curve-of-growth

September 8, 2018

1 Tarea 5 - Equivalent widths of absorption lines

Find the curve of growth: equivalent width versus line strength. Assume a Voigt (Hjelming) line profile and a Milne-Eddington model for the line formation.

```
In [1]: import numpy as np
        from astropy.convolution import convolve_fft, Gaussian1DKernel
        from scipy.integrate import quad
        from matplotlib import pyplot as plt
        %matplotlib inline
        import seaborn as sns
        sns.set(context='notebook',
                style='whitegrid',
                palette='dark',
                font_scale=1.5,
                color_codes=True,
                rc={'figure.figsize': (8,6)},
               )
```

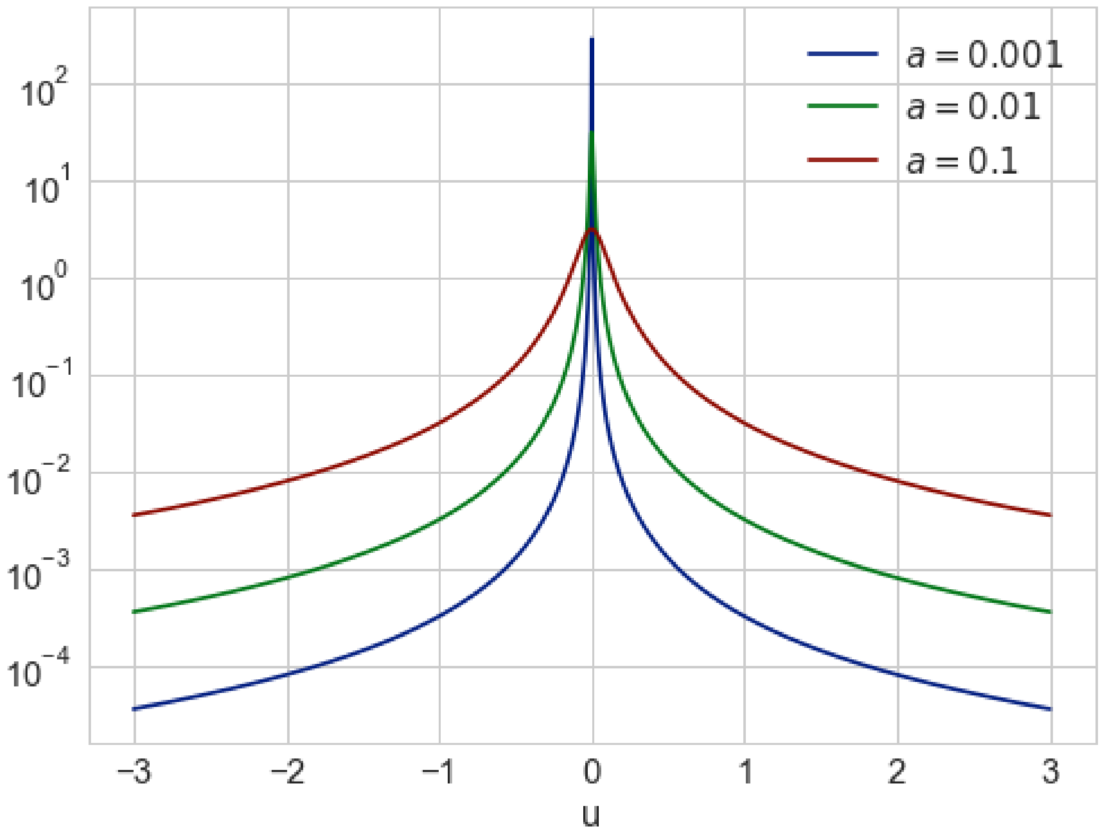
1.1 The absorption profile

The absorption profile ϕ_ν is the convolution of a Gaussian and a Lorentzian. We construct the Lorentzian explicitly and then use FFT to convolve with the Gaussian. We use a dimensional frequency shift, u, which is in units of the Doppler width: $u \equiv (\nu - \nu_0)/\Delta\nu_D$.

```
In [2]: def Lorentz(u, a=1e-6):
            return (a / np.pi) / (a**2 + u**2)
```

Test the Lorentz function

```
In [3]: fig, ax = plt.subplots()
        ugrid = np.linspace(-3.0, 3.0, 10000)
        for a in reversed([0.1, 0.01, 0.001]):
            ax.plot(ugrid, Lorentz(ugrid, a), label=f"$a = {a}$")
        ax.legend()
        ax.set(yscale="log", xlabel="u")
        None
```



So, this seems to work. Note that the central peak is higher for smaller a, since it is normalized to unit area under the curve.

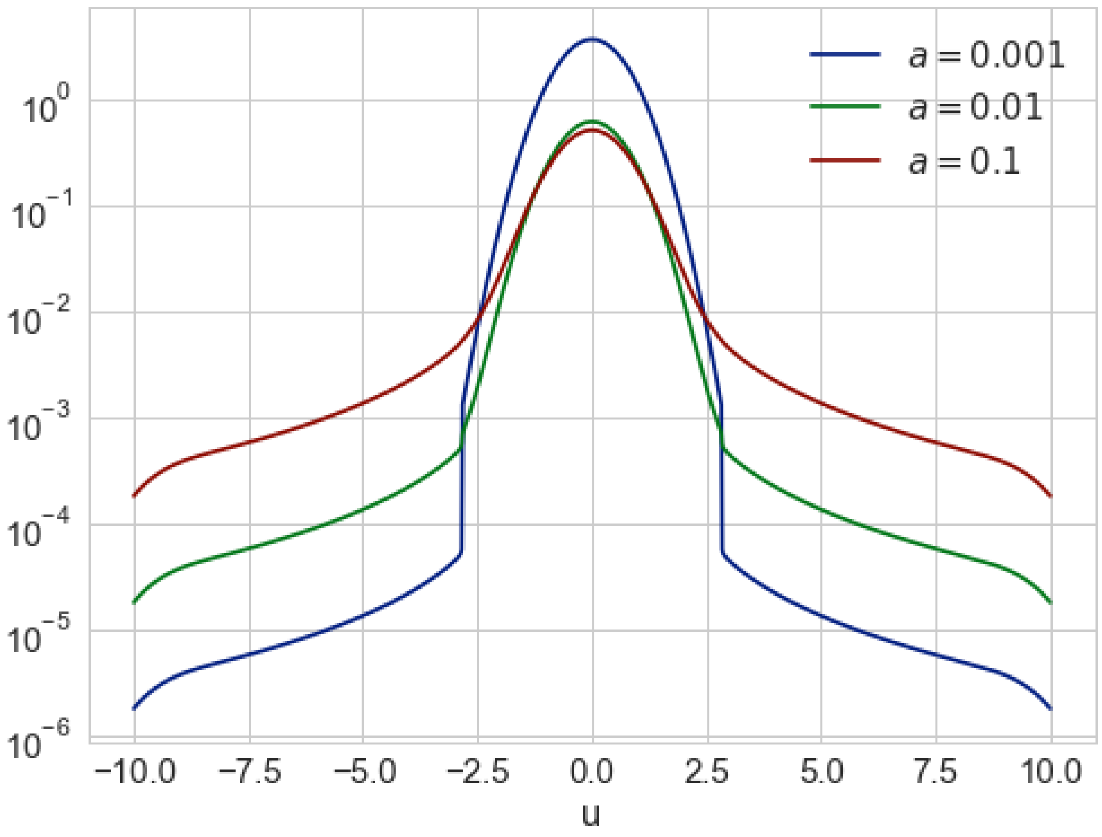
1.1.1 Convolution method for integral (mainly works, if we are careful)

First we use the default parameters for FFT convolution in `astropy.convolution`.
Note: *This does not work well, as we will see.*

```
In [4]: ugrid = np.linspace(-10.0, 10.0, 1001)
        ustep = ugrid[1] - ugrid[0]
        kernel = Gaussian1DKernel(stddev=1.0/np.sqrt(2)/ustep)
        def H_conv_naive(u, a=1e-6):
            return convolve_fft(Lorentz(u, a), kernel)
```

Note that the kernel width must be given in pixels, not in units of u, so we first calculate the pixel size `ustep` and use a standard deviation of `1.0/ustep` pixels, which corresponds to 1 in units of u.

```
In [5]: fig, ax = plt.subplots()
        for a in reversed([0.1, 0.01, 0.001]):
            ax.plot(ugrid, H_conv_naive(ugrid, a), label=f"$a = {a}$")
        ax.legend()
        ax.set(yscale="log", xlabel="u")
        None
```



So, there are three problems with this:

1. The turn down at the left and right edges.

2. The jump at $u = \pm 4$.
3. The normalization seems wrong

We fix these as follows:

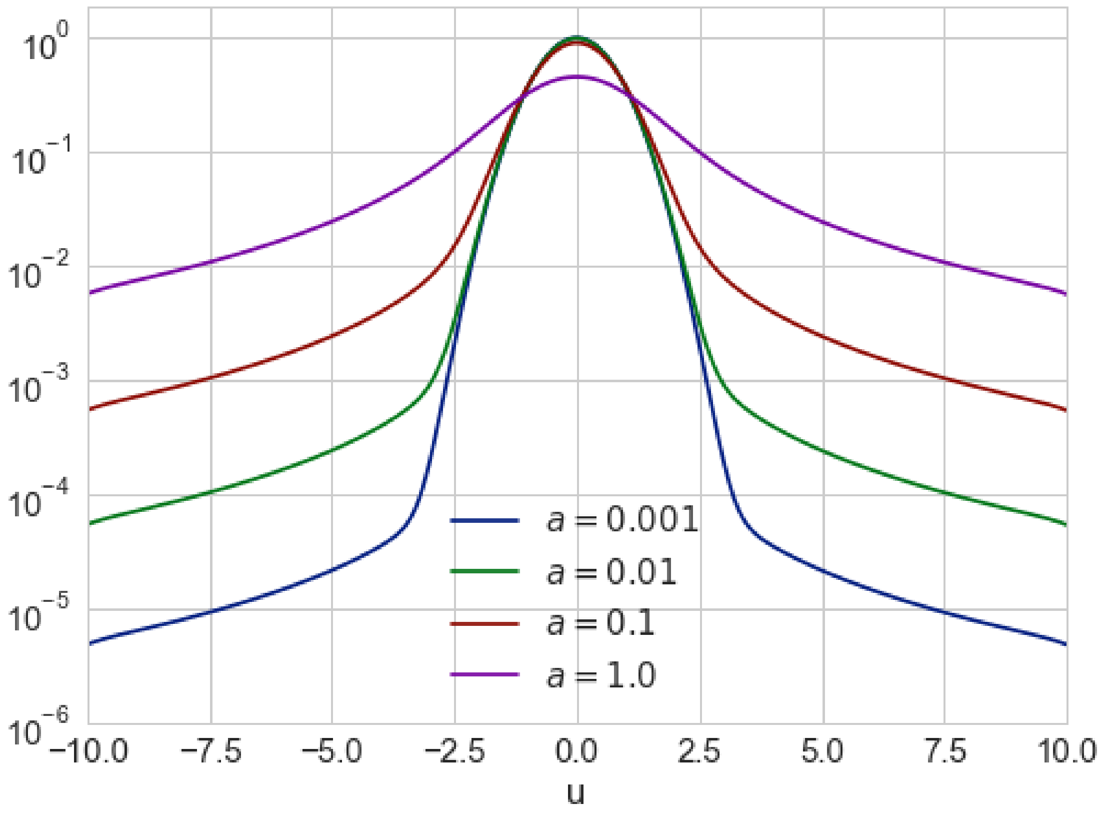
1. Extend the u range to $[-11, 11]$, but only plot the range $[-10, 10]$
2. Use the `x_size` optional parameter to make the kernel array the same size as `ugrid`, rather than the default of 8σ.
3. Just use more points (I don't understand why this makes a difference, and the normalization still doesn't look quite right).

I also plot the pure Gaussian kernel in black.

```
In [6]: def H_conv(u, a=1e-6):
            ustep = u[1] - u[0]
```

```
        kernel_wide = Gaussian1DKernel(stddev=1.0/np.sqrt(2)/ustep, x_size=len(u))
        kernel_wide.normalize("peak")
        result = convolve_fft(Lorentz(u, a), kernel_wide)
        return np.sqrt(np.pi)*result/np.trapz(result, u)
```

```
In [7]: ugrid = np.linspace(-11.0, 11.0, 10001)
        fig, ax = plt.subplots()
        for a in reversed([1.0, 0.1, 0.01, 0.001]):
            ax.plot(ugrid, H_conv(ugrid, a), label=f"$a = {a}$")
        ax.legend()
        ax.set(yscale="log", xlabel="u", xlim=[-10.0, 10.0], ylim=[1e-6, None])
        None
```



1.1.2 Quadrature method for integral (fails for small damping parameter)

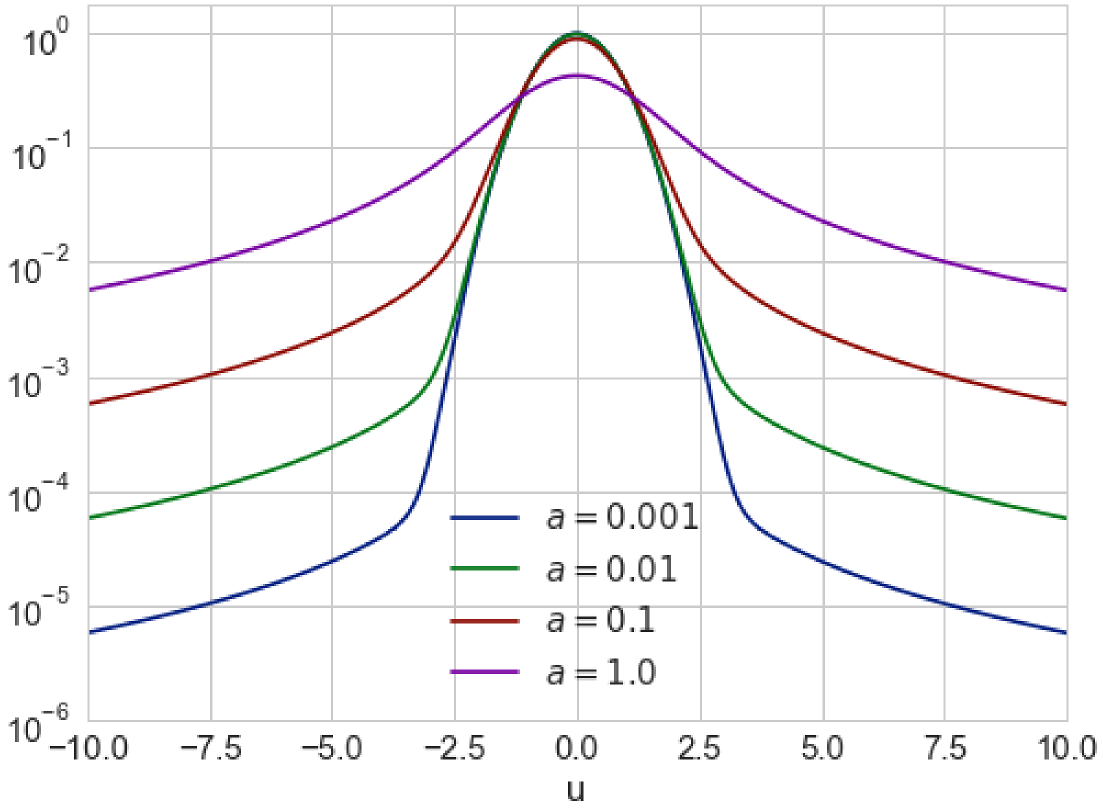
```
In [8]: def Gauss(u):
            return np.exp(-u**2)
```

```
In [9]: def H_integrand(y, u, a):
            return Gauss(y)*Lorentz(u-y, a)
```

```
In [10]: def H_quad_scalar(u, a):
             result, error = quad(H_integrand, -np.infty, np.infty, args=(u, a))
             return result
```

```
In [11]: @np.vectorize
         def H_quad(u, a):
             return H_quad_scalar(u, a)
```

```
In [12]: ugrid = np.linspace(-10.0, 10.0, 1000)
         fig, ax = plt.subplots()
         for a in reversed([1.0, 0.1, 0.01, 0.001]):
             ax.plot(ugrid, H_quad(ugrid, a), label=f"$a = {a}$")
         ax.legend()
         ax.set(yscale="log", xlabel="u", xlim=[-10.0, 10.0], ylim=[1e-6, None])
         None
```

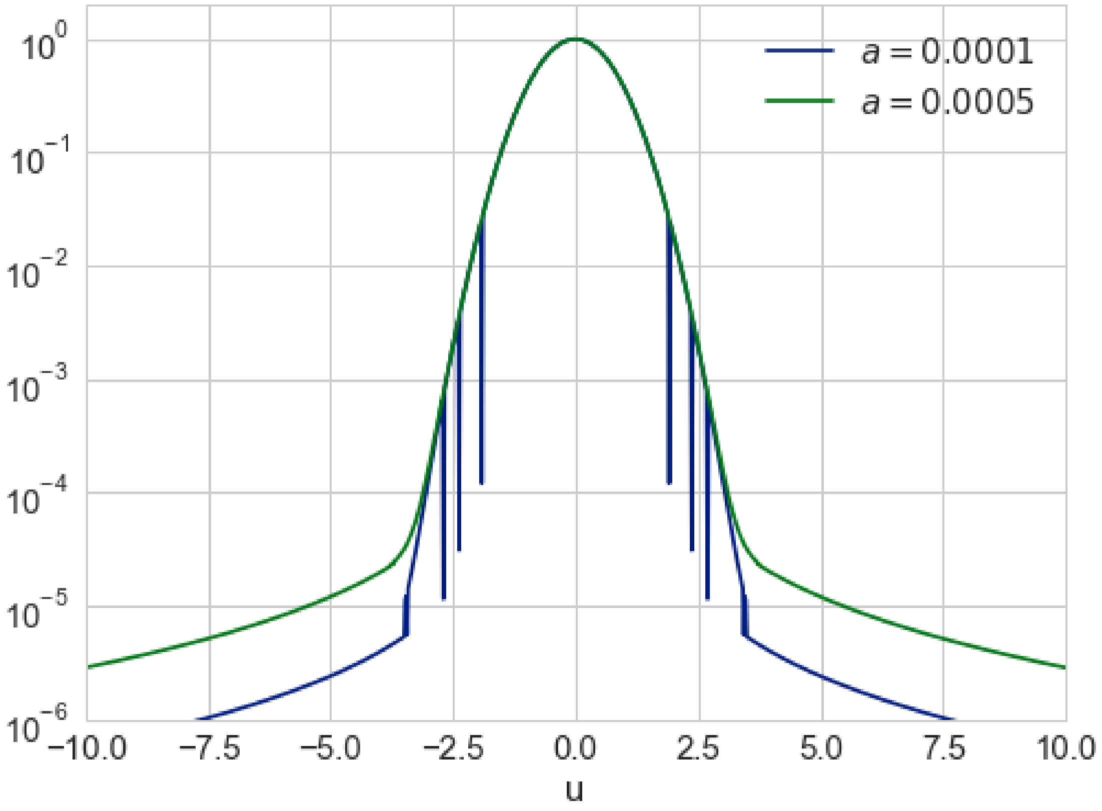


So that is fine for those a values, although it is much slower than the FFT method. And, the normalization looks fine, which is an improvement. But what if we make a smaller?

```
In [13]: ugrid = np.linspace(-10.0, 10.0, 1000)
         fig, ax = plt.subplots()
         for a in reversed([0.0005, 0.0001]):
             ax.plot(ugrid, H_quad(ugrid, a), label=f"$a = {a}$")
```

```
        ax.legend()
        ax.set(yscale="log", xlabel="u", xlim=[-10.0, 10.0], ylim=[1e-6, None])
        None
```

```
/Users/will/anaconda/lib/python3.6/site-packages/scipy/integrate/quadpack.py:364: IntegrationWa
  warnings.warn(msg, IntegrationWarning)
```



We can put off the inevitable by using more points, but this makes everything painfully slow.

1.1.3 Fadeeva function method (this is the best method: fast and accurate)

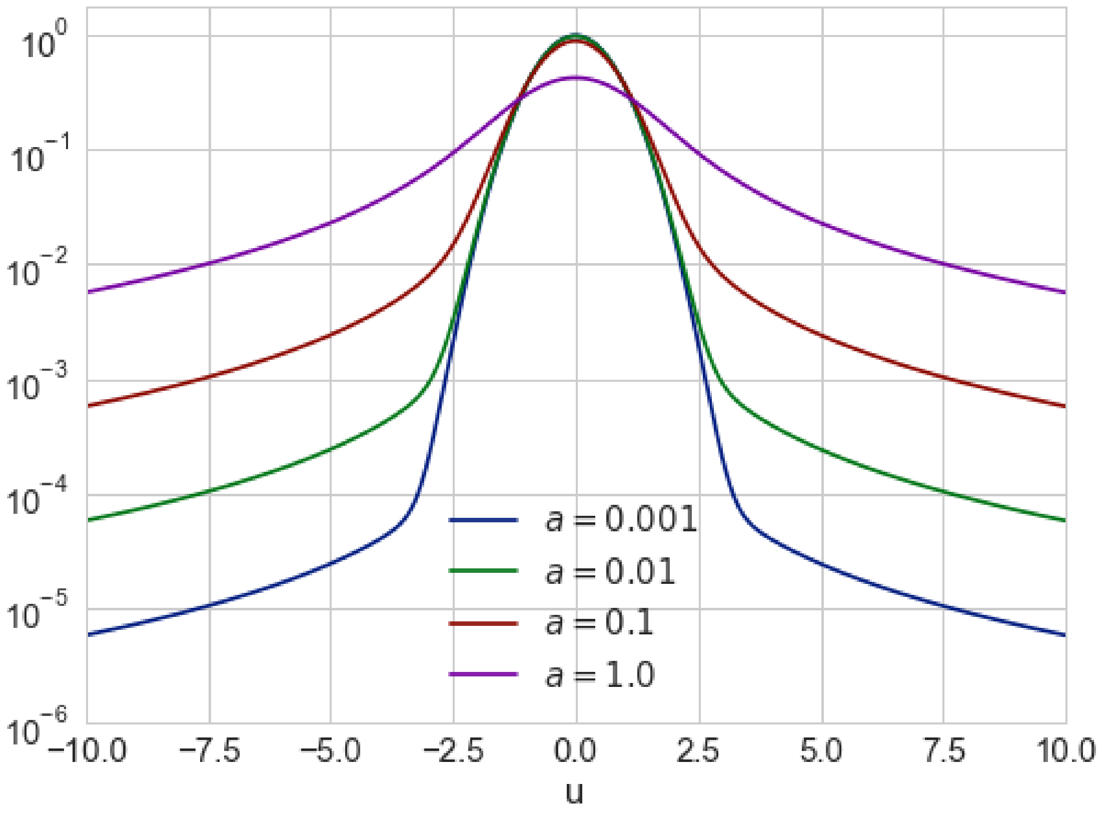
The Fadeeva function (see Wikipedia) is the scaled complementary error function of complex argument, and the Voigt function is its real part. It is implemented as `scipy.special.wofz`.

```
In [14]: from scipy.special import wofz

         def H_wofz(u, a):
             return np.real(wofz(u + 1j*a))

In [15]: ugrid = np.linspace(-10.0, 10.0, 1000)
         fig, ax = plt.subplots()
         for a in reversed([1.0, 0.1, 0.01, 0.001]):
```

```
    ax.plot(ugrid, H_wofz(ugrid, a), label=f"$a = {a}$")
ax.legend()
ax.set(yscale="log", xlabel="u", xlim=[-10.0, 10.0], ylim=[1e-6, None])
None
```

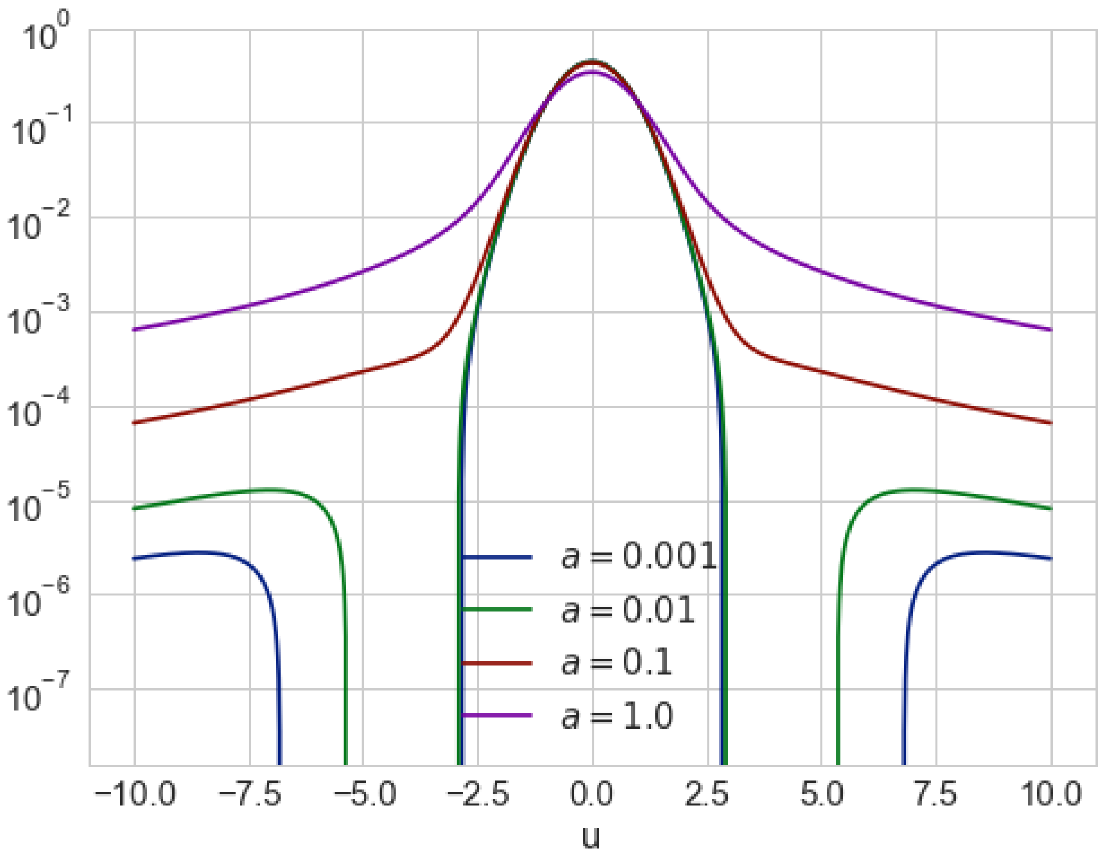


1.1.4 McLean algorithm method (very bad for small *a*)

```
In [16]: from astropy.modeling.functional_models import Voigt1D
```

We need to convert from Doppler width to FWHM, which is factor of $2\sqrt{\ln 2}$

```
In [17]: ugrid = np.linspace(-10.0, 10.0, 1000)
         fig, ax = plt.subplots()
         FWHM = 2*np.sqrt(np.log(2))
         for a in reversed([1.0, 0.1, 0.01, 0.001]):
             H_McL = Voigt1D(fwhm_G=FWHM, amplitude_L=1.0, fwhm_L=a/2)
             ax.plot(ugrid, H_McL(ugrid)/a, label=f"$a = {a}$")
         ax.legend()
         ax.set(yscale="log", xlabel="u")
         None
```



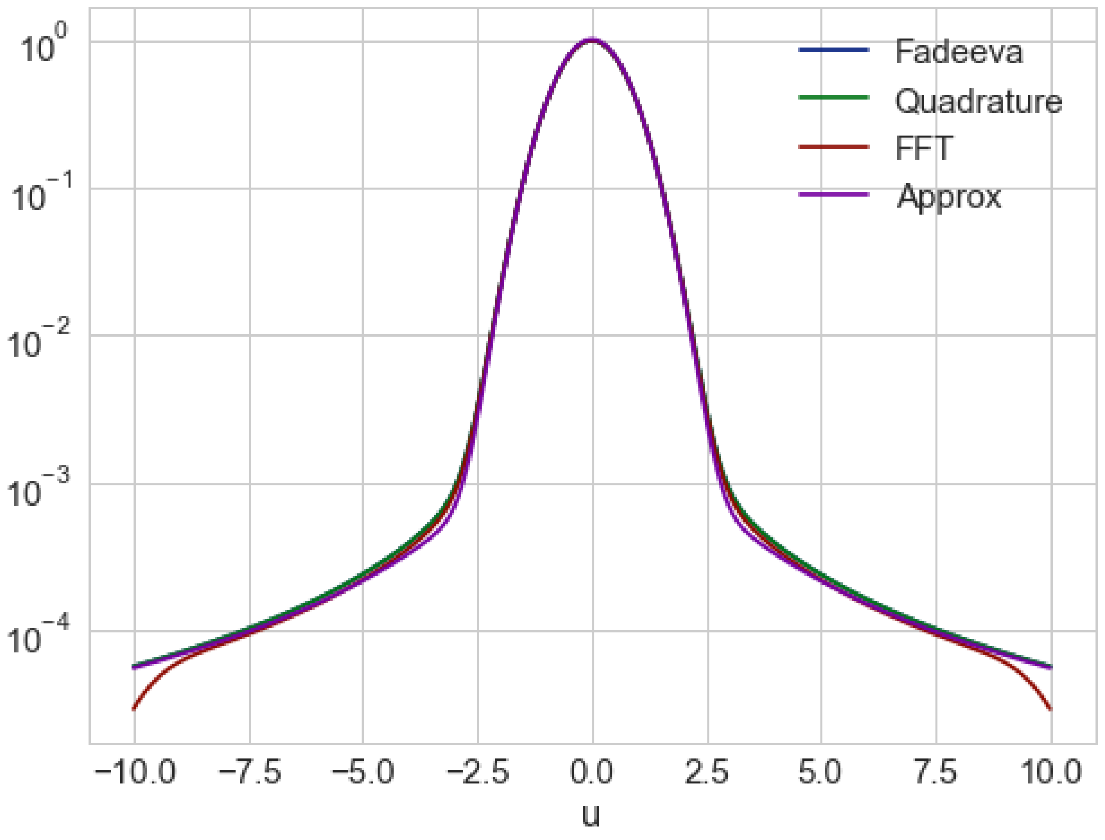
This is terrible. It goes negative for $a < 0.1$!
It turns out that there is a recent paper that points out these problems:

- Schreier (2008) JQSRT 213, 13 *Comments on the Voigt function implementation in the Astropy and SpectraPlot.com packages*

1.1.5 Comparison of methods

```
In [18]: def H_approx(u, a):
             return Gauss(u) + a/(1.0 + u**2)/np.sqrt(np.pi)
```

```
In [19]: a = 0.01
         ugrid = np.linspace(-10.0, 10.0, 1001)
         fig, ax = plt.subplots()
         for H, name in [
                 [H_wofz, "Fadeeva"],
                 [H_quad, "Quadrature"],
                 [H_conv, "FFT"],
                 [H_approx, "Approx"],
         ]:
             ax.plot(ugrid, H(ugrid, a), label=name)
         ax.legend()
         ax.set(yscale="log", xlabel="u")
         None
```



1.1.6 Timings

```
In [20]: for H, name in [
             [H_wofz, "Fadeeva"],
             [H_quad, "Quadrature"],
             [H_conv, "FFT"],
             [H_approx, "Approx"],
         ]:
             print(f"Timing for {name} method:")
             %timeit H(ugrid, a)
             print()
```

```
Timing for Fadeeva method:
287 ţs ś 11.2 ţs per loop (mean ś std. dev. of 7 runs, 1000 loops each)

Timing for Quadrature method:
2.55 s ś 209 ms per loop (mean ś std. dev. of 7 runs, 1 loop each)
```

```
Timing for FFT method:
2.93 ms ś 152 ţs per loop (mean ś std. dev. of 7 runs, 100 loops each)

Timing for Approx method:
46.9 ţs ś 3.12 ţs per loop (mean ś std. dev. of 7 runs, 10000 loops each)
```

1.1.7 Conclusions about methods

- The Fadeeva method is by far the best. It is very efficient and accurate.
- Quadrature is accurate for $a \geq 0.001$, but it is 5000 times slower.
- FFT is 10 times slower and suffers from edge effects
- McLean is hopelessly inaccurate for $a < 0.1$

1.2 The line flux profile F_ν

We define the frequency-dependent line opacity relative to the continuum as $\beta_\nu = \beta_0 \phi_\nu$, where $\beta_0 = \chi_\ell / \kappa_c$. In the Milne–Eddington approximation for LTE lines, the line absorption depth can be written as (see Hubeny & Mihalas, eq.~[17.189])

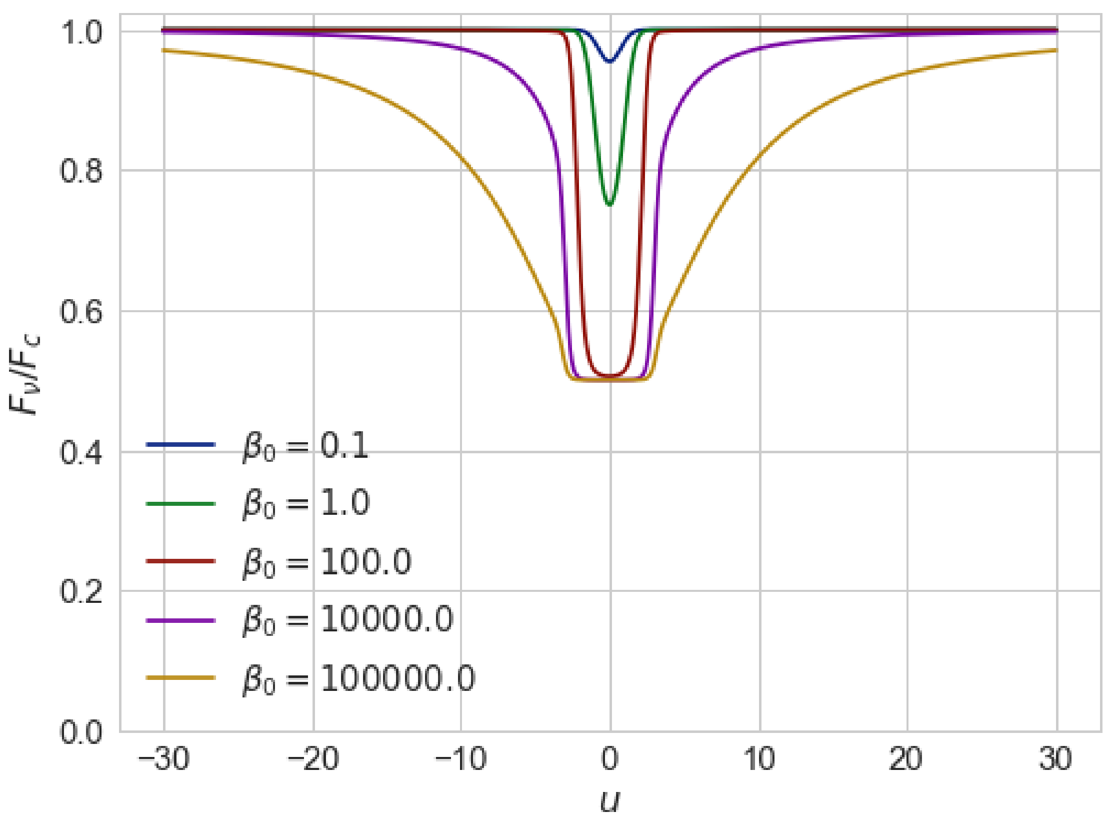
$$A_\nu = \frac{A_0 \beta_\nu}{1 + \beta_\nu}$$

where A_0 is the infinitely opaque limiting absorption depth, $A_0 = \left(1 + 3B_0/2B_1\right)^{-1}$, which depends on how the LTE source function varies with depth: $B_\nu(\tau_c) = B_0 + B_1 \tau_c$. The line flux is given by $F_\nu = F_c(1 - A_\nu)$.

```
In [21]: def A(u, a, beta0, A0):
             """Absorption depth"""
             beta_nu = beta0*H_wofz(u, a)
             return A0*beta_nu/(1.0 + beta_nu)
```

For illustration, we use $A_0 = 0.5$ and $a = 0.001$.

```
In [22]: ugrid = np.linspace(-30.0, 30.0, 1001)
         fig, ax = plt.subplots()
         A0 = 0.5
         a = 1.e-3
         for beta0 in [0.1, 1.0, 100.0, 1e4, 1e5]:
             label = fr"$\beta_0 = {beta0}$"
             ax.plot(ugrid, 1.0 - A(ugrid, a, beta0, A0), label=label)
         ax.legend()
         ax.set(ylim=[0.0, None], xlabel="$u$", ylabel=r"$F_\nu/F_c$")
         None
```



This shows the transition from weaker to stronger lines, showing saturation for $\beta_0 \geq 100$ and damping wings for $\beta_0 \geq a^{-1}$.

1.3 The equivalent width, W_ν

Defined as $W_\nu = \int_0^\infty A_\nu \, d\nu$.

```
In [23]: def W(a, beta0, A0):
             """Equivalent width in units of the Doppler width"""
             result, error = quad(A, -np.infty, np.infty, args=(a, beta0, A0))
             return result
```

Integration limits of u are $[-\infty, \infty]$. We just send those in directly, and let the quadrature routine sort it out.

```
In [24]: from astropy.table import Table

         Table(rows=[(x, W(a, x, A0)) for x in [0.1, 1.0, 100.0, 1e4, 1e6]], names=["beta0", "
```

```
Out[24]: <Table length=5>
           beta0           W
          float64       float64
         --------- ---------------
```

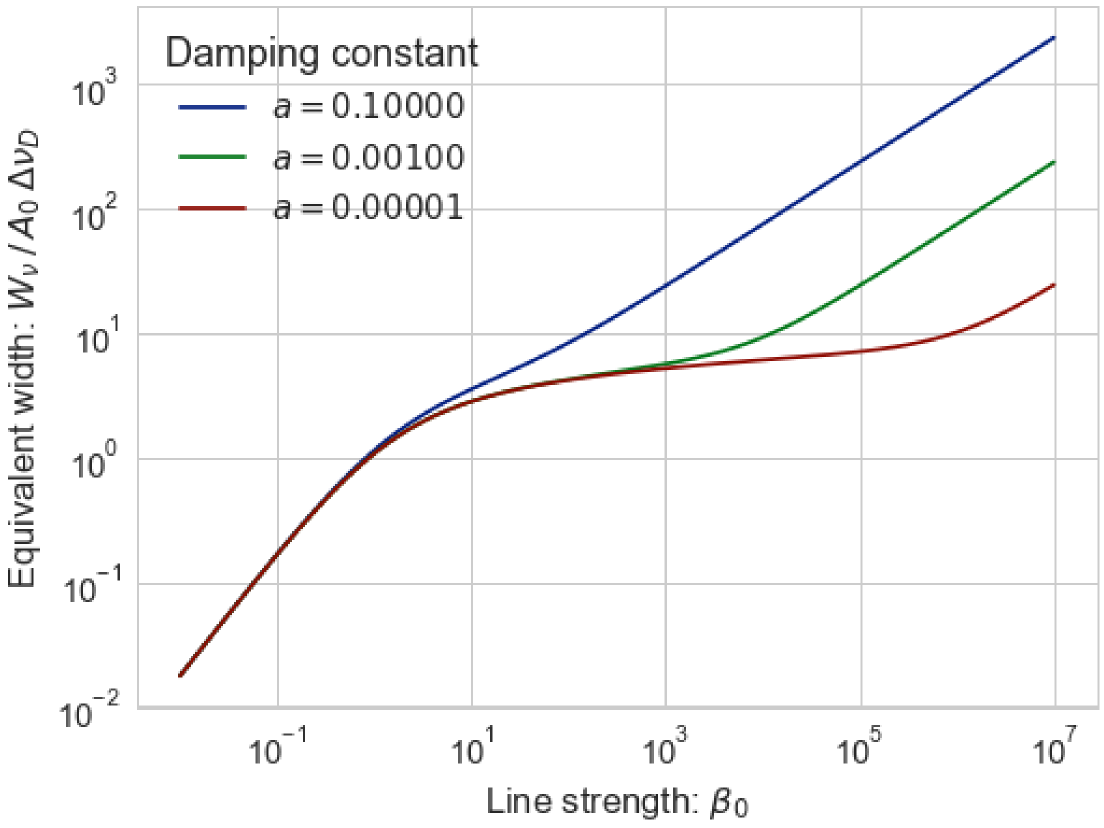
```
        0.1 0.0828358366521
        1.0   0.53645721327
      100.0   2.12332875198
    10000.0   4.62122393783
  1000000.0   37.3704253675
```

That seems to work.

1.4 The curve of growth

This is just a plot of $W_\nu(\beta_0)$ / $(A_0\,\Delta\nu_D)$.

```
In [25]: bgrid = np.logspace(-2.0, 7.0, 200)
         fig, ax = plt.subplots()
         for a in 1e-1, 1e-3, 1e-5:
             label = f"$a = {a:.5f}$"
             wgrid = np.array([W(a, b, A0)/A0 for b in bgrid])
             ax.plot(bgrid, wgrid, label=label)
         ax.legend(title="Damping constant")
         ax.set(
             xscale="log", yscale="log",
             xlabel=r"Line strength: $\beta_0$",
             ylabel=r"Equivalent width: $W_\nu \,/\, A_0\, \Delta\nu_D$"
         )
         None
```



So, we can clearly see the three regimes: linear, saturated, and damping (square-root).