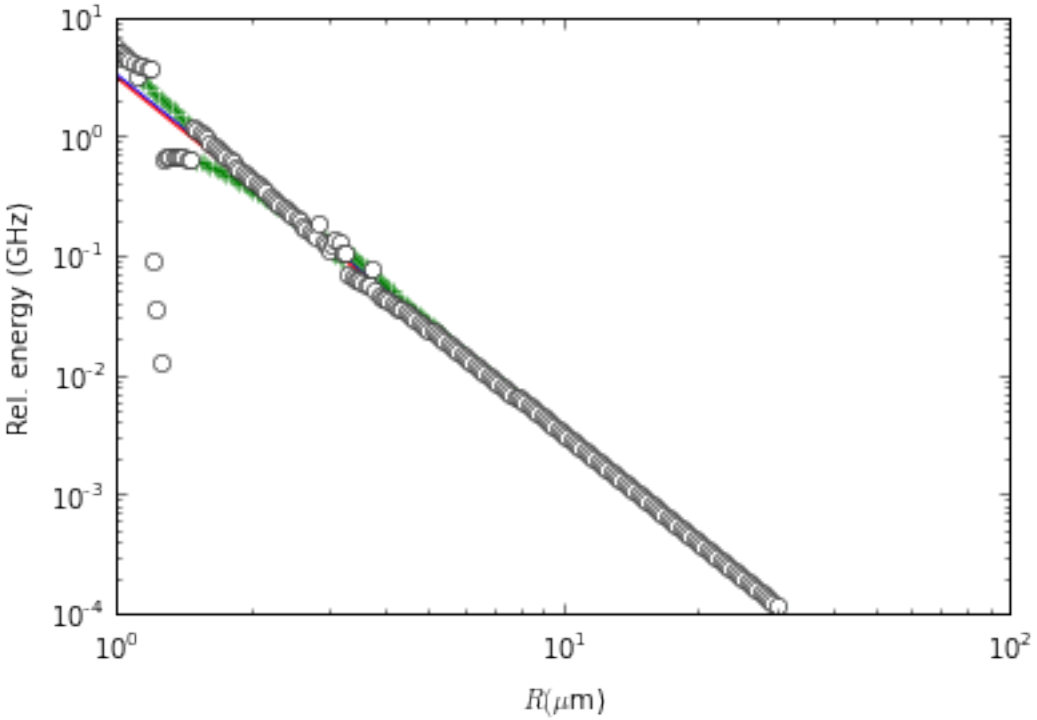
```
In [9]: builtins.theta = pi/2 # angle between magnetic field (quantization axis) and atom pair
        if __name__ == '__main__':
            if 'cal_VdW' not in locals():
                import cal_VdW
            else:
                reload(cal_VdW)
```

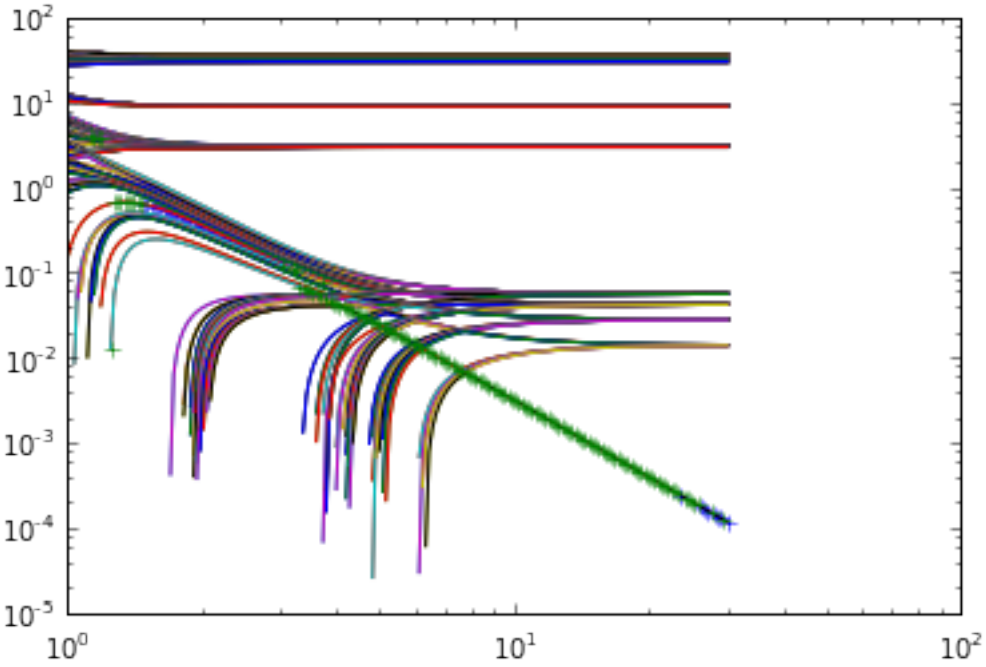
```
atom 60, 59, 59 and atom 61, 60, 60
theta = 90.0 deg
B_field = 10.0 G
F_field = 0.0 V/cm
theta_F = 0.09 deg
phi_F = 0.09 deg
0.0
Matrix size: 847
C6 = [ 3.27782365  3.        ] GHz.um^6
R_1 MHz = 14.63413375221298 um
[ 3.09313429  3.        ]
```

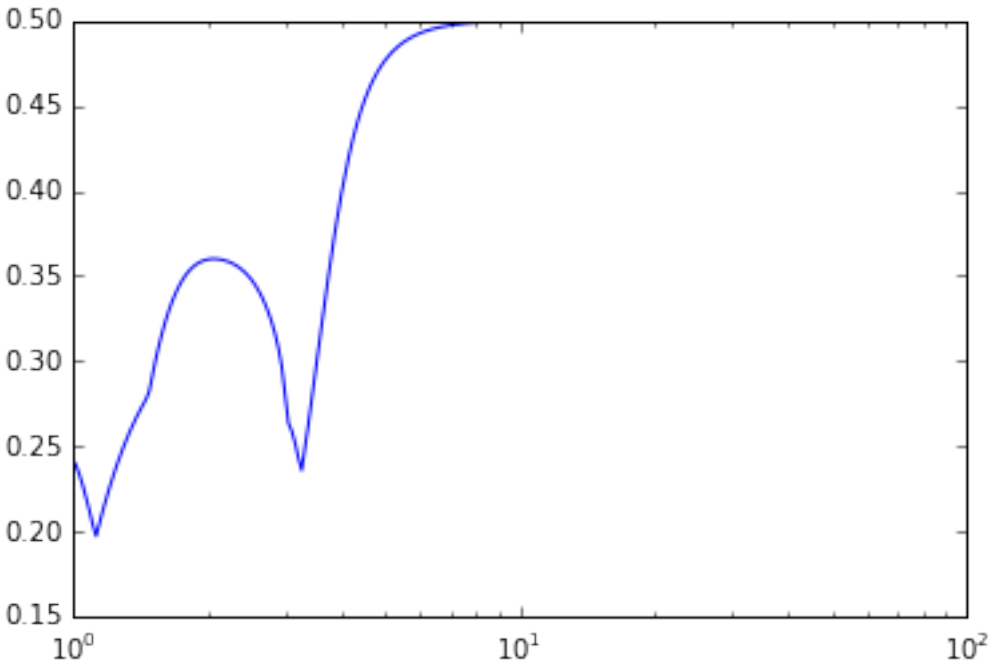



Rel. energy (GHz)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
60
40
20
0
−20
−40
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


Rel. energy (GHz)
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{0}
10^{1}
10^{2}

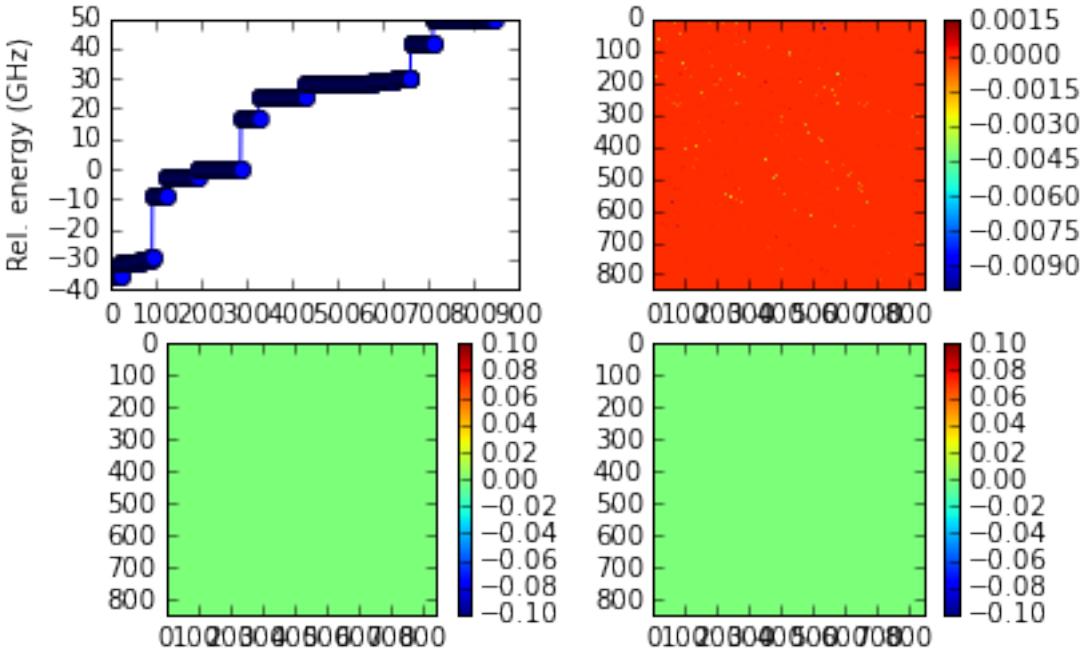


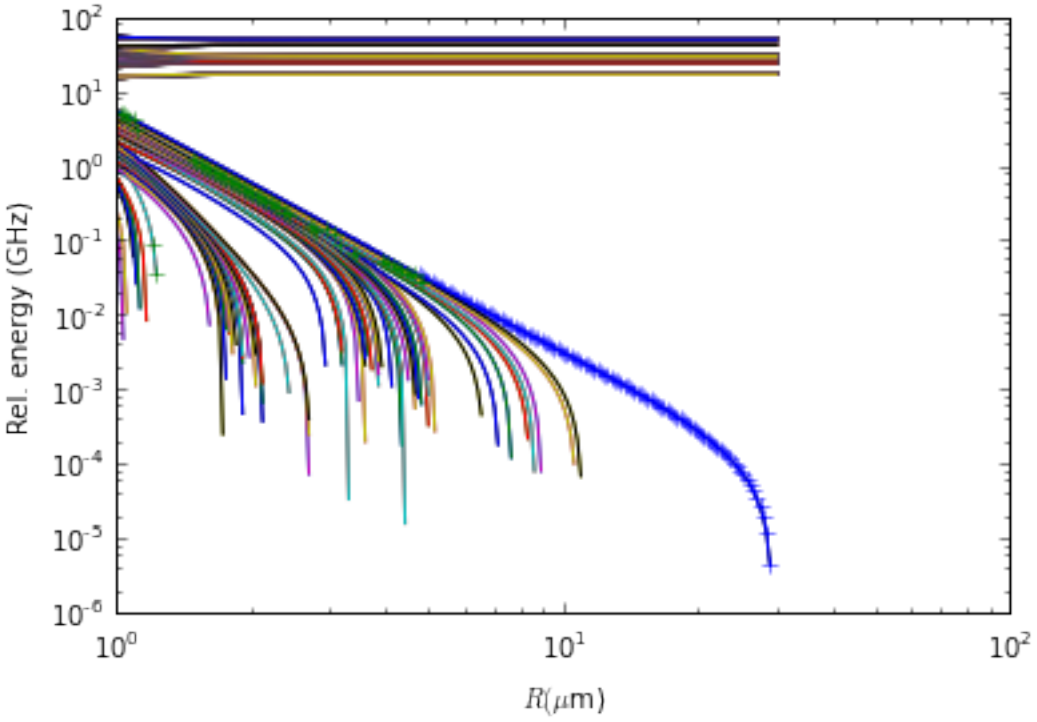
$C_3A =3.28, ; C_3S =3.09 $ GHzμm^3 The same $1/R^3$ behaviour with smaller coefficients.

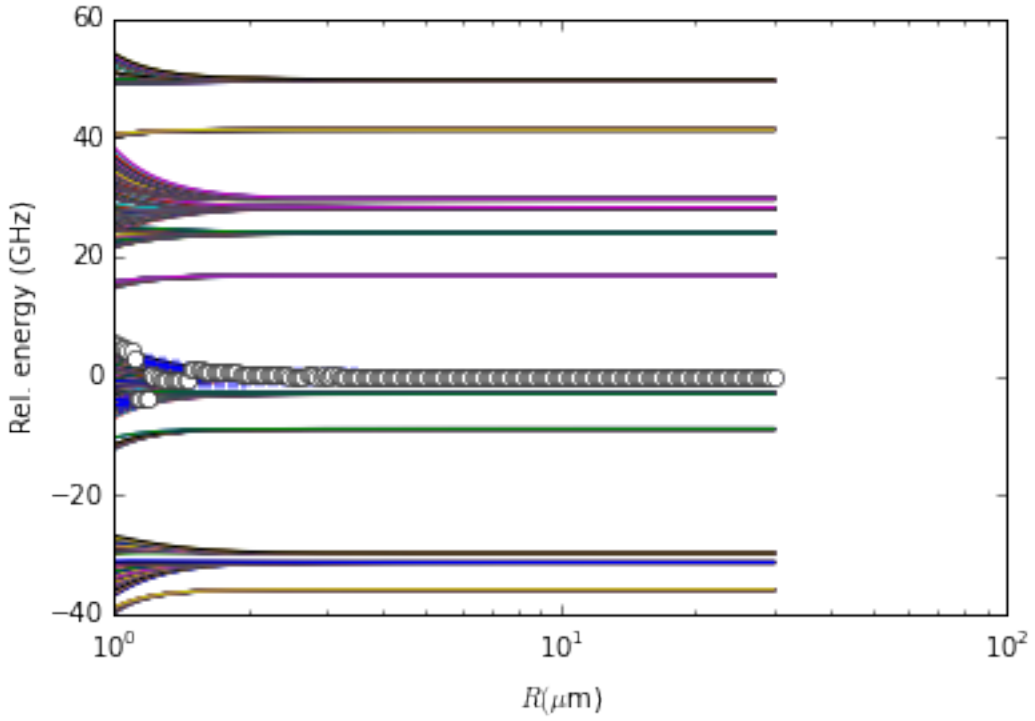
0.7.2 Adding an static electric field

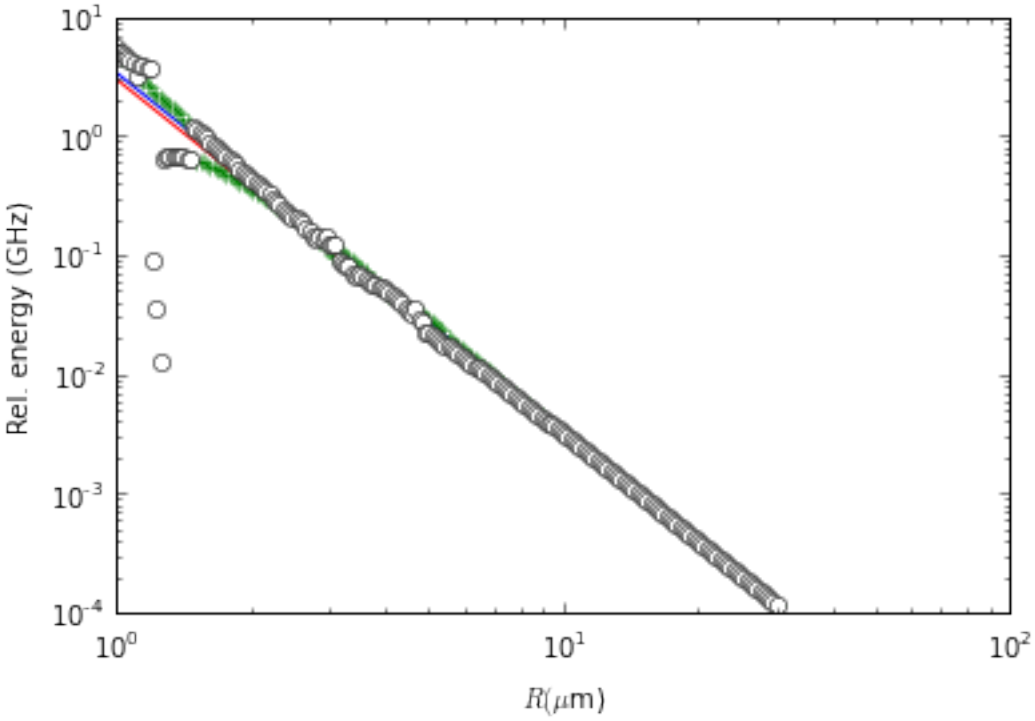
```
In [12]: builtins.Ffield = 0.1 #V/cm
         builtins.theta_F = 0
         if __name__ == '__main__':
             if 'cal_VdW' not in locals():
                 import cal_VdW
             else:
                 reload(cal_VdW)
```

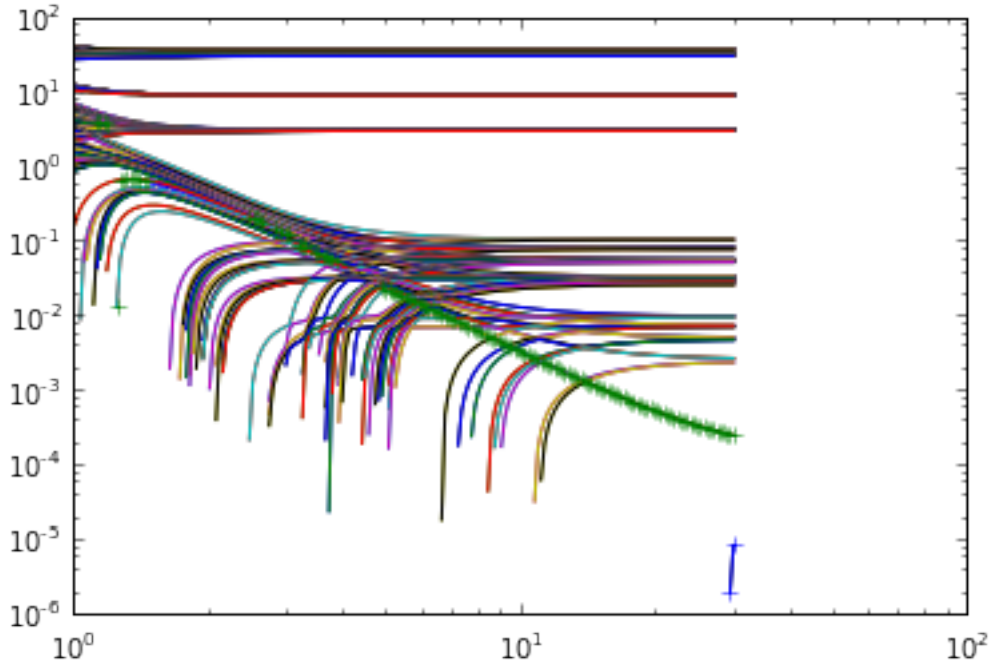
```
atom 60, 59, 59 and atom 61, 60, 60
theta = 90.0 deg
B_field = 10.0 G
F_field = 0.1 V/cm
theta_F = 0.0 deg
phi_F = 0.09 deg
10.0
Matrix size: 847
C6 = [ 3.37498889  3.        ] GHz.um^6
R_1 MHz = 14.63413375221298 um
[ 2.97884851  3.        ]
```

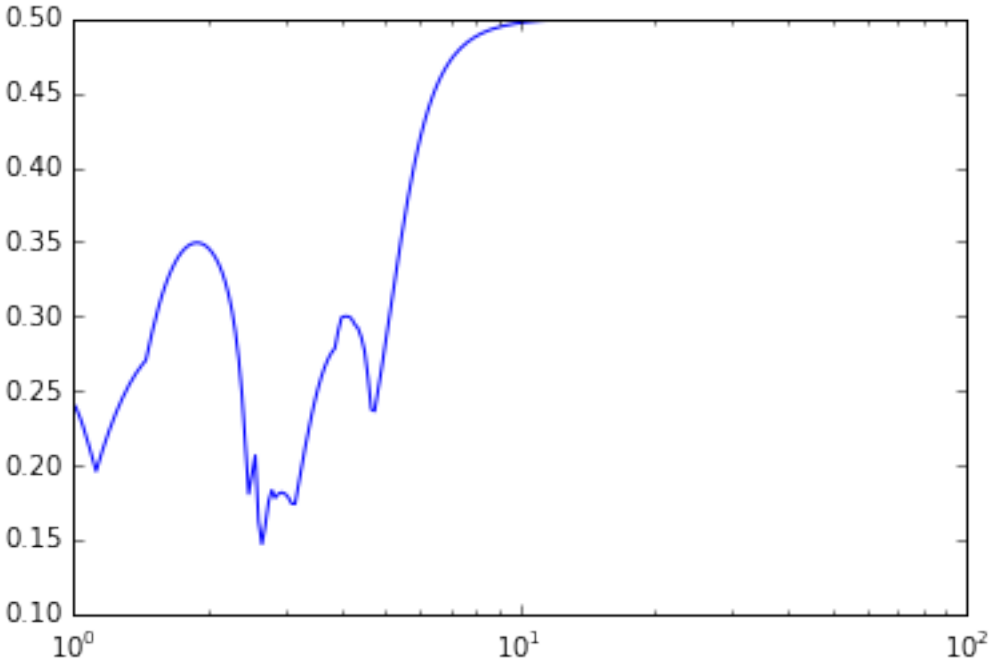

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0 100 200 300 400 500 600 700 800 900
0.0015
0.0000
−0.0015
−0.0030
−0.0045
−0.0060
−0.0075
−0.0090
0.10
0.08
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
−0.08
−0.10


Rel. energy (GHz)
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{0}
10^{1}
10^{2}
$R(\mu\mathrm{m})$


60
40
20
0
−20
−40
Rel. energy (GHz)
10^0
10^1
10^2
$R(\mu\mathrm{m})$


10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
Rel. energy (GHz)
10^0
10^1
10^2
$R(\mu\mathrm{m})$





The interaction is slightly modified but not that critical.
$C_3A \sim 3.37$ GHz.μm^3, $C_3S \sim 2.98$ GHz.μm^3,

In []: