Ch. 08
Ordinary Differential Equations (ODE)
[Boundary Value Problems]

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Two-Point Boundary Value Problems (BVP)

- When ODE are required to satisfy boundary conditions at more than one value of the independent variable, the resulting problem is called a *two point boundary value problem*.

- The most common case is when boundary conditions are supposed to be satisfied at two points — usually the starting and ending values of the integration.

- Unlike IVP, in BVP the boundary conditions at the starting point do not determine a unique solution to start with, and only certain (unknown) values will satisfy the boundary conditions at the other specified point.
- An iterative procedure is required and, for this reason, two point BVP require considerably more effort to solve than do IVP.

- You have to integrate your differential equations over the interval of interest, or perform an analogous "relaxation" procedure, at least several, and sometimes very many, times.

- Only in the special case of linear differential equations you can say in advance just how many such iterations will be required.

Boundary Value Problems: Definition

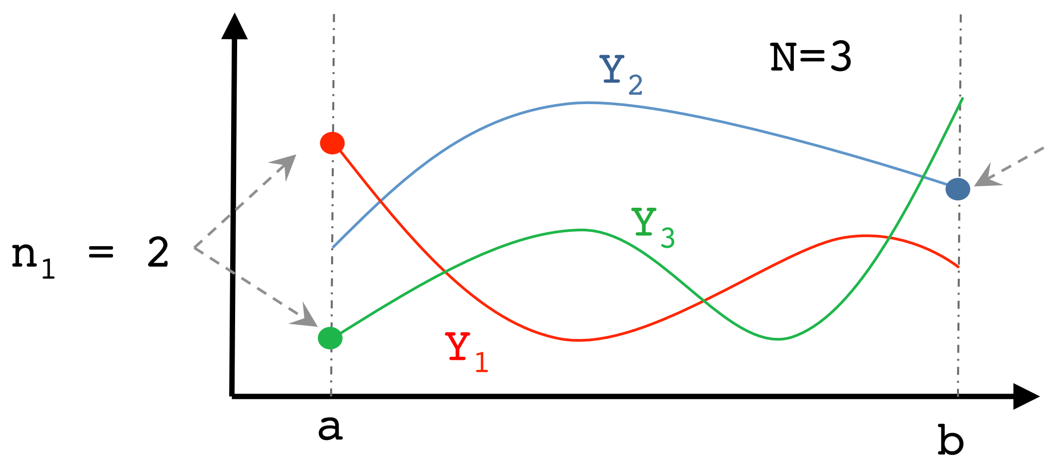
- The standard two point BVP has the following form: ***we seek for the solution to a set of N coupled first-order ODE, satisfying n_1 boundary conditions at the starting point a, and a remaining set of $n_2 = N - n_1$ boundary conditions at the final point b.*** (Recall that all differential equations of order higher than first can be written as coupled sets of first-order equations).

- The ODE are $$\frac{dY_i}{dx} = R_i(x, \vec{Y})\,, \quad i = 1, .., N$$

which are required to satisfy

$$\begin{aligned} Y_j = Y_j(a) &= \alpha_j\,, \quad j = 1 \ldots n_1 \\ Y_k = Y_k(b) &= \beta_k\,, \quad k = n_1 + 1 \ldots N \end{aligned}$$

- Here's an example with N=3:

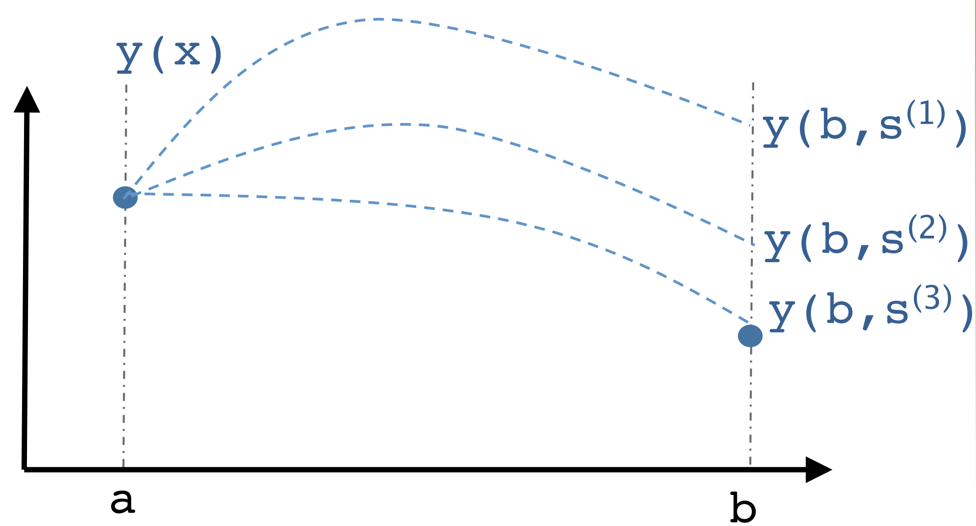


Single Shooting Method for BVP

- Consider the simple BVP $\dfrac{d^2y}{dx^2} = f(x, y, y')$, with $y(a) = \alpha, y(b) = \beta$

- A general strategy for solving a BVP is an iterative one: we guess a trial value for the derivative s=dy/dx at the starting point ***a*** and generate a solution by integrating the ODE as an IVP.

- If the resulting solution does not satisfy the b.c., we change the trial value s and iterate again, repeating the process until the b.c. are satisfied within a given tolerance.



- This is the <u>*shooting method*</u>.

Single Shooting Method for BVP

- Since for each trial value s of the derivative we generate, at the end of integration, a different function `y(b, s)`.
- Requiring that `y(b,s) =` β turns the BVP into a root-finder problem:

$$F(s) = y(b, s) - \beta$$

- If the BVP has a solution, then F(s) has a root.

- Note that Newton-Raphson is inappropriate since we cannot differentiate explicitly the resulting function with respect to k.

- Bisection, False Position or secant may be more appropriate.

BVP: Eigenvalue Problem

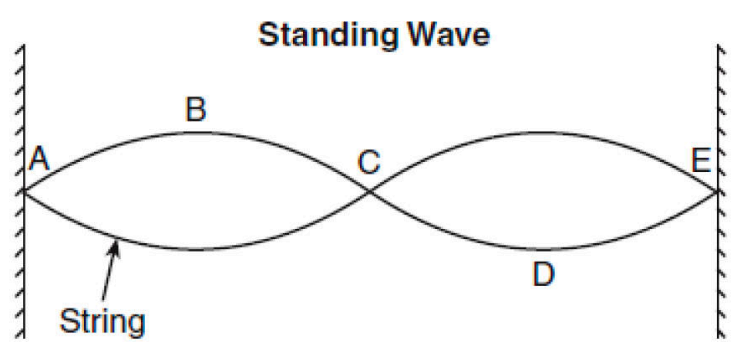
- A different variant of the BVP is given by an equation linear equation of the form

$$\frac{d^2y}{dx^2} = f(y, \lambda)\,, \quad \text{with} \quad y(a) = \alpha,\, y(b) = \beta$$

where λ is a free (unknown) parameter. The problem is *overdetermined* and there is no general solution for arbitrary values of λ.

- However, for certain special values of λ, the ODE does have a solution: this is *the eigenvalue problem for differential equation*.

- A typical example is that of a standing wave (a whirling string or rope) fixed at both ends. Here the the function is governed by the BVP



$$\frac{d^2\varphi}{dx^2} = -k^2\varphi \quad \text{with} \quad \varphi(0) = 0,\, \varphi(1) = 0$$

where φ has conditions specified at the boundaries of the independent variable.

- Solutions are possible only for discrete values of k (the eigenvalue):

$$y(x) = \sin(kx)\,, \quad k = n\pi$$

BVP: Eigenvalue Problem

- Eigenvalue problems can also be solved by means of the shooting method.

- Many physical problems can cast as linear homogenous second-order ODE depending on an unknown parameter.

- The stationary Schrodinger equation is an example:

$$\frac{d^2\psi}{dx^2} + k^2(x)\psi = 0 \qquad \text{where} \qquad \begin{cases} k^2(x) = \dfrac{2m}{\hbar^2}[E - V(x)] \\ \psi(a) = 0\,, \psi(b) = 0 \end{cases}$$

Solutions are possible only for certain value of E (the eigenvalue): the eigenfunction (ψ) will oscillate in the classically allowed region where E > V(x) and behave exponentially in the classical forbidden region (E < V(x)).

- Other well-known eigenvalue problems are the stationary vibration of a circular membrane, dispersion relations in fluid dynamics, wave propagation, etc…

BVP: Eigenvalue Problem

- Note that for linear homogenous equations (as it is the case for several problems)

$$\frac{d^2y}{dx^2} + k^2(x)y = 0 \quad \text{with} \quad y(a) = \alpha,\ y(b) = \beta$$

  the solution can always be rescaled by an arbitrary multiplicative constant and the normalization of the solution is not specified.

- In these cases, the value of the derivative ($s = dy/dx|_a$) is arbitrary and cannot be used to generate different solutions.

- Instead, we take the eigenvalue `k` as our free parameter and obtain trial solutions for different values of `k` until the b.c. are satisfied.

$$F(k) = y(b, k) - \beta$$

- Where `y(b,k)` means "*the solution generate by integrating the ODE from a to b using a trial value k*"

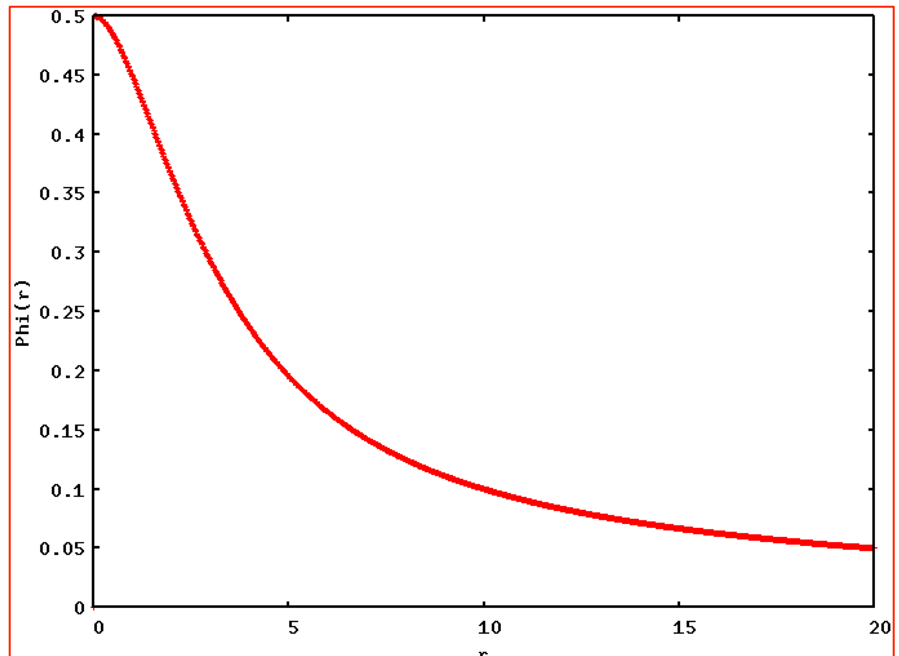
Practice Session #1

- `poisson.cpp`: we first consider a simple BVP problem given by the 1D spherically symmetric Poisson equation: we wish to find the electrostatic potential Φ generated by a localized charge distribution $\rho(r)$:

$$\nabla^2\Phi = -4\pi\rho \quad \rightarrow \quad \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) = -4\pi\rho \qquad (\text{with} \quad \rho(r) = \frac{1}{8\pi}e^{-r})$$

- In order to avoid dealing with the singularity at the origin we use the standard substitution

$$\Phi = \frac{\varphi}{r} \quad \rightarrow \quad \frac{d^2\varphi}{dr^2} = -4\pi r\rho$$



- Boundary conditions are imposed by requiring regularity of the solution:
  - At small r, the potential should vanish $\rightarrow \varphi = 0$ at $r=0$
  - At large r, the potential should behave as $1/r \rightarrow \varphi = 1$ at $r=b$ (use $b = 20$ or more)
- The value of the derivative $s = d\varphi/dr$ at $r = 0$ should be used as our free parameter.

Practice Session #1 (cont)

- We proceed step by step:

1. Generate solutions for different values of `s` = 0, 0.2, 0.4, 0.6, 0.8, 1.0 (the first derivative) by integrating the regularized ODE from r = 0 to r = b = 20 using RK4 (or similar) using 1000 points. Plot the solutions `φ(r,s)` that you have obtained.

2. Implement the residual function, $\mathrm{Residual}(s) = \varphi(b, s) - 1$

   and produce a plot of the residual as a function of s in the range [0,10]. Can you approximately identify the root ?

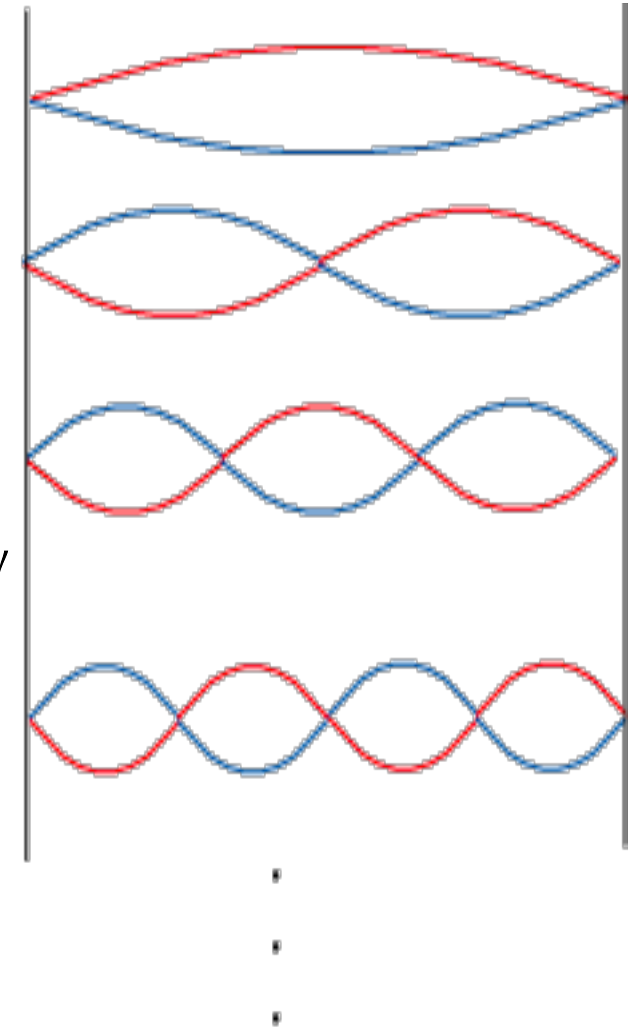
3. Now use Bisection or False position to refine the root s for which the residual vanishes. Make sure to supply a range in which the residual changes sign.

4. Compare your results against the analytical solution $\varphi(r) = 1 - \frac{1}{2}(r+2)e^{-r}$

Practice Session #2

- `wave.cpp`: solve the eigenvalue problem

$$\frac{d^2\varphi}{dx^2} = -k^2\varphi \quad \text{with} \quad \varphi(0)=0,\ \varphi(1)=0$$



1. start with a single forward integration from x=0 to x=1 using 100 points, `k=1` and `s = dy/dx`$|_0$`=1` (this is completely arbitrary). The code should contain, at this stage, only one single loop. The solution will largely overshoot the final value.

2. modify the code to loop over k=1,2,3,4,5 and generate 5 corresponding blocks to be plotted. Use gnuplot to verify that the actual solution lies between k = 3 and k =4

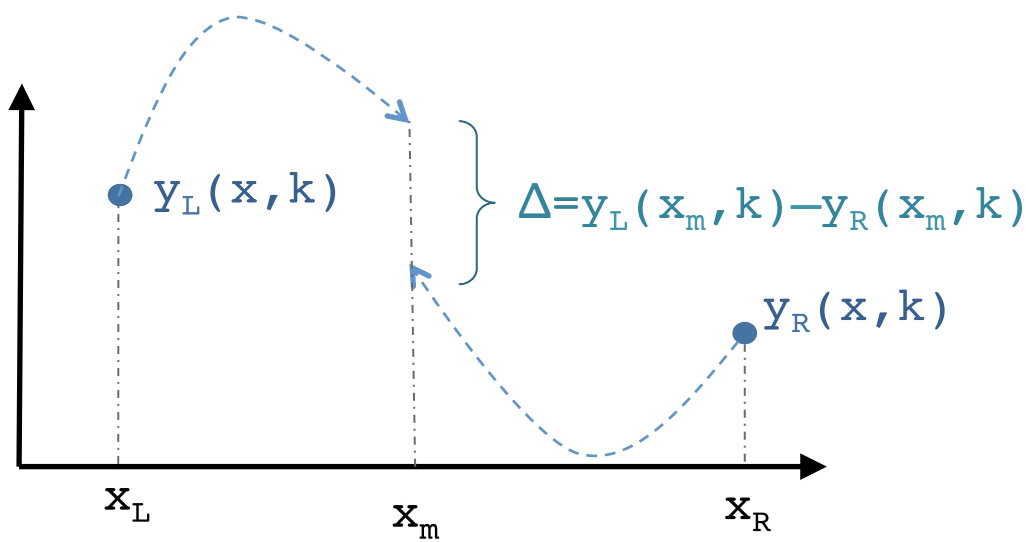
3. Move the integration to a function of the type `double Residual(double)` that we will later use for Bisection. Now use Bisection to find the first zero (pi).

4. Add a preliminary search using Bracket() and then find all of the zeros between 1 and 20.

Integrating to a Matching Point

- In some cases, the two solutions of the 2nd order ODE may be very different. A typical circumstance occurs when the solution, owing to inevitable numerical approximations, contain small admixtures of exponential growing and decaying functions.

- In such cases, it is more convenient to integrate from both ends up to a common point. Two numerical solutions must be generated: a forward integration starting at xL and a backward integration starting xR. Both integration stops at the "matching point" xm which is conveniently chosen by the user.



- At the matching point, we could compute the residual function as the difference between these two solutions: $\Delta = y_L(x_m,k) - y_R(x_m,k)$

Integrating to a Matching Point

- For linear problems, however, the two functions yL and yR may differ up to a multiplicative constant, so the residual is better constructed by matching the *logarithmic derivative:*

$$\left.\frac{y_L'}{y_L}\right|_{x_m} = \left.\frac{y_R'}{y_R}\right|_{x_m} \quad \rightarrow \quad \mathrm{Res}(k) = \frac{y_L'(x_m,k)\,y_R(x_m,k) - y_R'(x_m,k)\,y_L(x_m,k)}{D}$$

  where D is a normalization factor (if you have no clue, use D = 1).

- Thus we have again root-finding problem in the residual.

- Note that results must be independent on the choice of the matching point x_m.

Example: Quantum Eigenvalue Problem

- If a particle of energy E moving in one dimension experiences a potential V (x), its wave function is determined by an ODE (a PDE if greater than 1-D) known as the time-independent Schrödinger equation:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

- Setting $\kappa^2 = -\frac{2m}{\hbar^2}E = \frac{2m}{\hbar^2}|E|.$ we obtain $\frac{d^2\psi(x)}{dx^2} - \frac{2m}{\hbar^2}V(x)\psi(x) = \kappa^2\psi(x).$

- For a bounded particles, the wave function must decay exponentially as |x| → ∞.
- Although it is straightforward to solve the previous ODE with the techniques we have learned so far, we must *also require* that the solution ψ(x) simultaneously satisfies the boundary conditions at infinity.
- This extra condition turns the ODE problem into an *eigenvalue problem* that has solutions (*eigenvalues*) for only certain values of the energy E.
- The ground-state energy corresponds to the most negative eigenvalue. The corresponding psi(x) is our eigenfunction.

Practice Session #3

- `qho.cpp`: find the eigenvalues of the quantum harmonic oscillator,

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi\,, \qquad \text{with} \qquad V(x) = \frac{1}{2}kx^2$$

→ Rewrite the equation in a more suitable dimensionless form:

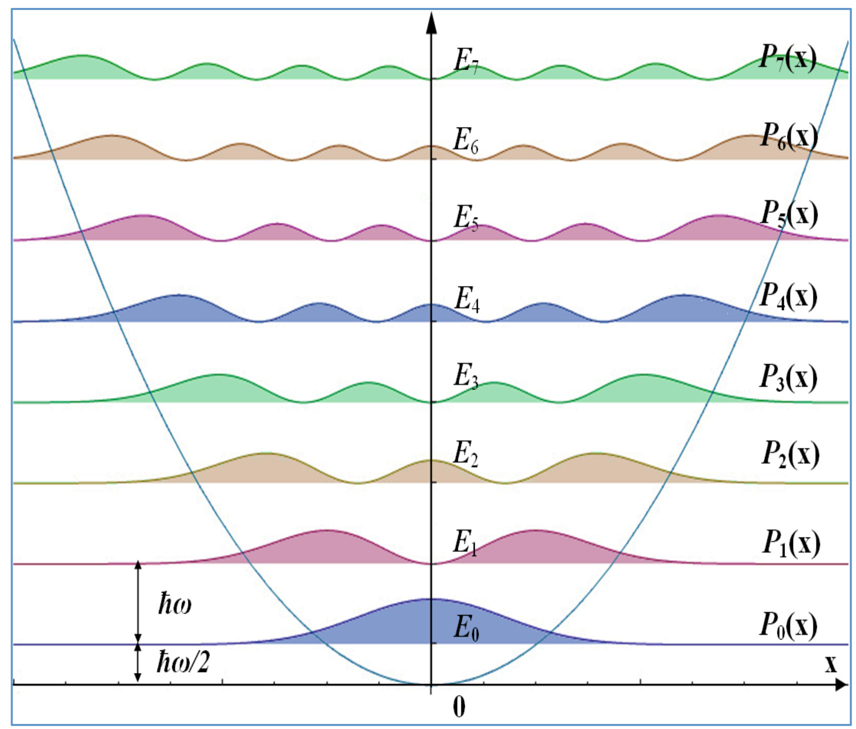
$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi\,, \qquad \text{with} \qquad V(x) = \frac{1}{2}x^2$$

what is the natural scale for energy and length ?

→ In dimensionless form the exact analytical eigenfunctions and the corresponding eigenvalues are

$$\psi_n(x) = \langle x \mid n\rangle = \frac{1}{\sqrt{2^n n!}}\,\pi^{-1/4}\exp(-x^2/2)\,H_n(x),$$

$$E_n = n + \tfrac{1}{2}\,,$$



Practice Session #3

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi\,, \qquad \text{with} \qquad V(x) = \frac{1}{2}x^2$$

1. Solve the equation in the domain [-10,10] using, as initial condition the eigenfunction for the ground state `exp(-x²/2),` its derivative and the exact eigenvalue (E = ½). Solve the equation forward (from x=-10 to x=10) and backwards (from x=10 to x=-10). What happens ?

2. Now construct the residual by matching forward and backward numerical solutions at the matching point. Use the logarithmic derivative. Produce a plot with 0 < E < 5. How many zero do you see ?

3. Use bisection or false position to refine your search and converge to the eigenvalues.

Practice Session #3: Useful Tips

- *Matching point*: if x_m=0 is chosen to be the interval midpoint, then the logarithmic derivative may become ill-behaved due to the fact that the eigenfunctions of odd order have a zero. Therefore, it is advisable to use a point close to 0.

- *Initial condition*: to obtain a more accurate expression for the initial condition, one could use an asymptotic expansion of the original ODE. This can be rather complicated and outside this course objective; however we can obtain a simple expression by neglecting E:

$$\frac{d^2y}{dx^2} = x^2 y \qquad \rightarrow \qquad y(x) = \sqrt{x}\left[c_1 I_{\frac{1}{4}}\left(\frac{x^2}{2}\right) + c_2 K_{\frac{1}{4}}\left(\frac{x^2}{2}\right)\right]$$

where $I_\nu()$ and $K_\nu()$ are the modified Bessel functions. The physical admissible solution is $K_\nu()$ and an asymptotic expansion for large x is

$$y(x) \sim \sqrt{\pi} e^{-\frac{x^2}{2}} \frac{1}{\sqrt{|x|}}$$

- *Residual*: a convenient way to normalize the residual is $\mathrm{Res}(E) = \dfrac{A - B}{\sqrt{A^2 + B^2}}$ where `A=yL'yR, B=yR'yL.`