VdW for circular Rydberg atoms

April 20, 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
        %config InlineBackend.figure_format='svg'
```

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

1 $|60C60C\rangle$

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 [3]: # 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 [4]: # 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
```

1.1 B field aligned with pair of atoms

1.1.1 No electric field

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

```
In [6]: 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 = [ 49.14201786   6.        ] GHz.um^6
R_1 MHz = 6.017077242542638 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}
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

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

```
In [7]: 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
```

```
Matrix size: 482
C6 = [ 49.5523487   6.       ] GHz.um^6
R_1 MHz = 6.017077242542638 um
```

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0
100
200
300
400
500
0.006
0.005
0.004
0.003
0.002
0.001
0.000
−0.001
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}
$R(\mu\mathrm{m})$

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

$C_6 = 49.55$ 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.

1.1.3 F field perpendicular to B field which is aligned to pair of atoms

```
In [4]: builtins.theta = 0*pi/2 # angle between magnetic field (quantization axis) and atom pair
        builtins.Ffield = 1.e-2 # V/cm
        builtins.theta_F = 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 = 0.0 deg
B_field = 10.0 G
F_field = 0.01 V/cm
theta_F = 90.0 deg
phi_F = 0.0 deg
```

```
Matrix size: 482
C6 = [ 28.08752755   6.        ] GHz.um^6
R_1 MHz = 6.898701369505688 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
0.006
0.005
0.004
0.003
0.002
0.001
0.000
−0.001
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}
$R(\mu\mathrm{m})$

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

It is complicated due to Stark effect. Let's try with a smaller F field

```
In [6]: builtins.theta = 0*pi/2 # angle between magnetic field (quantization axis) and atom pair
        builtins.Ffield = 5.e-3 # V/cm
        builtins.theta_F = 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 = 0.0 deg
B_field = 10.0 G
F_field = 0.005 V/cm
theta_F = 90.0 deg
phi_F = 0.0 deg
```

```
Matrix size: 482
C6 = [ 0.25332649  3.        ] GHz.um^6
R_1 MHz = 6.226314108246262 um
```

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0
100
200
300
400
500
0.006
0.005
0.004
0.003
0.002
0.001
0.000
−0.001
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}
$R(\mu\mathrm{m})$

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

There is a change from $1/R^3$ to $1/R^6$ which is not yet understood >“<

1.2 B field perpendicular to pair of atoms

1.2.1 No electric field

```
In [8]: 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
```

```
Matrix size: 482
C6 = [ 30.76966515   6.        ] 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
0.0000
−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}
$R(\mu\mathrm{m})$

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.

1.2.2 Weak electric field

```
In [9]: 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
```

```
Matrix size: 482
C6 = [ 54.42595878   6.        ] GHz.um^6
R_1 MHz = 6.120801657107568 um
```

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0
100
200
300
400
500
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}
$R(\mu\mathrm{m})$

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 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)

1.2.3 Strong electric field

```
In [10]: 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
```

```
Matrix size: 482
C6 = [ 21.50986621   6.        ] 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
0.0000
−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}
$R(\mu\mathrm{m})$

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
$R(\mu\mathrm{m})$

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**.

1.2.4 Effect of electric field alignment

In plan of B field and atomic pair

```
In [11]: 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 = [ 29.24132198   6.        ] 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
0.0000
−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}
$R(\mu\mathrm{m})$

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.

Perpendicular to plan of B field and atomic pair

```
In [12]: 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 = 1.*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 = 90.0 deg
```

```
Matrix size: 482
C6 = [ 32.00307111   6.        ] GHz.um^6
R_1 MHz = 5.619461591120331 um
```

Rel. energy (GHz)
50
40
30
20
10
0
−10
−20
−30
−40
0
100
200
300
400
500
0.0000
−0.0015
−0.0030
−0.0045
−0.0060
−0.0075
−0.0090
1e−7
2.4
1.6
0.8
0.0
−0.8
−1.6
−2.4

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

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 declination of the electric field has small effect on the interaction as expected. However it modifies a little bit when the atoms are furthur away as the Stark effect increases the detuning b/w levels. $C_6 = 33$ GHz.μm^6

1.2.5 B parallel to pair of atoms, F perpendicular

2 $|60C61C\rangle$

2.1 No electric field, B field parallel pair of atoms

In [14]:
```
# 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
```

```
Matrix size: 847
C6 = [ 6.41010324  3.        ] GHz.um^6
R_1 MHz = 18.27521009584531 um
[ 6.31527539  6.        ]
```

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

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

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

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

2.1.1 pair of atoms perpendicular to the B field

```
In [15]: 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
```

```
Matrix size: 847
C6 = [ 3.27782365  3.        ] GHz.um^6
R_1 MHz = 14.63413375221298 um
[ 3.09313429  6.        ]
```

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

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

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

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

2.1.2 Adding an static electric field

```
In [16]: 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
```

```
Matrix size: 847
C6 = [ 3.37498889  3.        ] GHz.um^6
R_1 MHz = 14.63413375221298 um
[ 2.97884851  6.        ]
```

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

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

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

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 [8]: 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 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 = 90.0 deg
```

```
Matrix size: 482
C6 = [ 13.32865257   6.        ] GHz.um^6
R_1 MHz = 6.120801657107568 um
```

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

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

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

```
In []:
```