EPR

February 19, 2022

[1]:
```
%matplotlib inline
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from scipy.optimize import curve_fit
```

[2]:
```
def chi_sq(x, y, err):
    function = lambda x, a, b: a * x + b
    popt, pcov = curve_fit(function, xdata=x, ydata=y, sigma=err)

    sigma_a = np.sqrt(pcov[0, 0])
    sigma_b = np.sqrt(pcov[1, 1])

    return popt[0], popt[1], sigma_a, sigma_b
```

[3]:
```
# Gaussian
def func(x, a, x0, sigma):
    return a*np.exp(-(x-x0)**2/(2*sigma**2))
```

[4]:
```
sns.set_theme()
plt.rcParams['mathtext.fontset'] = 'stix'
plt.rcParams['font.family'] = 'STIXGeneral'
```

[5]:
```
#DPPG

file_1 = open('DPPG_0,1A_200.epr.txt')
str_1 = file_1.read().splitlines()

file_2 = open('DPPG_0,3A_200.epr.txt')
str_2 = file_2.read().splitlines()

file_3 = open('DPPG_0,5A_100.epr.txt')
str_3 = file_3.read().splitlines()

file_4 = open('DPPG_0,8A_100.epr.txt')
str_4 = file_4.read().splitlines()
```

```
file_5 = open('DPPG_1,2A_100.epr.txt')
str_5 = file_5.read().splitlines()

file_6 = open('DPPG_1,5A_100.epr.txt')
str_6 = file_6.read().splitlines()

file_7 = open('DPPG_1,8A_50.epr.txt')
str_7 = file_7.read().splitlines()

field_01 = []
field_03 = []
field_05 = []
field_08 = []
field_12 = []
field_15 = []
field_18 = []

intense_01 = []
intense_03 = []
intense_05 = []
intense_08 = []
intense_12 = []
intense_15 = []
intense_18 = []
```

[6]:
```
#for e in str_1[1::]:
 #   e.replace('\t', ' ')
  #  print(e)#

for i in range(1, len(str_1),1):
    tmp = str_1[i].split()
    field_01.append(float(tmp[0]))
    intense_01.append(float(tmp[1]))
```

[7]:
```
for i in range(1, len(str_2),1):
    tmp = str_2[i].split()
    field_03.append(float(tmp[0]))
    intense_03.append(float(tmp[1]))
for i in range(1, len(str_3),1):
    tmp = str_3[i].split()
    field_05.append(float(tmp[0]))
    intense_05.append(float(tmp[1]))
for i in range(1, len(str_4),1):
    tmp = str_4[i].split()
    field_08.append(float(tmp[0]))
```

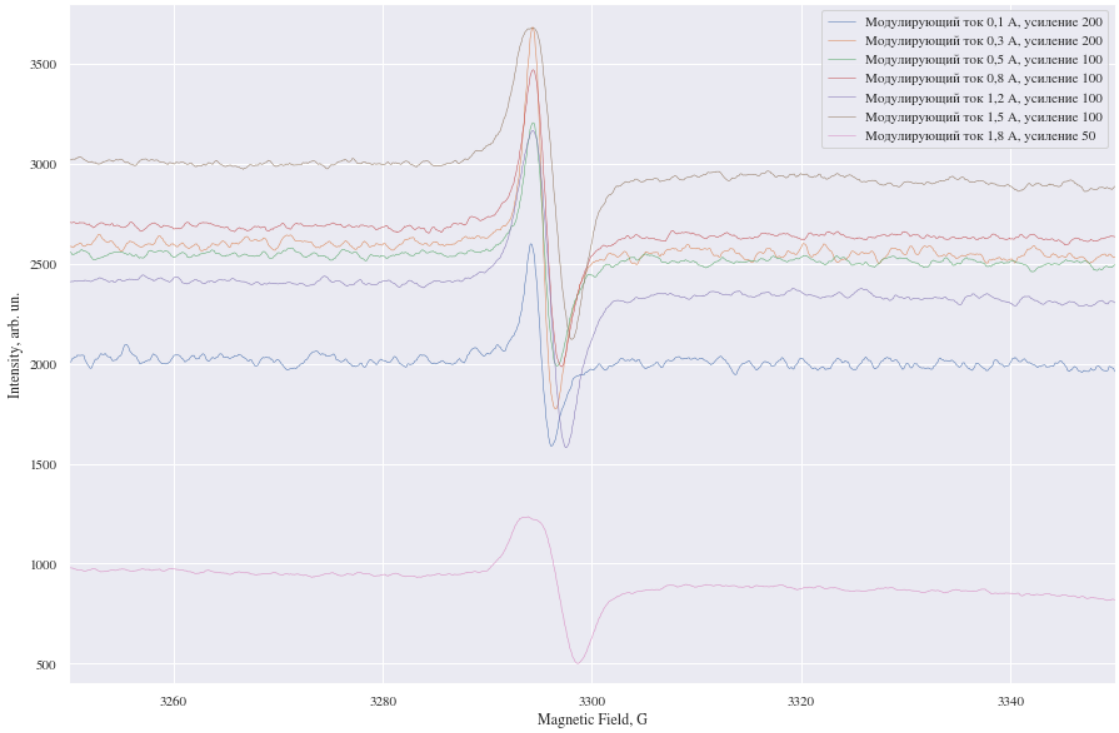
```
    intense_08.append(float(tmp[1]))
for i in range(1, len(str_5),1):
    tmp = str_5[i].split()
    field_12.append(float(tmp[0]))
    intense_12.append(float(tmp[1]))
for i in range(1, len(str_6),1):
    tmp = str_6[i].split()
    field_15.append(float(tmp[0]))
    intense_15.append(float(tmp[1]))
for i in range(1, len(str_7),1):
    tmp = str_7[i].split()
    field_18.append(float(tmp[0]))
    intense_18.append(float(tmp[1]))
```

[8]:
```
file_1.close()
file_2.close()
file_3.close()
file_4.close()
file_5.close()
file_6.close()
file_7.close()
```

[9]:
```
def Lorentzian(x, amp1, cen1, wid1):
    return (amp1*wid1**2/((x - cen1)**2 - wid1**2))
```

[10]:
```
plt.rcParams["figure.figsize"] = (15,10)
plt.plot(field_01, intense_01, lw = 0.5, label = '          0,1  ,      200')
plt.plot(field_03, intense_03, lw = 0.5, label = '          0,3  ,      200')
plt.plot(field_05, intense_05, lw = 0.5, label = '          0,5  ,      100')
plt.plot(field_08, intense_08, lw = 0.5, label = '          0,8  ,      100')
plt.plot(field_12, intense_12, lw = 0.5, label = '          1,2  ,      100')
plt.plot(field_15, intense_15, lw = 0.5, label = '          1,5  ,      100')
plt.plot(field_18, intense_18, lw = 0.5, label = '          1,8  ,      50')

plt.xlabel('Magnetic Field, G')
plt.ylabel('Intensity, arb. un.')

plt.axis([3250, 3350, 400, 3800])
plt.legend()
```

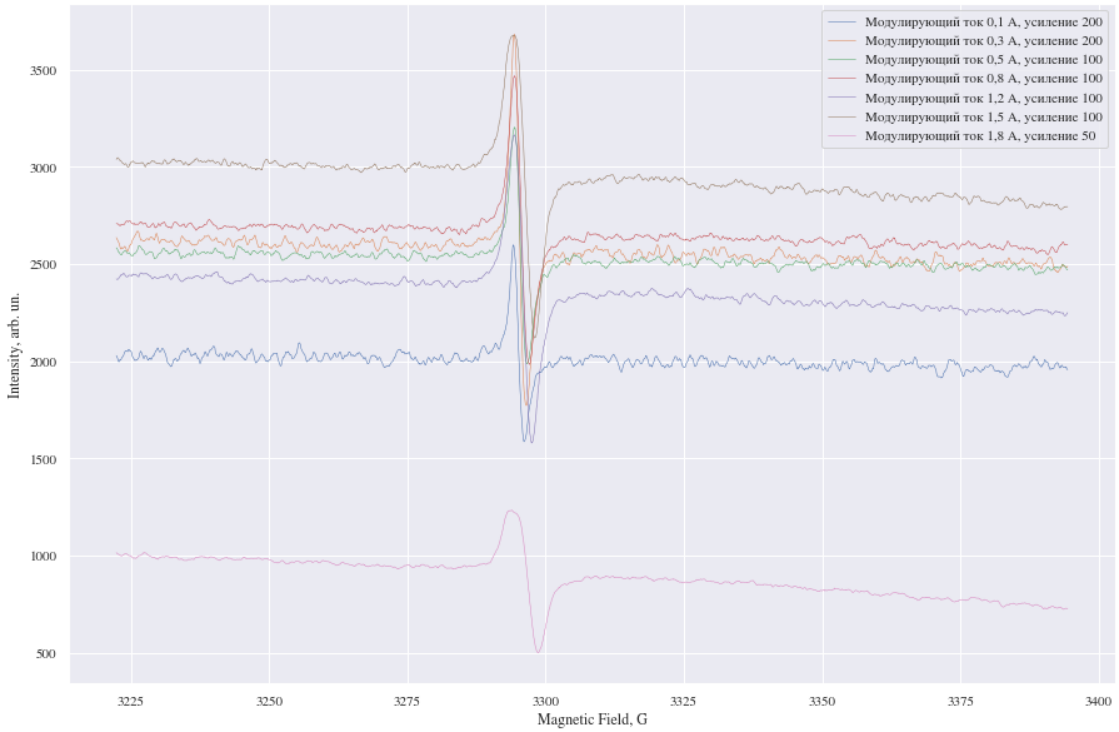
[10]:
```
<matplotlib.legend.Legend at 0x29ad9523340>
```



,

[11]:
```
plt.plot(field_01[3250:6000], intense_01[3250:6000], lw = 0.5, label = '
 ↪   0,1  ,       200')
plt.plot(field_03[3250:6000], intense_03[3250:6000], lw = 0.5, label = '
 ↪   0,3  ,       200')
plt.plot(field_05[3250:6000], intense_05[3250:6000], lw = 0.5, label = '
 ↪   0,5  ,       100')
plt.plot(field_08[3250:6000], intense_08[3250:6000], lw = 0.5, label = '
 ↪   0,8  ,       100')
plt.plot(field_12[3250:6000], intense_12[3250:6000], lw = 0.5, label = '
 ↪   1,2  ,       100')
plt.plot(field_15[3250:6000], intense_15[3250:6000], lw = 0.5, label = '
 ↪   1,5  ,       100')
plt.plot(field_18[3250:6000], intense_18[3250:6000], lw = 0.5, label = '
 ↪   1,8  ,       50')
plt.xlabel('Magnetic Field, G')
plt.ylabel('Intensity, arb. un.')


plt.legend()
```

[11]: <matplotlib.legend.Legend at 0x29ad97defd0>



[12]:
```
# All Lorentzian
mx_01 = max(intense_01[3250:6000])
imx_01 = intense_01[3250:6000].index(mx_01)
mx_03 = max(intense_03[3250:6000])
imx_03 = intense_03[3250:6000].index(mx_03)
mx_05 = max(intense_05[3250:6000])
imx_05 = intense_05[3250:6000].index(mx_05)
mx_08 = max(intense_08[3250:6000])
imx_08 = intense_08[3250:6000].index(mx_08)
mx_12 = max(intense_12[3250:6000])
imx_12 = intense_12[3250:6000].index(mx_12)
mx_15 = max(intense_15[3250:6000])
imx_15 = intense_15[3250:6000].index(mx_15)
mx_18 = max(intense_18[3250:6000])
imx_18 = intense_18[3250:6000].index(mx_18)

min_01 = min(intense_01[3250:6000])
imn_01 = intense_01[3250:6000].index(min_01)
min_03 = min(intense_03[3250:6000])
imn_03 = intense_03[3250:6000].index(min_03)
min_05 = min(intense_05[3250:6000])
imn_05 = intense_05[3250:6000].index(min_05)
min_08 = min(intense_08[3250:6000])
```

```
imn_08 = intense_08[3250:6000].index(min_08)
min_12 = min(intense_12[3250:6000])
imn_12 = intense_12[3250:6000].index(min_12)
min_15 = min(intense_15[3250:6000])
imn_15 = intense_15[3250:6000].index(min_15)
min_18 = min(intense_18[3250:6000])
imn_18 = intense_18[3250:6000].index(min_18)
```

[13]:
```
dH = []
cur = [0.1, 0.3, 0.5, 0.8, 1.2, 1.5, 1.8]

dH.append(np.sqrt(3)/2 * (field_01[imn_01] - field_01[imx_01]))
dH.append(np.sqrt(3)/2 * (field_03[imn_03] - field_03[imx_03]))
dH.append(np.sqrt(3)/2 * (field_05[imn_05] - field_05[imx_05]))
dH.append(np.sqrt(3)/2 * (field_08[imn_08] - field_08[imx_08]))
dH.append(np.sqrt(3)/2 * (field_12[imn_12] - field_12[imx_12]))
dH.append(np.sqrt(3)/2 * (field_15[imn_15] - field_15[imx_15]))
dH.append(np.sqrt(3)/2 * (field_18[imn_18] - field_18[imx_18]))
```

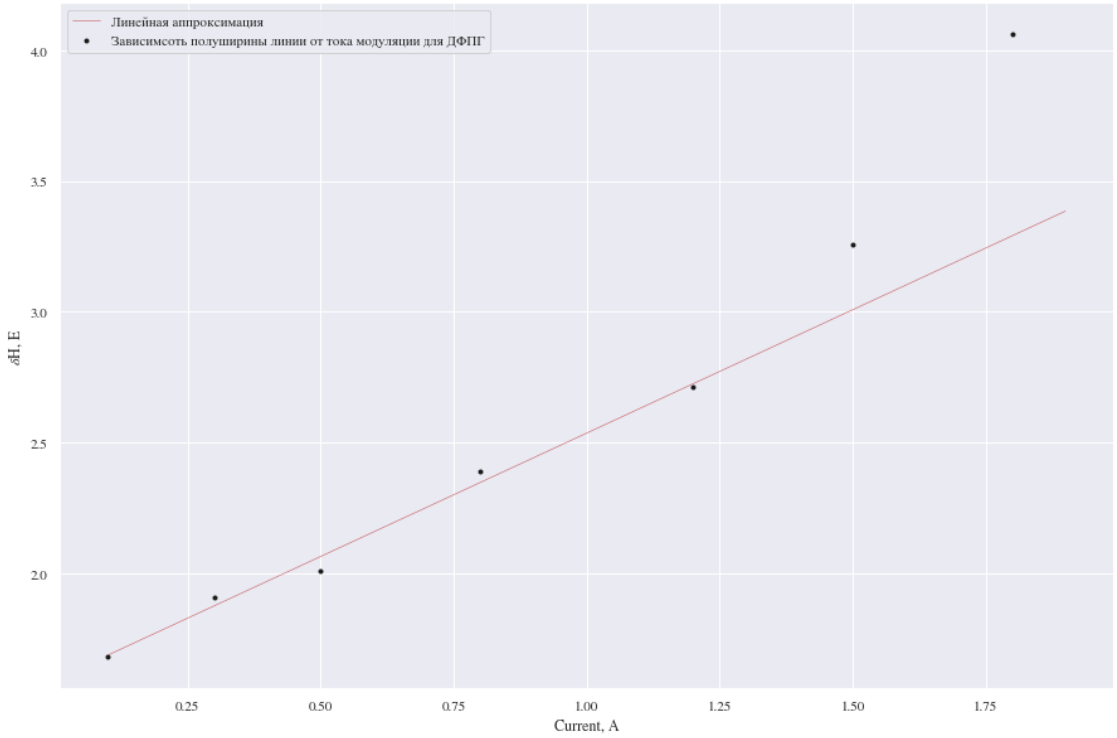
[14]:
```
dH # dH = sqrt(3)/2 * DeltaH_max
```

[14]:
```
[1.6800892833414642,
 1.9052558883256074,
 2.0091789367800392,
 2.390230114444846,
 2.7106595138453873,
 3.2562555182292843,
 4.06165914374867]
```

[15]:
```
plt.scatter(cur, dH, marker = '.', color = 'k', label = '
 ↪           ')

x = np.linspace(0.1, 1.9, 100)
a, b, s, e = chi_sq(cur[0:5], dH[0:5], None)
y = a * x + b
print(a,b,s,e)

plt.plot(x,y, lw = 0.5, color = 'r', label = '            ')
plt.xlabel('Current, A')
plt.ylabel('$\delta$H, E')

plt.legend()
```

```
0.9435971989272619 1.5917963719696568 0.0517044476788302 0.03604508422427963
```

[15]:
```
<matplotlib.legend.Legend at 0x29ad9a984c0>
```



1,5 , -

[16]:
```
#Mn

file_1m = open('Mn0,1_20.epr.txt')
str_1m = file_1m.read().splitlines()

file_2m = open('Mn0,05_50.epr.txt')
str_2m = file_2m.read().splitlines()

file_3m = open('Mn0,5_10.epr.txt')
str_3m = file_3m.read().splitlines()

file_4m = open('Mn1_10.epr.txt')
str_4m = file_4m.read().splitlines()

file_5m = open('Mn0,8_10.epr.txt')
str_5m = file_5m.read().splitlines()


field_01m = []
field_005m = []
field_05m = []
field_1m = []
```

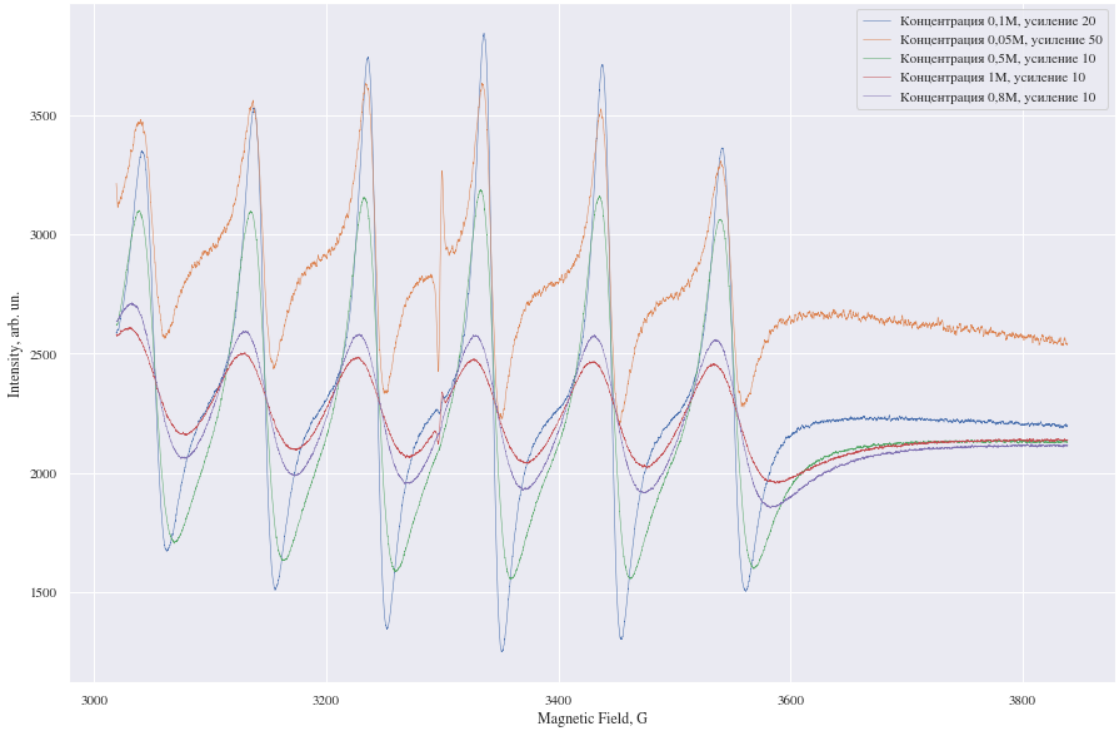
```
field_08m = []

intense_01m = []
intense_005m = []
intense_05m = []
intense_1m = []
intense_08m = []
```

[17]:
```
for i in range(1, len(str_1m),1):
    tmp = str_1m[i].split()
    field_01m.append(float(tmp[0]))
    intense_01m.append(float(tmp[1]))
for i in range(1, len(str_2m),1):
    tmp = str_2m[i].split()
    field_005m.append(float(tmp[0]))
    intense_005m.append(float(tmp[1]))
for i in range(1, len(str_3m),1):
    tmp = str_3m[i].split()
    field_05m.append(float(tmp[0]))
    intense_05m.append(float(tmp[1]))
for i in range(1, len(str_4m),1):
    tmp = str_4m[i].split()
    field_1m.append(float(tmp[0]))
    intense_1m.append(float(tmp[1]))
for i in range(1, len(str_5m),1):
    tmp = str_5m[i].split()
    field_08m.append(float(tmp[0]))
    intense_08m.append(float(tmp[1]))
```

[18]:
```
file_1m.close()
file_2m.close()
file_3m.close()
file_4m.close()
file_5m.close()
```

[19]:
```
plt.rcParams["figure.figsize"] = (15,10)
plt.plot(field_01m, intense_01m, lw = 0.5, label = '       0,1 ,       20')
plt.plot(field_005m, intense_005m, lw = 0.5, label = '       0,05 ,       50')
plt.plot(field_05m, intense_05m, lw = 0.5, label = '       0,5 ,       10')
plt.plot(field_1m, intense_1m, lw = 0.5, label = '       1 ,       10')
plt.plot(field_08m, intense_08m, lw = 0.5, label = '       0,8 ,       10')

plt.xlabel('Magnetic Field, G')
plt.ylabel('Intensity, arb. un.')

#plt.axis([3250, 3350, 400, 3800])
plt.legend()
```

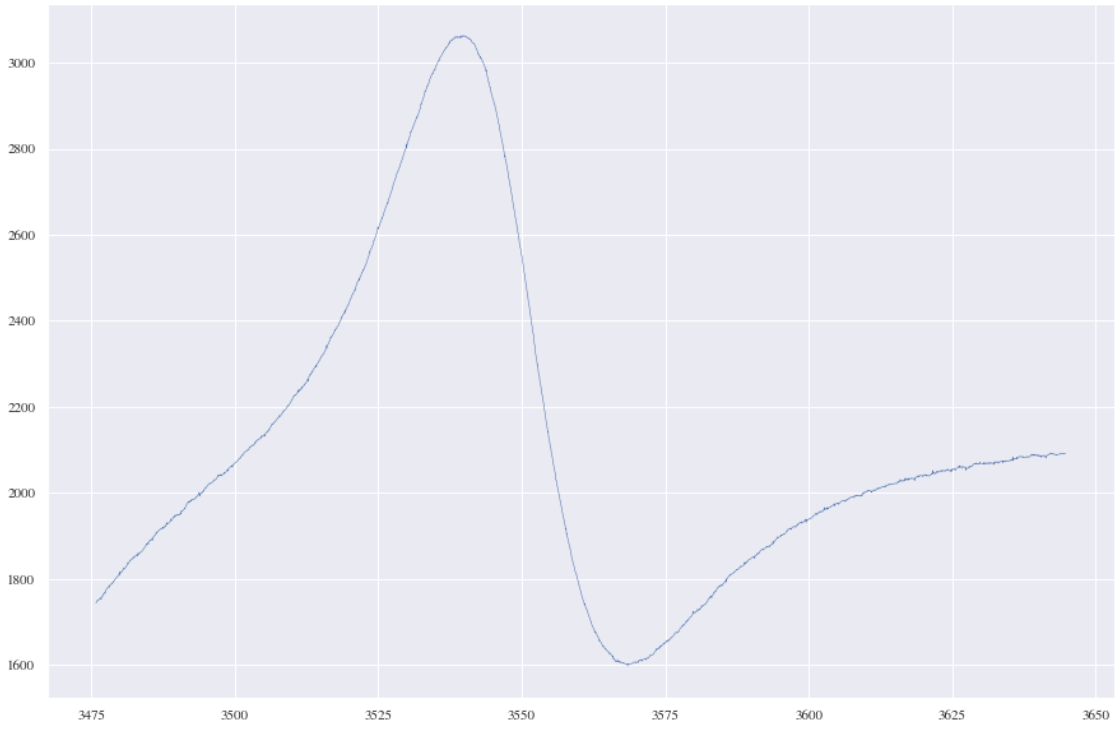
[19]: <matplotlib.legend.Legend at 0x29ad9dadc70>



0,5 . 1 ,

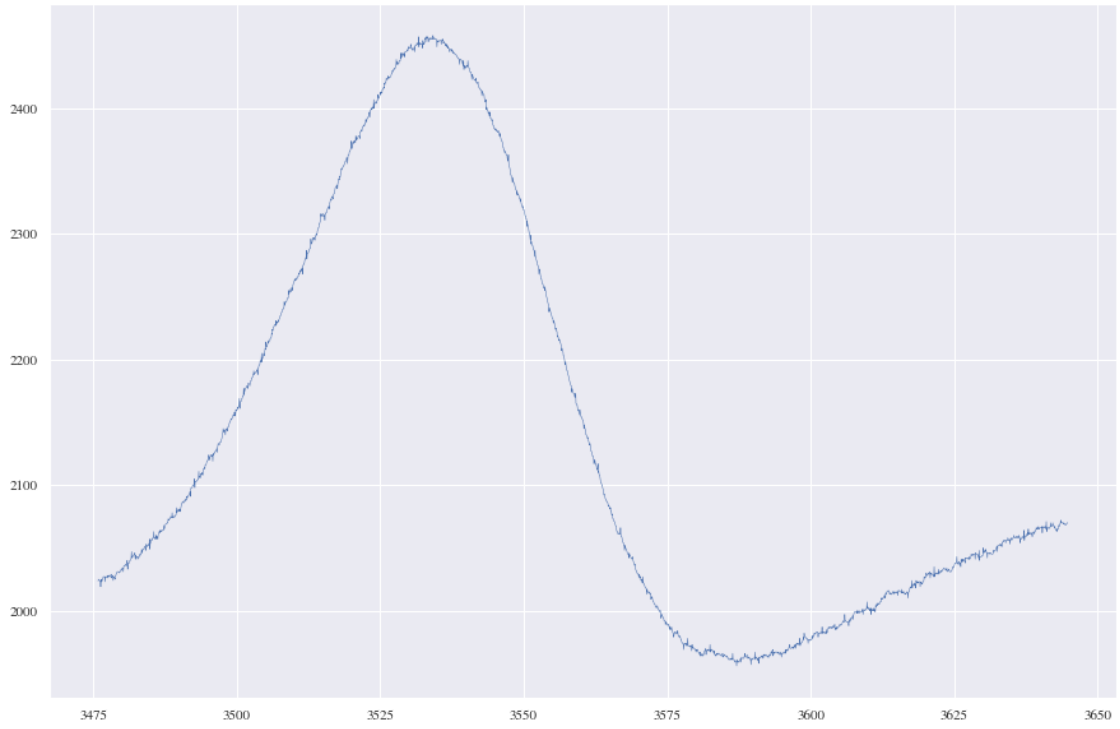
[20]:
```
plt.plot(field_05m[7300:10000], intense_05m[7300:10000], lw = 0.5, label =␣
↪'       0,5 ,      10')
```

[20]: [<matplotlib.lines.Line2D at 0x29adbfb9340>]



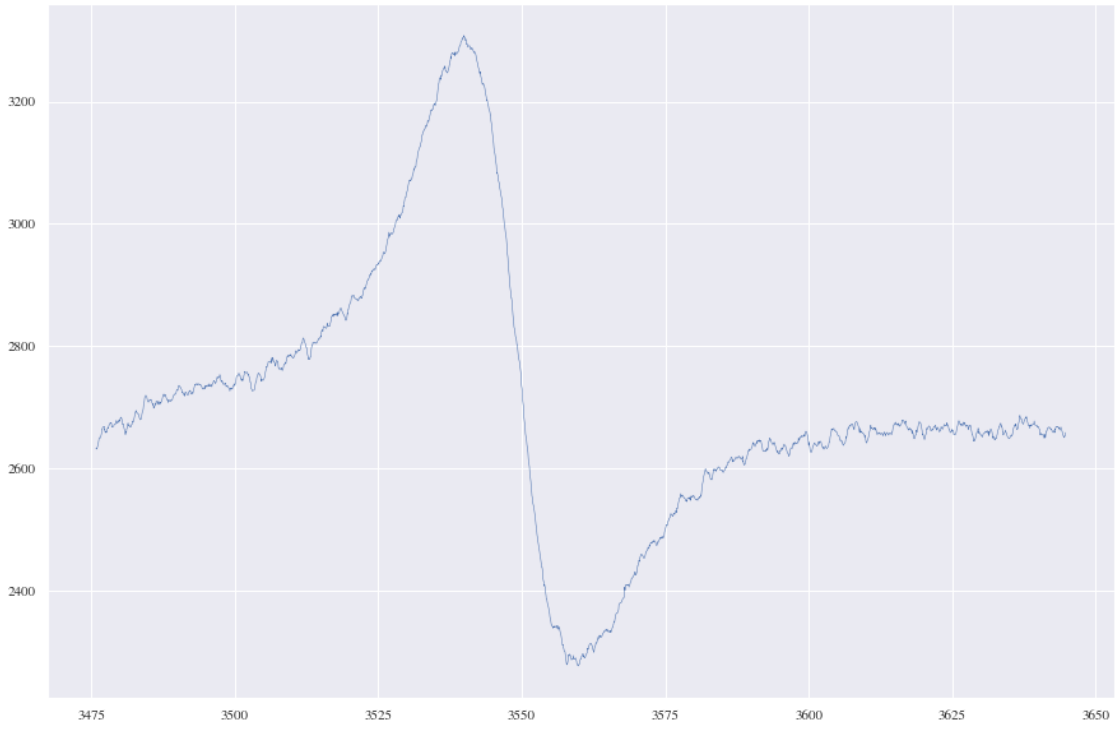
[21]:
```
plt.plot(field_1m[7300:10000], intense_1m[7300:10000], lw = 0.5, label =␣
↪'        1 ,       10')
```

[21]:
```
[<matplotlib.lines.Line2D at 0x29adbecac10>]
```



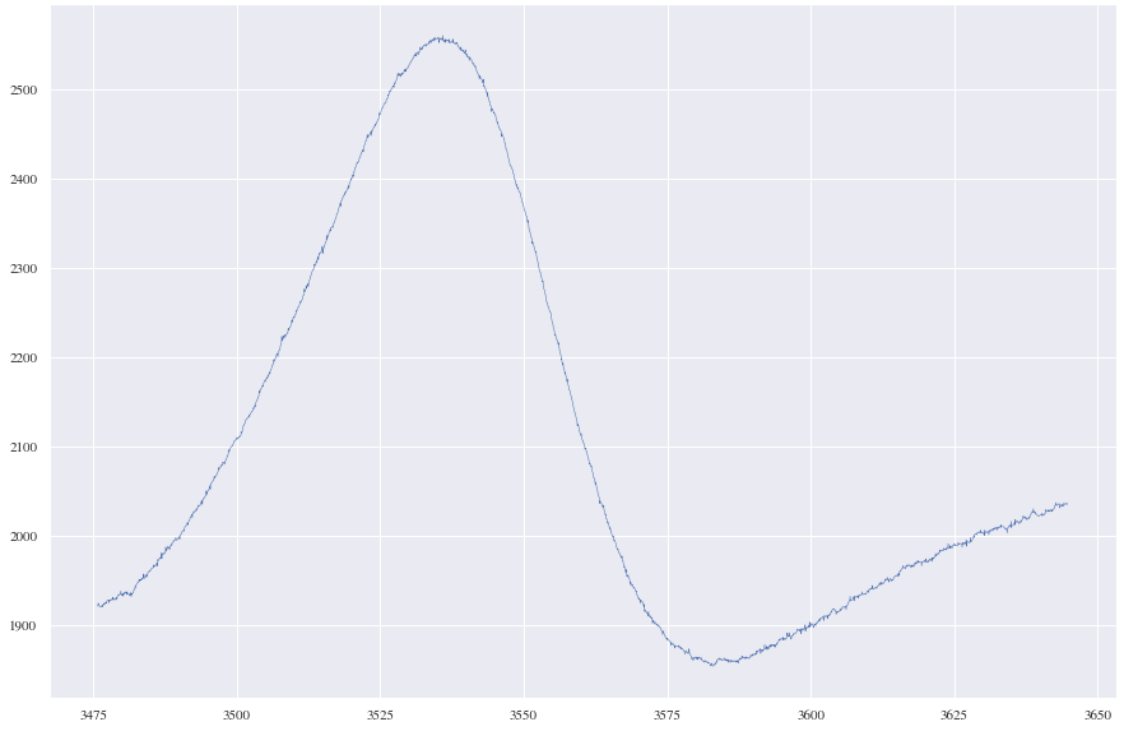
[22]:
```
plt.plot(field_005m[7300:10000], intense_005m[7300:10000], lw = 0.5, label =␣
↪'       0,05 ,      20')
```

[22]: [<matplotlib.lines.Line2D at 0x29adbf21670>]



[23]:
```
plt.plot(field_08m[7300:10000], intense_08m[7300:10000], lw = 0.5, label =␣
↪'       0,8 ,      10')
```

[23]:
```
[<matplotlib.lines.Line2D at 0x29adbf782e0>]
```



[24]:
```
mx_01m = max(intense_01m[7300:10000])
imx_01m = intense_01m[7300:10000].index(mx_01m)
mx_005m = max(intense_005m[7300:10000])
imx_005m = intense_005m[7300:10000].index(mx_005m)
mx_05m = max(intense_05m[7300:10000])
imx_05m = intense_05m[7300:10000].index(mx_05m)
mx_1m = max(intense_1m[7300:10000])
imx_1m = intense_1m[7300:10000].index(mx_1m)
mx_08m = max(intense_08m[7300:10000])
imx_08m = intense_08m[7300:10000].index(mx_08m)


min_01m = min(intense_01m[7300:10000])
imn_01m = intense_01m[7300:10000].index(min_01m)
min_005m = min(intense_005m[7300:10000])
imn_005m = intense_005m[7300:10000].index(min_005m)
min_05m = min(intense_05m[7300:10000])
imn_05m = intense_05m[7300:10000].index(min_05m)
min_1m = min(intense_1m[7300:10000])
imn_1m = intense_1m[7300:10000].index(min_1m)
min_08m = min(intense_08m[7300:10000])
imn_08m = intense_08m[7300:10000].index(min_08m)
```

[25]:
```
len(intense_08m), len(field_08m)
```

[25]: (13104, 13104)

[26]:
```
field_08m[7300:10000][imx_08m], field_08m[7300:10000][imn_08m]
```

[26]: (3535.9, 3582.58)

[27]:
```
dH_m = []
conc = [0.1, 0.05, 0.5, 1, 0.8]

dH_m.append(np.sqrt(3)/2 * (field_01m[7300:10000][imn_01m] - field_01m[7300:
↪10000][imx_01m])) #Lorentz
dH_m.append(np.sqrt(3)/2 * (field_005m[7300:10000][imn_005m] - field_005m[7300:
↪10000][imx_005m])) #Lorentz
dH_m.append(np.sqrt(2/np.log(2)) * (field_05m[7300:10000][imn_05m] -␣
↪field_05m[7300:10000][imx_05m])) #Gauss
dH_m.append(np.sqrt(2/np.log(2))* (field_1m[7300:10000][imn_1m] - field_1m[7300:
↪10000][imx_1m])) #Gauss
dH_m.append(np.sqrt(2/np.log(2))* (field_08m[7300:10000][imn_08m] -␣
↪field_08m[7300:10000][imx_08m])) #Gauss
```

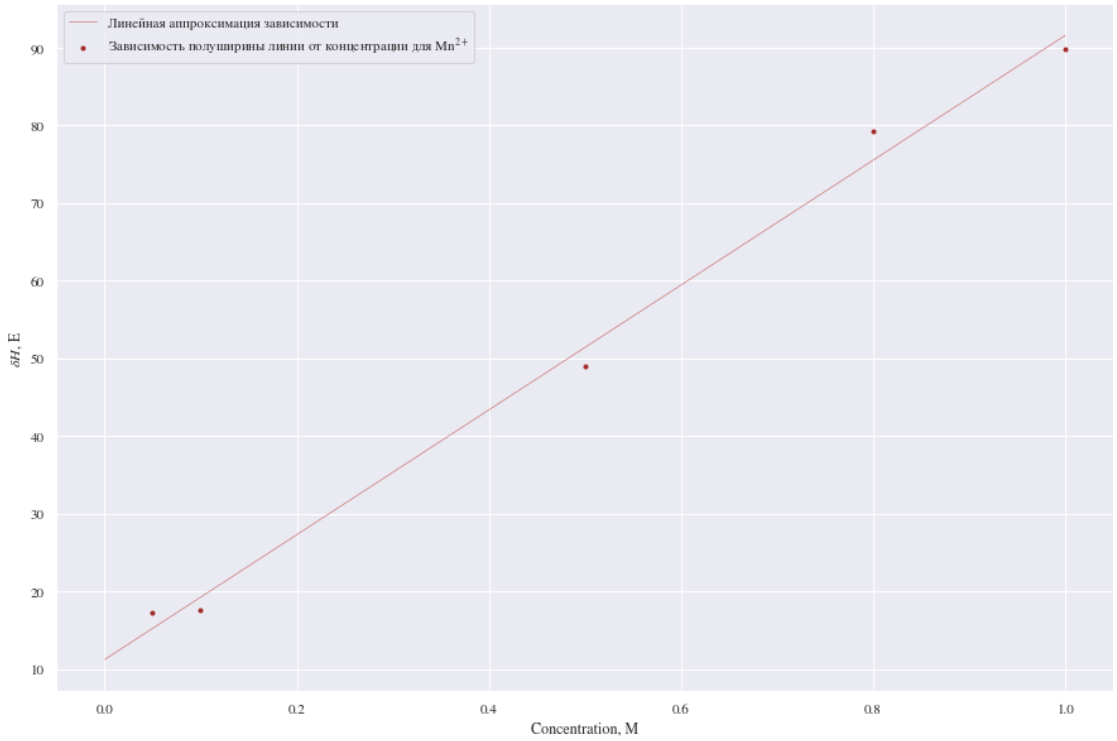
[28]:
```
dH_m
```

[28]:
```
[17.562995188748193,
 17.285867059537427,
 49.005867876618545,
 89.82427359846108,
 79.29268327488919]
```

[29]:
```
plt.scatter(conc, dH_m, marker = '.', color = 'brown', label = '                ␣
↪                Mn$^{2+}$')

x = np.linspace(0, 1, 100)

am, bm, sm, em = chi_sq(conc, dH_m, None)
y = am * x + bm

print(am, bm, sm, em)

plt.plot(x,y, lw = 0.5, color = 'r', label = '                    ')

plt.xlabel('Concentration, M')
plt.ylabel('$\delta H$, E')

plt.legend()
```

```
80.37866160105034 11.208793215136174 3.786693222398202 2.335809694158027
```

[29]: <matplotlib.legend.Legend at 0x29ad981d5b0>



[30]:
```
#Y' * DeltaH^2 = S

S = []
S.append((mx_01m - min_01m)/2 * (field_01m[7300:10000][imn_01m] -␣
 ↪field_01m[7300:10000][imx_01m])**2)
S.append((mx_005m - min_005m)/2 * (field_005m[7300:10000][imn_005m] -␣
 ↪field_005m[7300:10000][imx_005m])**2)
S.append((mx_05m - min_05m)/2 * (field_05m[7300:10000][imn_05m] -␣
 ↪field_05m[7300:10000][imx_05m])**2)
S.append((mx_1m - min_1m)/2 * (field_1m[7300:10000][imn_1m] - field_1m[7300:
 ↪10000][imx_1m])**2)
S.append((mx_08m - min_08m)/2 * (field_08m[7300:10000][imn_08m] -␣
 ↪field_08m[7300:10000][imx_08m])**2)
```

[31]:
```
S
```

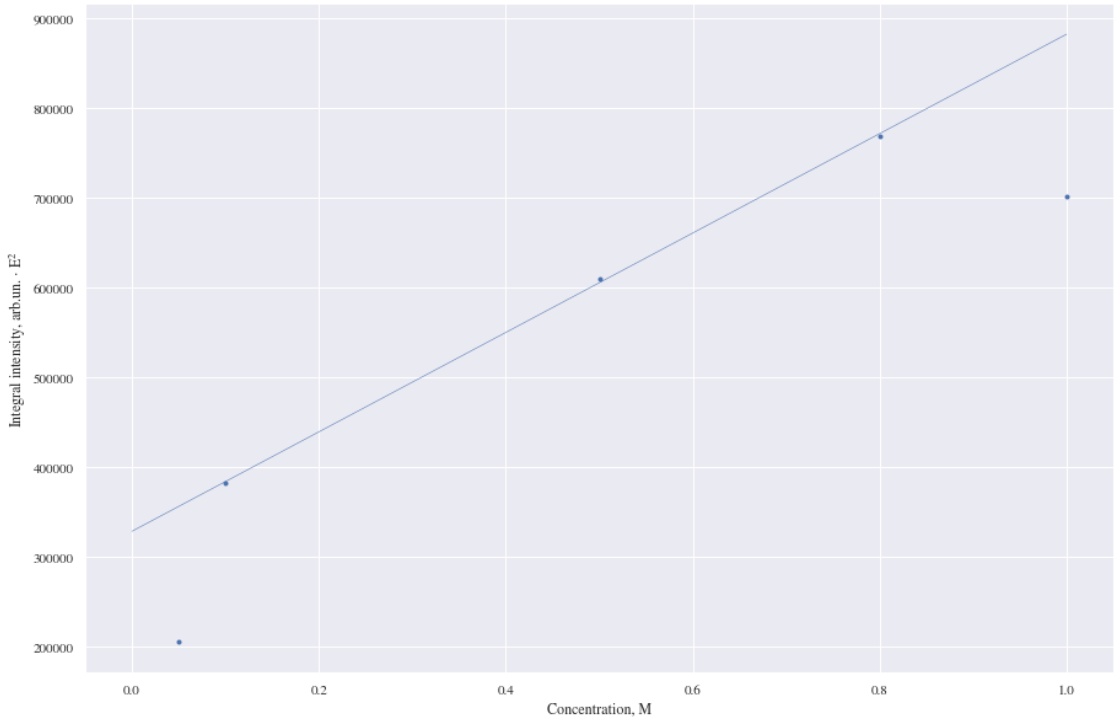
[31]:
```
[382283.27279999043,
 205575.22560000076,
 609676.2312499961,
 701869.8944000029,
 769194.9071999947]
```

[ ]:
```
# I prop S intensivnost pogloschenia
```

[32]:
```
plt.scatter(conc, S, marker = '.')
c = [0.1, 0.5, 0.8]
s = [382283.27279999043,609676.2312499961, 769194.9071999947 ]

a_s, b_s, s_s, e_s = chi_sq(c,s, None)
print(a_s, b_s, s_s, e_s)
y_s = a_s * x + b_s

plt.plot(x, y_s, lw = 0.5)

plt.xlabel('Concentration, M')
plt.ylabel('Integral intensity, arb.un. $\cdot$ E$^{2}$')
```

```
553582.3381689254 328713.04593782854 10323.062866231612 5654.1744354513385
```

[32]:
```
Text(0, 0.5, 'Integral intensity, arb.un. $\\cdot$ E$^{2}$')
```



[ ]:
```

```

[33]:
```
gamma = 17.6 * 10**6 #1/(E*s)
K_e = gamma * am
sig_K_e = K_e * sm/am
```

[34]:
```
K_e, sig_K_e #1/(M * s)
```

[34]:
```
(1414664444.1784859, 66645800.71420835)
```

[35]:
```
tau_e = []
for i in range(5):
    tau_e.append(1/(K_e * conc[i]))
```

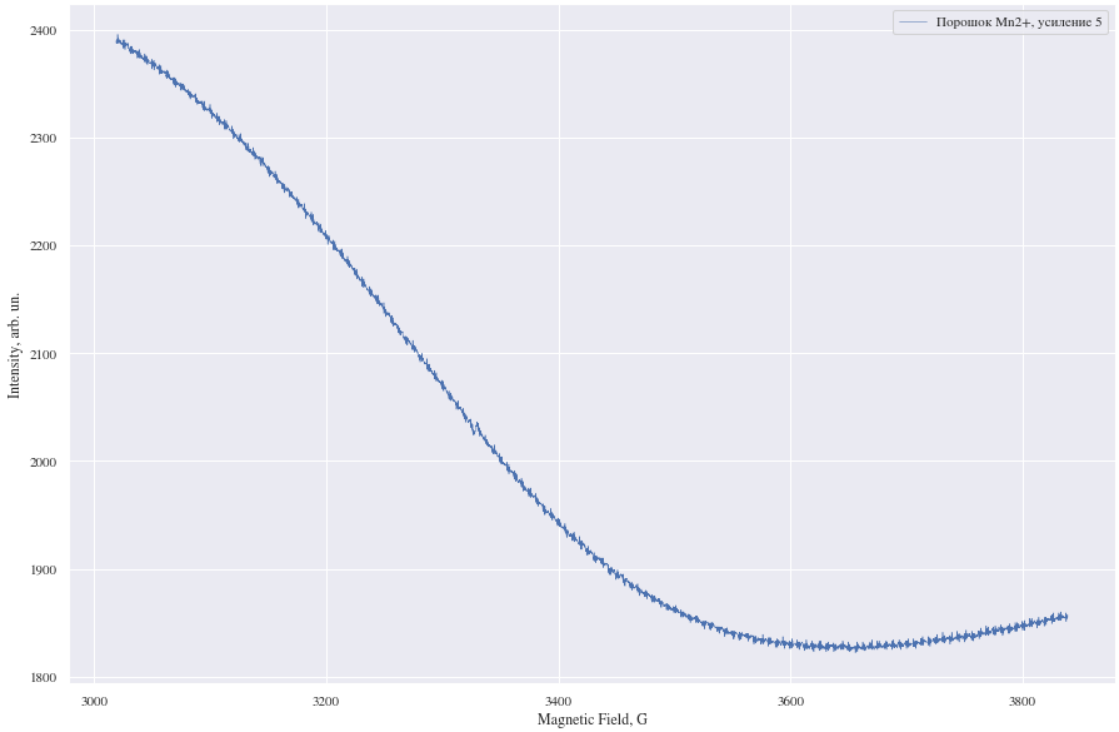
[36]:
```
tau_e
```

[36]:
```
[7.068814121363693e-09,
 1.4137628242727385e-08,
 1.4137628242727384e-09,
 7.068814121363692e-10,
 8.836017651704616e-10]
```

[37]:
```
# solid Mn

file_sMn = open('Mn_solid_5.epr.txt')
str_sMn = file_sMn.read().splitlines()

field_sMn = []
intense_sMn = []

for i in range(1, len(str_sMn),1):
    tmp = str_sMn[i].split()
    field_sMn.append(float(tmp[0]))
    intense_sMn.append(float(tmp[1]))

file_sMn.close()
```

[38]:
```
plt.plot(field_sMn, intense_sMn, lw = 0.5, label = '     Mn2+,      5')

plt.xlabel('Magnetic Field, G')
plt.ylabel('Intensity, arb. un.')

#plt.axis([3250, 3350, 400, 3800])
plt.legend()
```

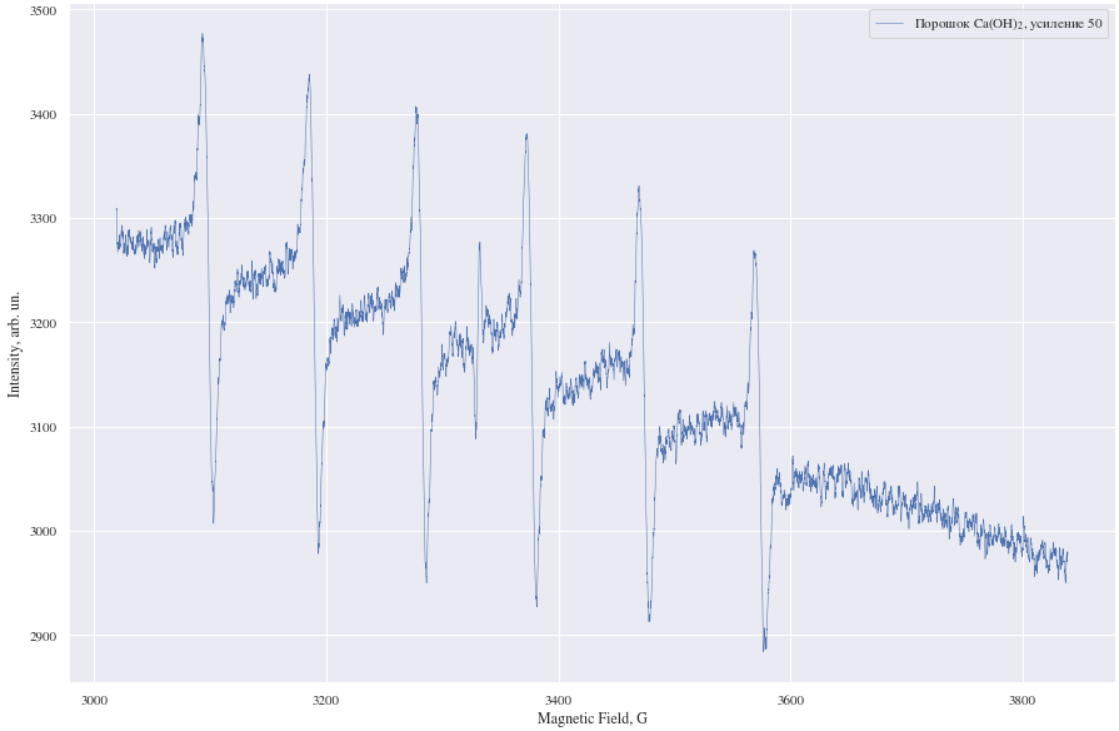
[38]:
```
<matplotlib.legend.Legend at 0x29adbee7a90>
```



[39]:
```
# solid Ca

file_sCa = open('Ca_solid_50.epr.txt')
str_sCa = file_sCa.read().splitlines()

field_sCa = []
intense_sCa = []

for i in range(1, len(str_sCa),1):
    tmp = str_sCa[i].split()
    field_sCa.append(float(tmp[0]))
    intense_sCa.append(float(tmp[1]))

file_sCa.close()
```

[40]:
```
plt.plot(field_sCa, intense_sCa, lw = 0.5, label = '    Ca(OH)$_2$,      50')

plt.xlabel('Magnetic Field, G')
plt.ylabel('Intensity, arb. un.')

#plt.axis([3250, 3350, 400, 3800])
plt.legend()
```

[40]: <matplotlib.legend.Legend at 0x29add202850>

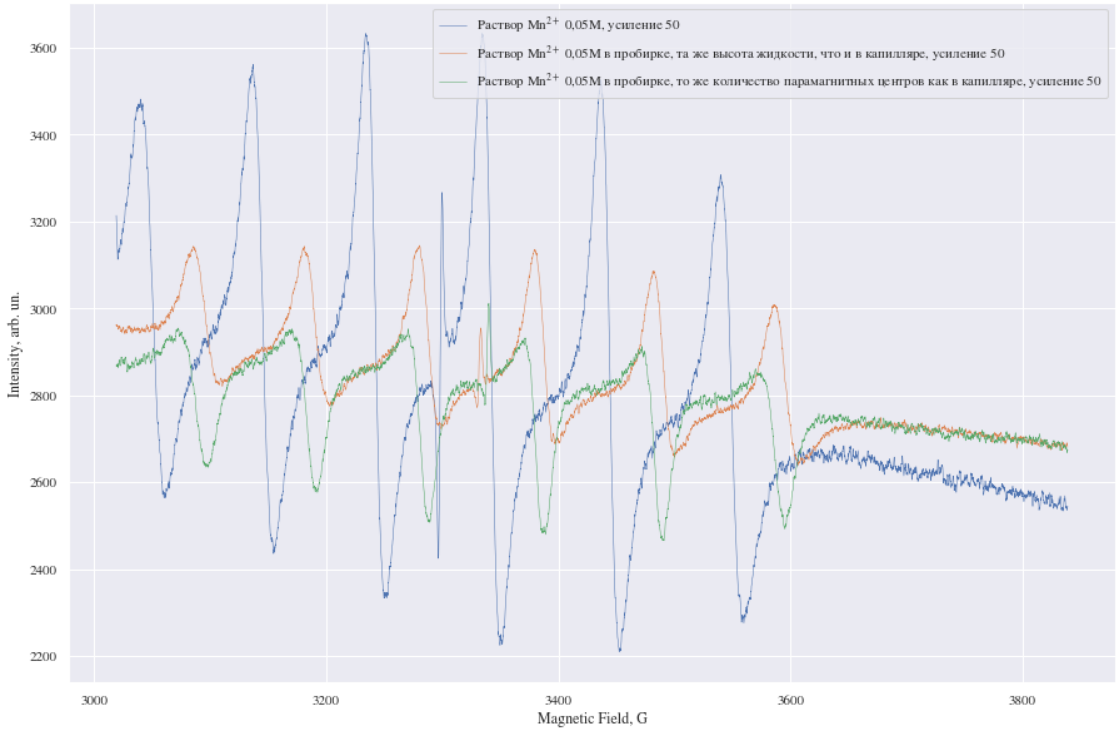


[41]:
```
#dielectric loss

file_005_pr = open('Mn0,05_prob_50.epr.txt')
str_005_pr = file_005_pr.read().splitlines()

file_005_pr_b = open('Mn0,05_prob(b)_50.epr.txt')
str_005_pr_b = file_005_pr_b.read().splitlines()

field_005_pr = []
field_005_pr_b = []
intense_005_pr = []
intense_005_pr_b = []

for i in range(1, len(str_005_pr),1):
    tmp = str_005_pr[i].split()
    field_005_pr.append(float(tmp[0]))
    intense_005_pr.append(float(tmp[1]))
for i in range(1, len(str_005_pr_b),1):
    tmp = str_005_pr_b[i].split()
    field_005_pr_b.append(float(tmp[0]))
    intense_005_pr_b.append(float(tmp[1]))
```

```
file_005_pr.close()
file_005_pr_b.close()
```

[42]:
```
plt.plot(field_005m, intense_005m, lw = 0.5, label = '     Mn$^{2+}$ 0,05M,␣
↪     50')
plt.plot(field_005_pr, intense_005_pr, lw = 0.5, label = '     Mn$^{2+}$ 0,05M ␣
↪    ,              ,           ,      50')
plt.plot(field_005_pr_b, intense_005_pr_b, lw = 0.5, label = '     Mn$^{2+}$$␣
↪0,05M       ,                                  ,      50')
plt.xlabel('Magnetic Field, G')
plt.ylabel('Intensity, arb. un.')

#plt.axis([3250, 3350, 400, 3800])
plt.legend()
```

[42]:
```
<matplotlib.legend.Legend at 0x29add3fe4c0>
```



[ ]:
```

```

[ ]:
```

```