

# The solution of singular Schrödinger problems using a piecewise perturbation method

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# Outline

- 1 Introduction
  - The Schrödinger problem
  - The Piecewise Perturbation Methods
- 2 Truncation of an infinite integration interval
  - Regularization of infinite problems
  - Selection of the cutoff point
- 3 Adapted boundary conditions for Coulomb-like potentials
  - Improved boundary conditions at large distance
  - Solution near the origin
- 4 Conclusion

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# The Schrödinger problem

## The one-dimensional Schrödinger problem

$$y'' = (V(x) - E)y, \quad x \in [a, b]$$

- $V(x)$ : potential function
- $E$ : energy level

## The Boundary Value Problem

- BCs: e.g.  $\alpha_1 y(a) + \alpha_2 y'(a) = 0$  and  $\beta_1 y(b) + \beta_2 y'(b) = 0$
- **eigenvalue**: a value for the parameter  $E$  for which there is a non-zero solution  $y$ .
- **eigenfunction**: the corresponding solution  $y$ .

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# The Piecewise Perturbation Methods

## The perturbation approximation

$$y'' = (V(x) - E)y, \quad x \in [a, b]$$

- the given diff. eq. is replaced piecewisely by a reference diff. eq. which can be solved exactly
- the deviation between the two diff. eqs. is used to construct some correction terms
- CPM (Constant Perturbation Methods) - LPM (Line Perturbation Methods)

# The Piecewise Perturbation Methods

## The Piecewise Perturbation Methods

$$y'' = (V(x) - E)y, \quad x \in [a, b]$$

- The piecewise perturbation methods are used in a shooting procedure to compute the eigenvalues upto high accuracy
- The main focus was on regular problems defined on a finite integration interval
- Now we want to apply the piecewise perturbation methods on some singular problems, the problem is regularized by using interval truncation

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# Regularization of infinite problems

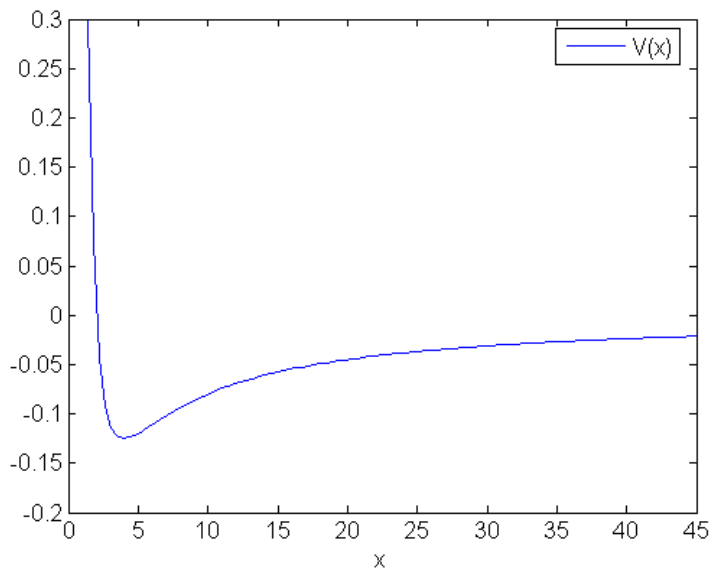
## Example

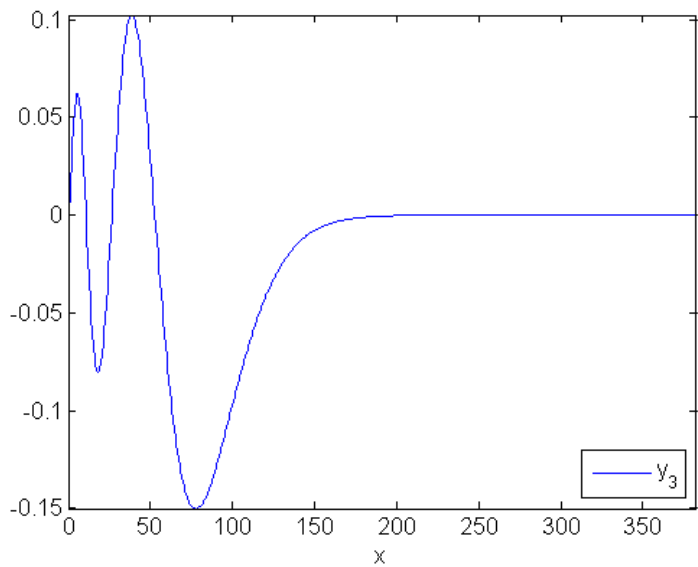
The hydrogen problem

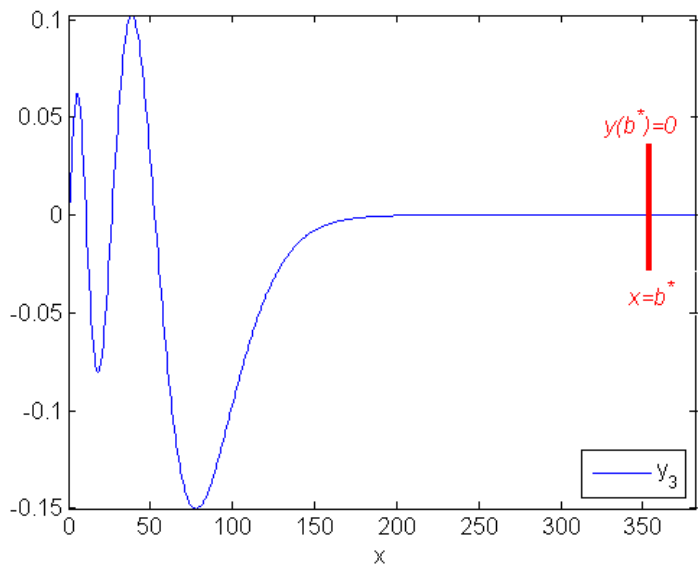
$$y''(x) = \left( \frac{l(l+1)}{x^2} - \frac{1}{x} - E \right) y(x), \quad x \in (0, +\infty),$$

exact eigenvalues  $E_k = -1/(2k+4)^2$ ,  $k = 0, 1, 2, \dots$  when  $l = 1$ .

- Where to truncate the integration interval?







# Regularization of infinite problems

## Example

The hydrogen problem

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exact eigenvalues  $E_k = -1/(2k+4)^2$  when  $l = 1$ .

- Where to truncate the integration interval?
- Impose BCs  $y(\epsilon) = y(b^*) = 0$  and solve as a regular problem on  $[\epsilon, b^*]$ .
- With  $\epsilon = 0.00001$  and  $b^* = 1000$ , the first 4 eigenvalues agree with those of the infinite problem. However, when  $k$  is further increased the agreement deteriorates.
- an increase with  $k$  of  $b^*$  is necessary

## Regularization of infinite problems

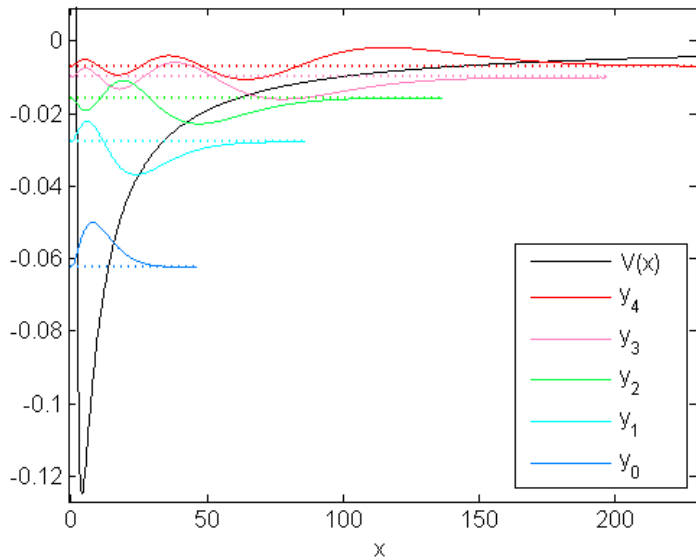
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# Regularization of infinite problems

## Selection of the cutoff value $b^*$

- an infinite endpoint  $a$  can be treated in the same way
- aim is to determine  $b^*$  as the leftmost point such that the cut does not affect the accuracy
- $b^*$  must be to the right of the outer turningpoint  $x_t$
- Via derivation based on the WKB approximation, the following condition is obtained

$$e^{-2 \int_{x_t}^{b^*} [V(x) - E]^{1/2} dx} \leq \text{machine accuracy}$$

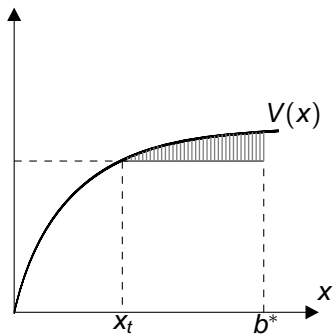
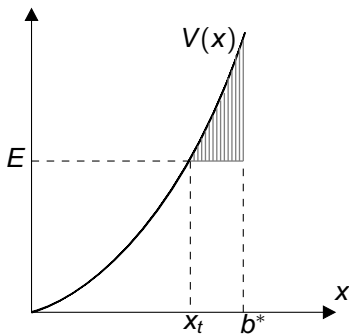
- In double precision calculations, this means:

$$\int_{x_t}^{b^*} [V(x) - E]^{1/2} dx \geq 18$$

# Regularization of infinite problems

Selection of the cutoff value  $b^*$

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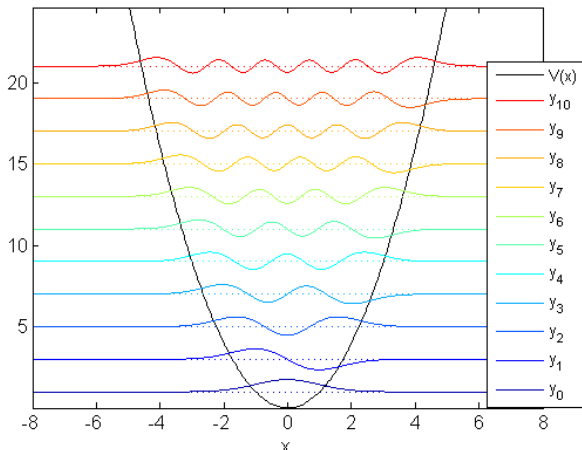


## Some illustrations

- The harmonic oscillator

$$y'' = (x^2 - E) y, \quad x \in (-\infty, +\infty)$$

with exact eigenvalues given by  $E_k = 2k + 1$ ,  $k = 0, 1, \dots$



## Some illustrations

**Table:** The first eigenvalues of the harmonic oscillator calculated with CPM{16,14} and  $tol = 10^{-12}$ . ( $a^* = -b^*$ )

$k$	$b^*$	$E_k$
0	5.7306	0.999999999998
1	6.1815	2.999999999999
2	6.6459	4.999999999999
3	6.6459	6.999999999998
4	7.0940	8.999999999997
5	7.5422	10.999999999996
6	7.9903	12.999999999995
7	7.9903	14.999999999994
8	8.4360	16.999999999999
9	8.4360	18.999999999995
10	8.4360	20.999999999995

## Some illustrations

**Table:** Some higher eigenvalues of the harmonic oscillator calculated with CPM{16,14} and  $tol = 10^{-12}$ .

$k$	$b^*$	$E_k$
100	17.4590	201.0000000000003
500	35.0838	1000.9999999999998
1000	50.1788	2001.0000000000012

## Some illustrations

- The hydrogen equation

$$y''(x) = \left( \frac{l(l+1)}{x^2} - \frac{1}{x} - E \right) y(x), \quad x \in (0, +\infty),$$

exact eigenvalues  $E_k = -1/(2k+4)^2$  when  $l = 1$ .

**Table:** Some eigenvalues of the hydrogen problem calculated with CPM{16,14} and  $tol = 10^{-12}$ .

$k$	$b^*$	$E_k$
0	1.05E2	-0.0625000000000
10	1.27E3	-0.0017361111111
100	5.32E4	-0.0000240292195
1000	4.25E6	-0.0000000249003

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## The Coulomb equation

$$y'' + \left( E + \frac{Z}{x} - \frac{l(l+1)}{x^2} \right) y = 0, \quad x > 0$$

### adapted BCs

- For potentials which behave as a Coulomb potential at large distance, the truncation algorithm can be improved
- an approximation of the asymptotic Coulomb function is used to construct more precise BCs
- smaller cutoff values can be chosen

## The Coulomb equation

$$y'' + \left( E + \frac{Z}{x} - \frac{l(l+1)}{x^2} \right) y = 0, \quad x > 0$$

- change of variables  $x = r/(2\sqrt{-E})$
- divide by  $-4E$
- $\mu = l + \frac{1}{2}$ ,  $\kappa = \frac{Z}{2\sqrt{-E}}$

$$\frac{d^2 w}{dr^2} + \left( -\frac{1}{4} + \frac{\kappa}{r} + \frac{\frac{1}{4} - \mu^2}{r^2} \right) w = 0$$

Whittaker equation

## The Coulomb equation

$$\frac{d^2 w}{dr^2} + \left( -\frac{1}{4} + \frac{\kappa}{r} + \frac{\frac{1}{4} - \mu^2}{r^2} \right) w = 0$$

Abramowitz and Stegun, Handbook of Mathematical Functions:

- $W_{\kappa, \mu}(t) = e^{-\frac{r}{2}} r^{\mu + \frac{1}{2}} U\left(\frac{1}{2} + \mu - \kappa, 1 + 2\mu, r\right)$
- for large  $r$ :

$$U(a, b, r) = r^{-a} \sum_n \frac{(a)_n (1 + a - b)_n}{n!} (-r)^{-n}$$

with

$$(a)_0 = 1,$$

$$(a)_n = a(a+1) \dots (a+n-1).$$

## The Coulomb equation

- For large  $r$ :

$$W_{\kappa,\mu}(r) = e^{-\frac{r}{2}} r^{\kappa} \sum_n c_n r^{-n}$$

where the coefficients  $c_n$  are defined by

$$\begin{aligned} c_0 &= 1, \\ (n+1)c_{n+1} &= -(l+1-\kappa+n)(-l-\kappa+n)c_n \end{aligned}$$

- First derivative:

$$\frac{dW_{\kappa,\mu}}{dx} = 2\sqrt{-E} \frac{dW_{\kappa,\mu}}{dr}$$

with for large  $r$ :

$$\frac{dW_{\kappa,\mu}}{dr} = -\frac{1}{2}W_{\kappa,\mu}(r) + \frac{\kappa}{r}W_{\kappa,\mu}(r) - e^{-\frac{r}{2}} r^{\kappa} \sum_n n c_n r^{-n-1}$$

- These expressions allow us to cut off the interval at points where the solution is not yet zero.

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## The Coulomb equation

$$W_{\kappa,\mu}(r) = e^{-\frac{r}{2}} r^{\kappa} \sum_n c_n r^{-n} \quad (\text{for large } r)$$

$$\frac{dW_{\kappa,\mu}}{dx} = 2\sqrt{-E} \left[ \left(-\frac{1}{2} + \frac{\kappa}{r}\right) W_{\kappa,\mu}(r) - e^{-\frac{r}{2}} r^{\kappa} \sum_n n c_n r^{-n-1} \right]$$

- For a Coulomb problem  $\kappa = Z/(2\sqrt{-E})$  increases very rapidly with the eigenvalue index. The factor  $r^{\kappa}$  may cause overflow problems.
- Therefore we use scaled wavefunctions  $\bar{W}_{\kappa,\mu}$  to obtain BCs in  $b^*$ :

$$\bar{W}_{\kappa,\mu}(r) = 1,$$
$$\frac{d\bar{W}_{\kappa,\mu}}{dx}(r) = 2\sqrt{-E} \left[ -\frac{1}{2} + \frac{\kappa}{r} - \frac{\sum_n n c_n r^{-n-1}}{\sum_n c_n r^{-n}} \right]$$

## Adapted BCs for Coulomb-like problems

### Example

The Hydrogen equation

$$y''(x) = \left( \frac{l(l+1)}{x^2} - \frac{1}{x} - E \right) y(x), \quad x \in (0, +\infty),$$

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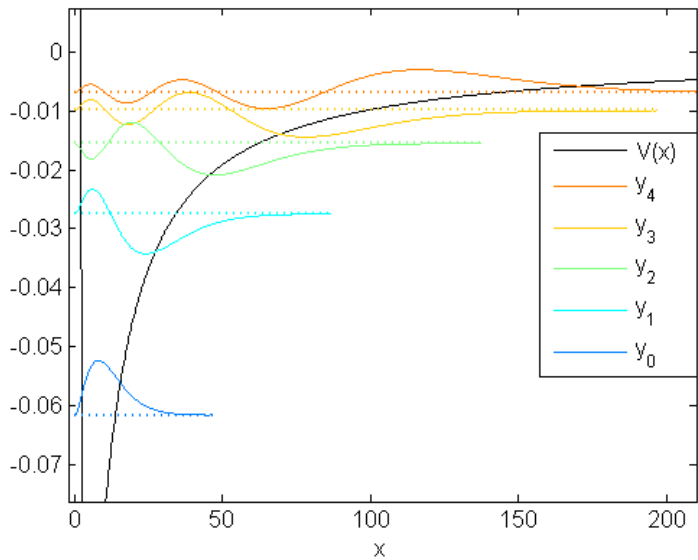
### Example

$$y''(x) = \left( \frac{l(l+1)}{x^2} + \frac{-1 + 5e^{-2x}}{x} - E \right) y(x), \quad x \in (0, +\infty)$$

with  $l = 1$ .

**Table:** The first eigenvalues calculated with CPM{16,14},  $tol = 10^{-12}$ .

$k$	$b^*$	$b^*_a$	$E_k$
0	110.80	18.35	-0.061681846633
1	137.13	42.56	-0.027498099943
2	203.53	88.74	-0.015501561691
3	243.83	110.80	-0.009935496851
4	340.03	168.07	-0.006906701382



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## Solution near the origin

$$y'' = \left( \frac{l(l+1)}{x^2} + V(x) - E \right) y, \quad x > 0$$

- singular at the origin
- on a short interval around the origin a specially tuned implementation is used
- $l(l+1)/x^2$  is seen as the reference potential and the rest of the potential as a perturbation
- the algorithm computes  $y(\epsilon)$  where  $\epsilon \neq 0$  small enough such that the centrifugal term is numerically dominating w.r.t. the other terms of the potential.

## Solution near the origin

### Algorithm

- potential =  $\frac{l(l+1)}{x^2} + \frac{S(x)}{x} + R(x)$
- We assume that  $S(x)$  and  $R(x)$  can be approximated by a second degree polynomial over  $[0, \epsilon]$ :

$$S(x) = S_0 + S_1x + S_2x^2, \quad R(x) = R_0 + R_1x + R_2x^2$$

- The potential is then approximated over  $[0, \epsilon]$  by

$$\frac{l(l+1)}{x^2} + \frac{V_{-1}}{x} + V_0 + V_1x + V_2x^2$$

where

$$V_{-1} = S_0, \quad V_0 = S_1 + R_0, \quad V_1 = S_2 + R_1, \quad V_2 = R_2$$

## Solution near the origin

### Algorithm (Cont'd)

- The Schrödinger eq. can then be written as

$$Ly(x) = \Delta V(x)y(x)$$

where

$$L = \frac{d^2}{dx^2} - \frac{l(l+1)}{x^2}$$

and

$$\Delta V(x) = \frac{V_{-1}}{x} + V_0 + V_1x + V_2x^2 - E.$$

- Perturbative approach:

$$y(x) = y_0(x) + y_1(x) + y_2(x) + \dots$$

where

$$Ly_0(x) = 0, \quad Ly_{q+1}(x) = \Delta V(x)y_q(x), \quad q = 0, 1, \dots$$

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## Solution near the origin

### Algorithm (Cont'd)

- $\mathcal{L}y_0(x) = 0$  with  $\mathcal{L} = \frac{d^2}{dx^2} - \frac{l(l+1)}{x^2}$

Thus:

$$y_0(x) = x^{l+1}, \quad y_0'(x) = (l+1)x^l$$

- Expressions for the higher order perturbations are obtained from

$$\mathcal{L}y_{q+1}(x) = \Delta V(x)y_q(x), \quad q = 0, 1, \dots$$

- $y(x) = y_0(x) + y_1(x) + y_2(x) + \dots$  is used to compute  $y(\epsilon)$  and  $y'(\epsilon)$ .
- The problem is then integrated using a CPM (or LPM) on  $[\epsilon, b^*]$ .

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## Conclusion

- We constructed a WKB- based algorithm to regularize infinite problems by interval truncation
- For a problem with a Coulomb-like potential both around the origin and in the asymptotic range a more accurate treatment of the boundaries is possible
  - asymptotic expressions for the Coulomb equation are used to obtain more precise BCs in the right truncation point
  - in a small region around the origin a special algorithm is applied