Exploring Heavy Mesons

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Motivation

- Mesons, quark and anti-quark pairs united by the exchange of gluons, are excellent cases for the study of the strong nuclear force.
- **bottomonium** ($b\bar{b}$) and **charmonium** ($c\bar{c}$).
- The motivation of this body of work is to solve the TISE for these particles and compare them with momentum space calculations

The generalized Breit–Fermi Hamiltonian

The Hamiltonian used will include as a base the resting masses of the particles, their kinetic energy, a non relativistic potential that describes their general behaviour and other corrections.

$$H = m_1 + m_2 + \frac{p^2}{2\mu} + V_{NR}(r) + H_{LS} + H_{SS} + H_T \,, \qquad (1)$$

The non-relativistic potential is the Cornell potential:

$$V_{NR}(r) = -\frac{\alpha_s}{r} + \sigma r \qquad (2)$$

Where the linear term (σr) represents the binding properties of a gluon tube formed between two quarks as they separate, and the vectrial term (-$\frac{\alpha_s}{r}$) represents the attractive force created by the exchange of a single gluon at short distances.

From the 3D equation to a 1D radial problem

Beginning with the time independent Schrödinger equation:

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi(\mathbf{r}) + V(r)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{3}$$

We can separate the state Ψ as such:

$$\Psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi) \tag{4}$$

Defining the function $u(r)$ as such:

$$R(r) = \frac{u(r)}{r} \tag{5}$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2}u(r) = (E - \underbrace{\left[V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}\right]}_{V_{eff}(r)})u(r) \tag{6}$$

The differential equation can now be numerically solved using the Numerov method.

Solving the Schrödinger equation with Numerov's method

Numerov form: $f''(x) = g(x)f(x)$

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The radial Schrödinger equation:

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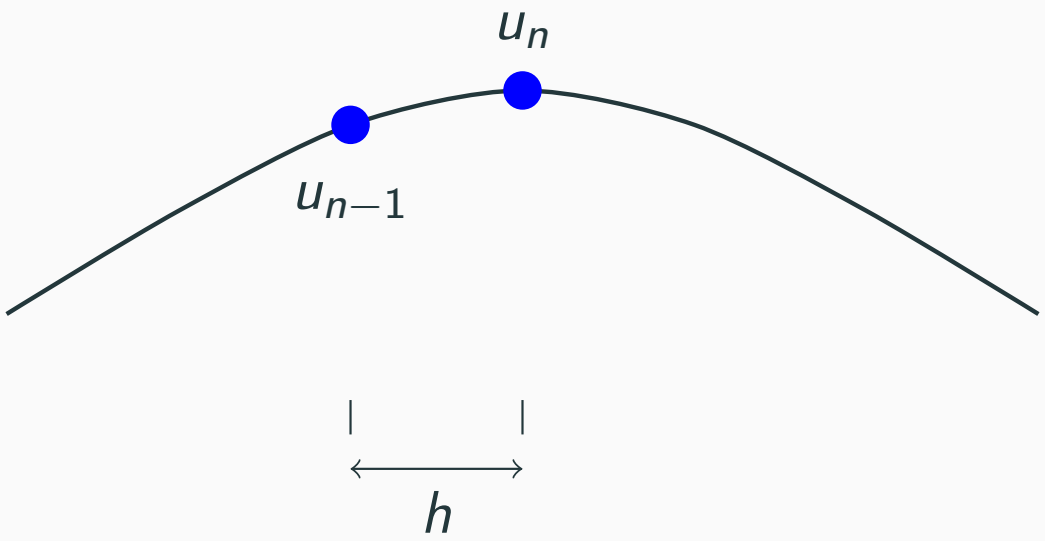
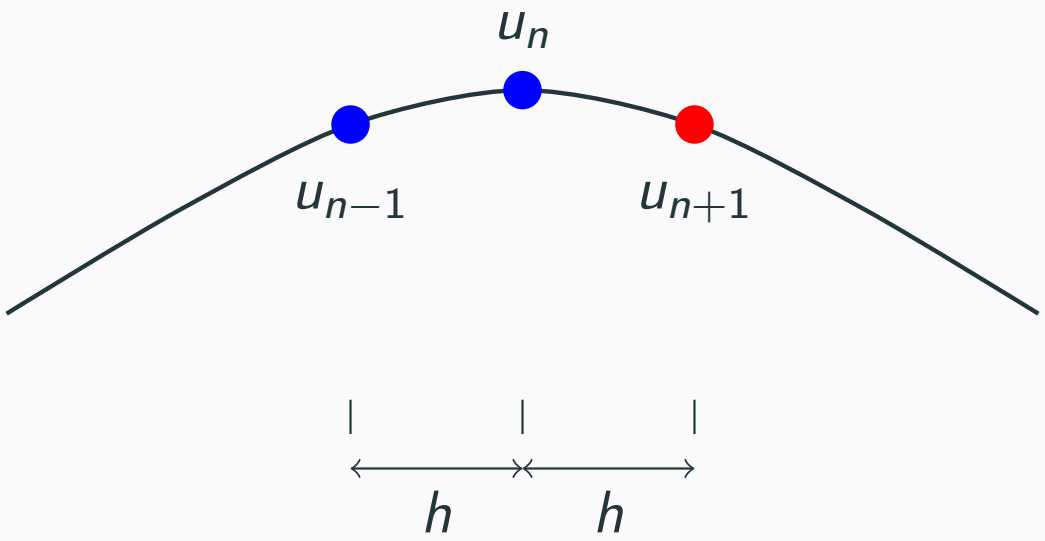
where $g(r) = -\frac{2m}{\hbar^2}(E - V_{eff}(r))$

The Numerov idea: use three neighbouring points



Known: u_{n-1}, u_n

The Numerov idea: use three neighbouring points



$$\boxed{u_{n-1}, u_n \quad \Longrightarrow \quad u_{n+1}}$$

The Numerov recurrence

$$u_{n+1} = u_n + hu'_n + \frac{h^2}{2}u''_n + \frac{h^3}{6}u'''_n + \frac{h^4}{24}u''''_n + \frac{h^5}{120}u^{(5)}_n + \mathcal{O}(h^6)$$

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$$\begin{aligned} u_n'''' &= (u_n'')'' = (gu)_n'' \\ &= \frac{g_{n+1}u_{n+1} - 2g_n u_n + g_{n-1}u_{n-1}}{h^2} + \mathcal{O}(h^2) \end{aligned}$$

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Numerov recurrence relation:

$$\boxed{u_{n+1} = \frac{2\left(1 + \frac{5h^2 g_n}{12}\right) u_n - \left(1 - \frac{h^2 g_{n-1}}{12}\right) u_{n-1}}{1 - \frac{h^2 g_{n+1}}{12}}}$$

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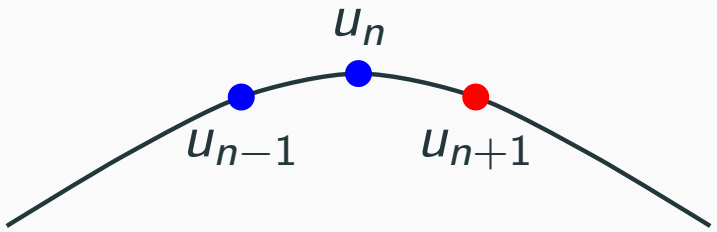
Forward vs backward propagation

Forward propagation



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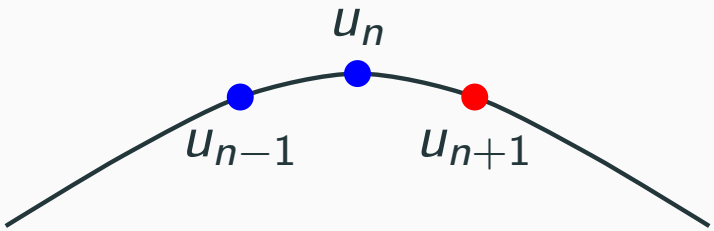

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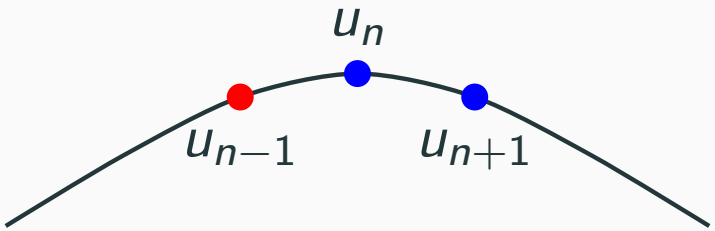

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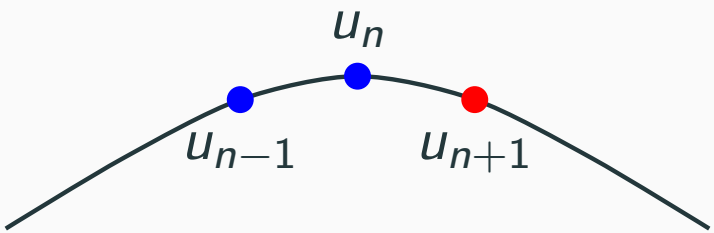

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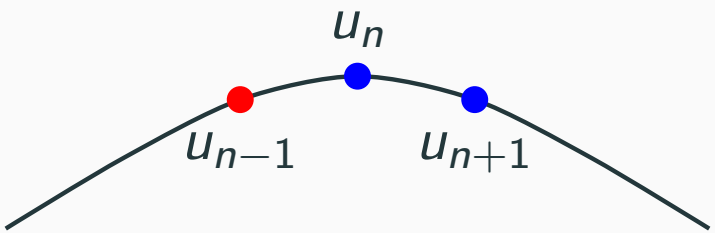

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Boundary conditions for the radial Schrödinger equation:

$$u(0) = 0$$

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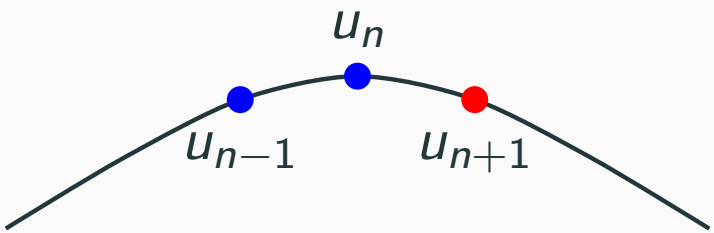

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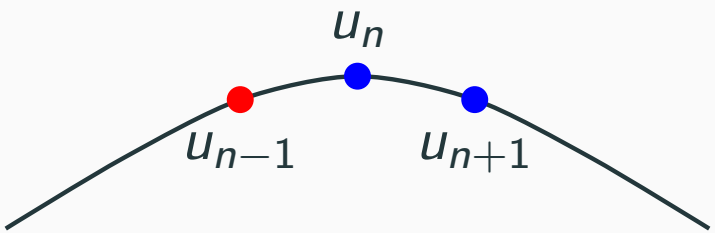

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Boundary conditions for the radial Schrödinger equation:

$$u(0) = 0 \qquad u(r) \to 0 \quad \text{as} \quad r \to \infty$$

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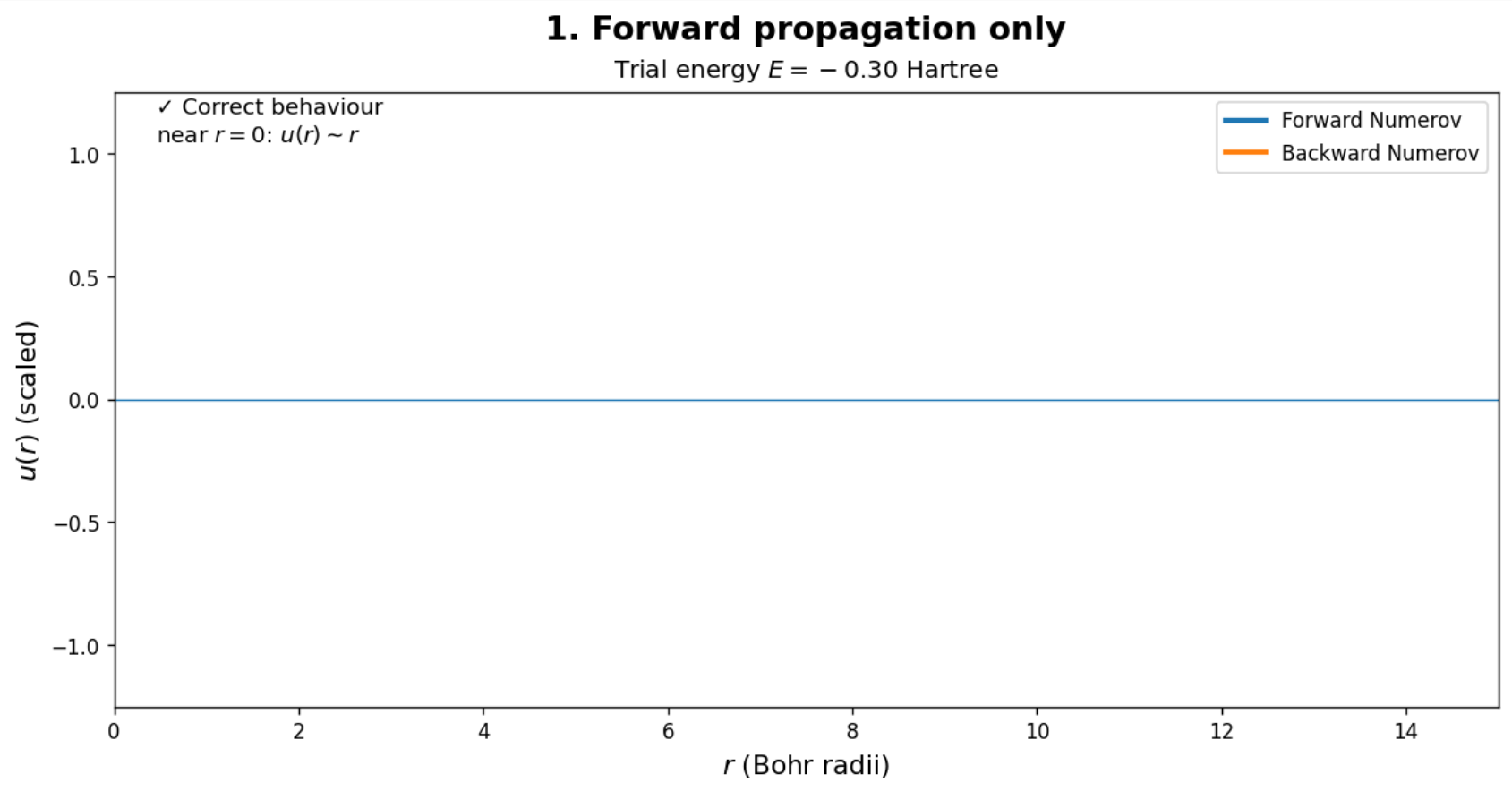

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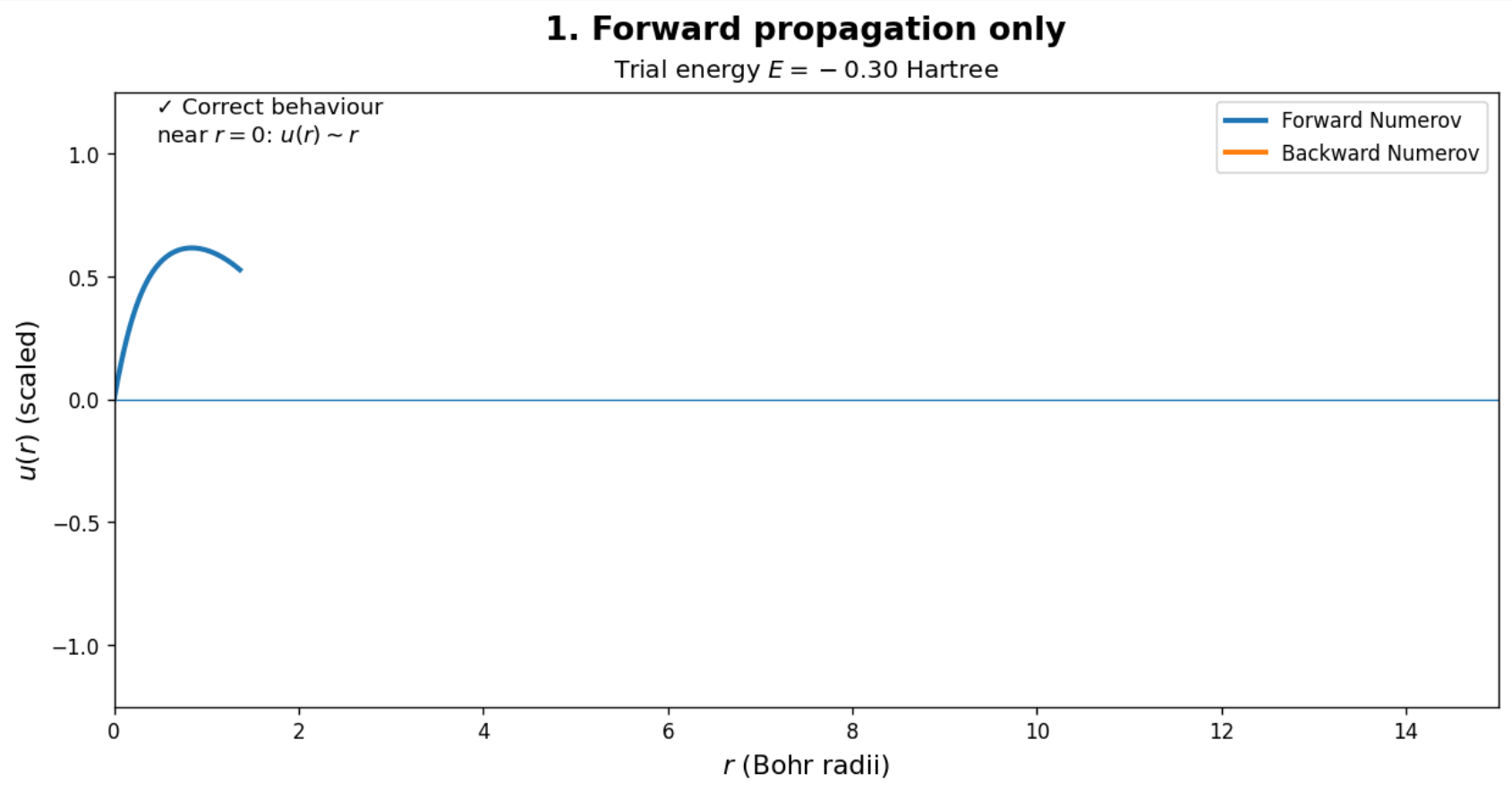

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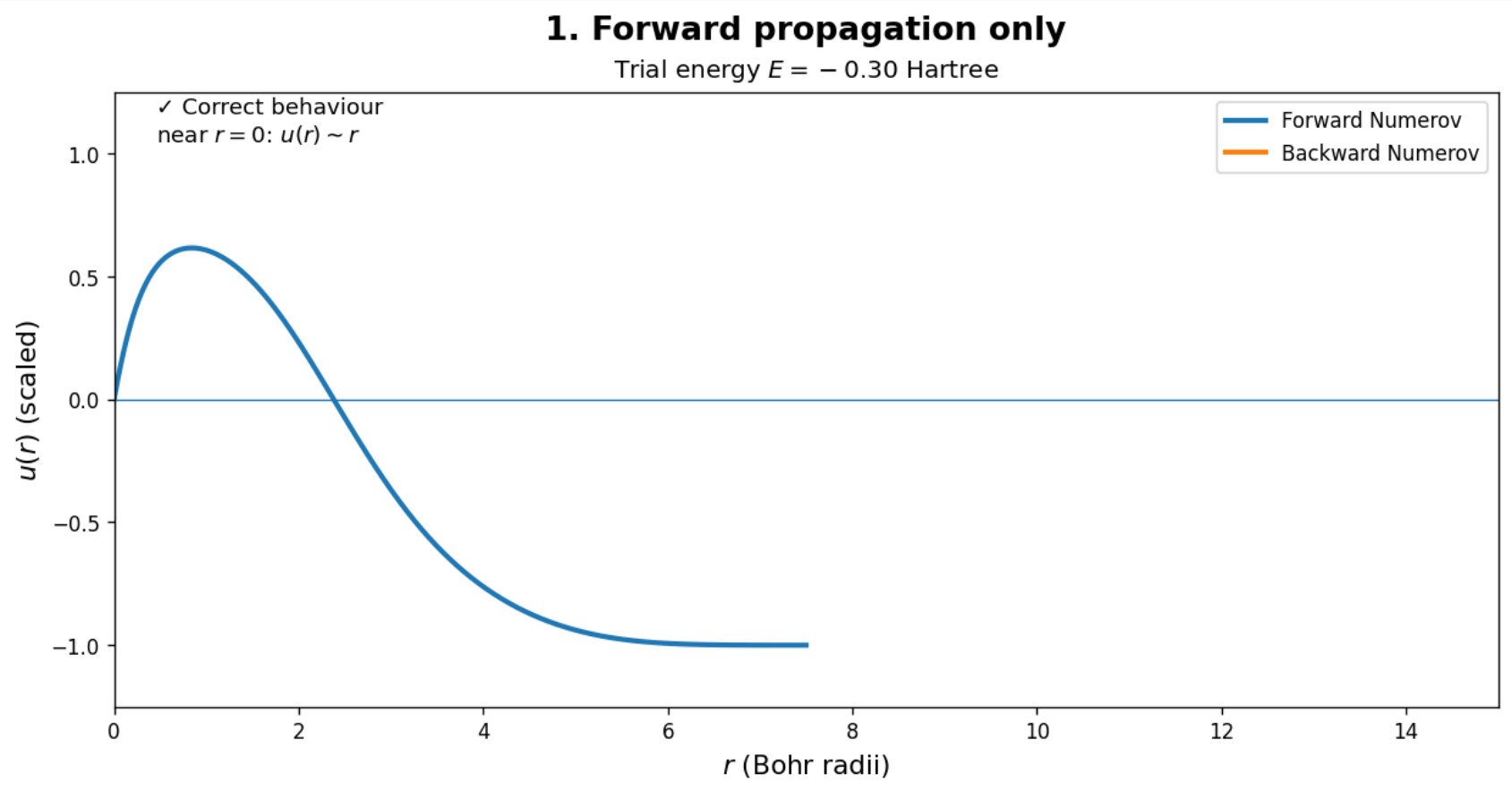

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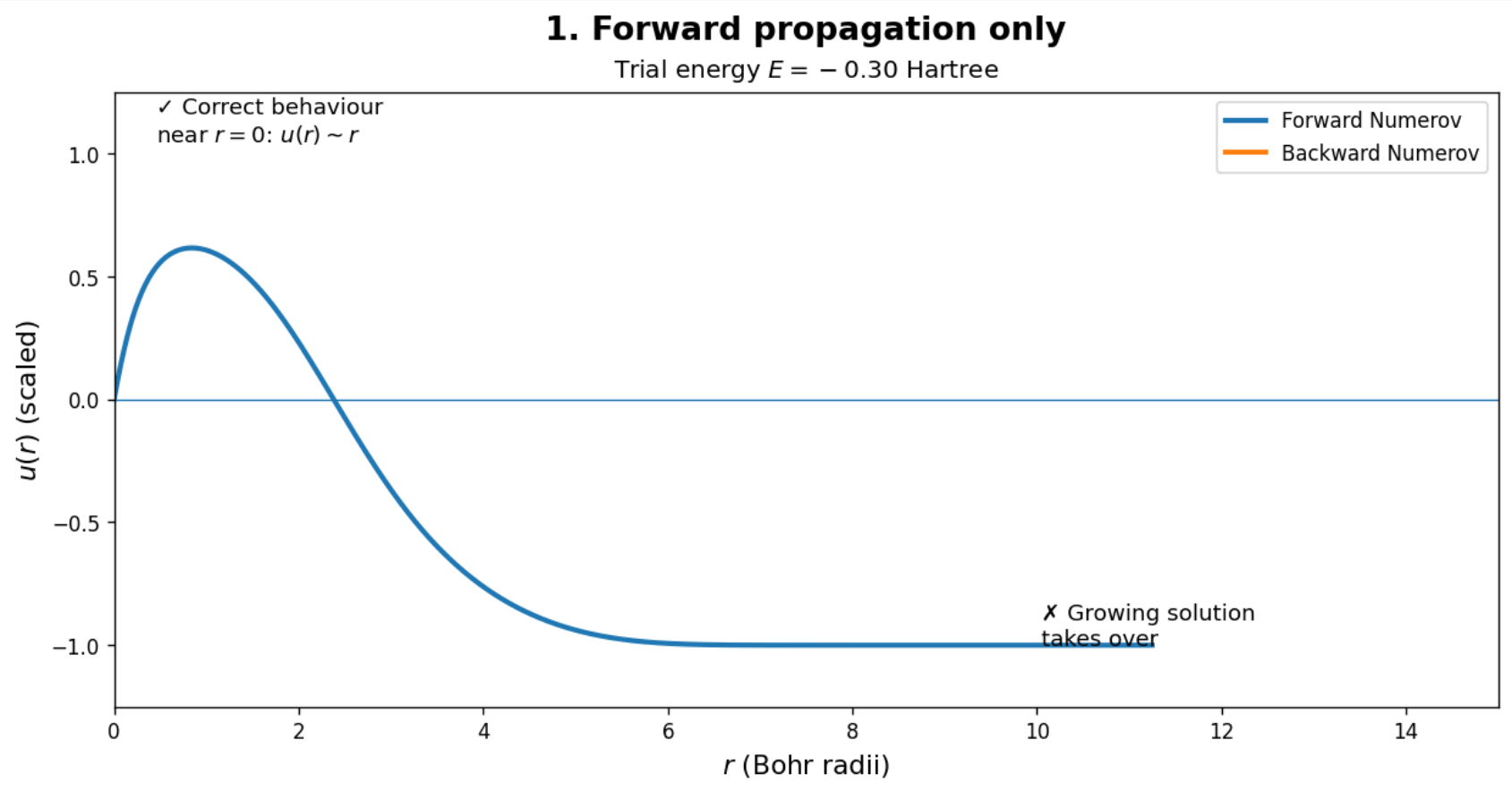

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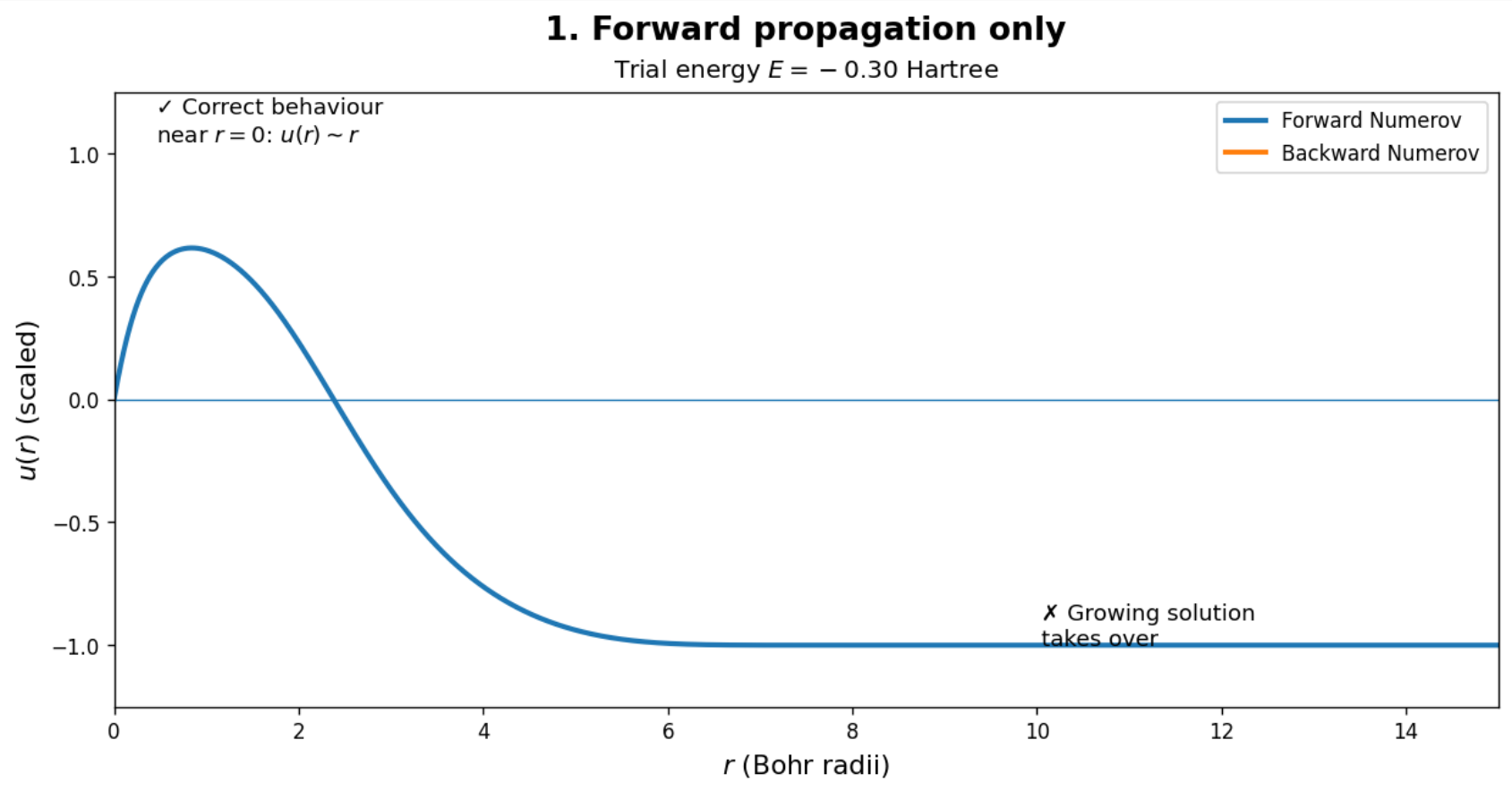

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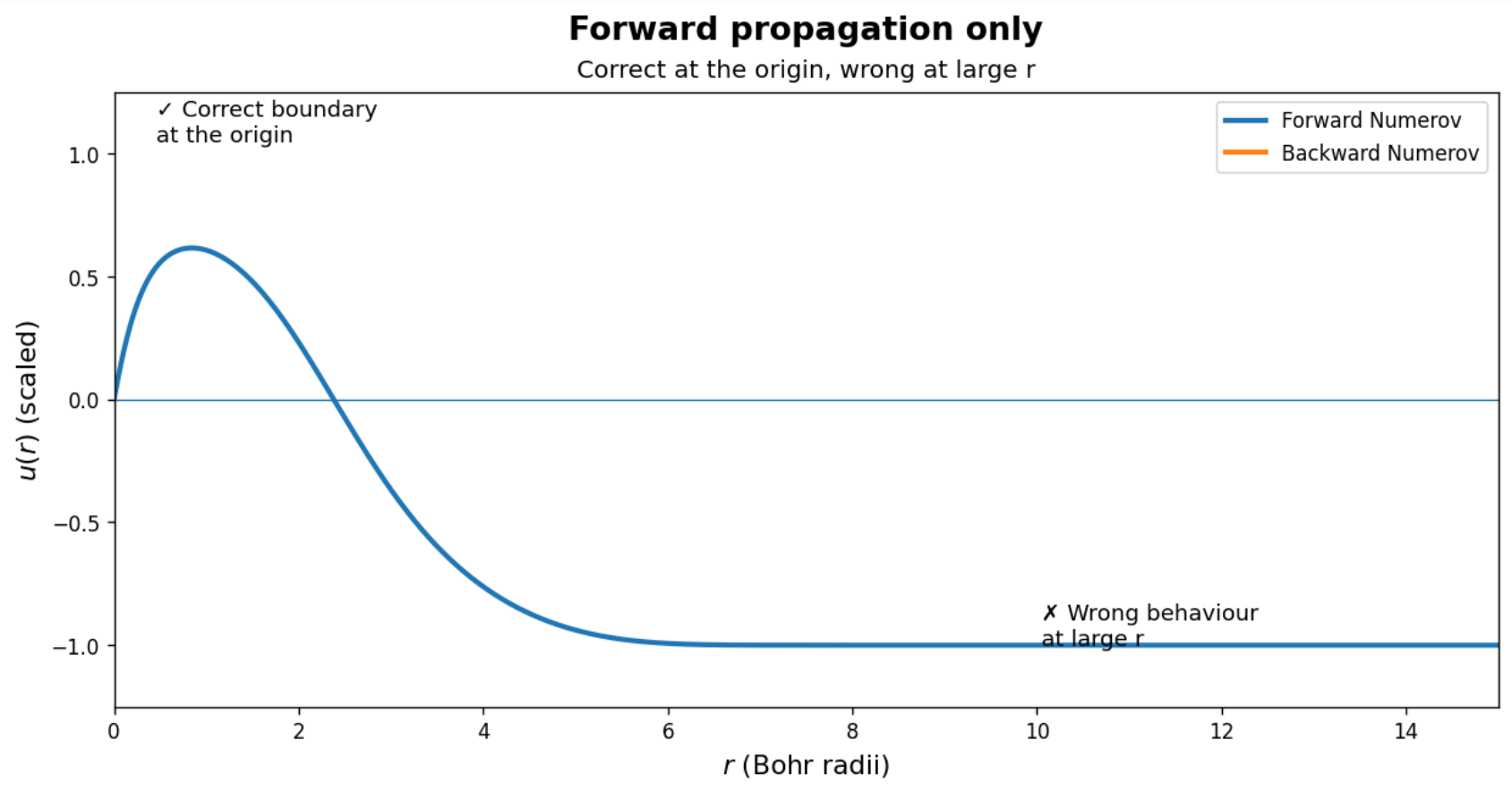

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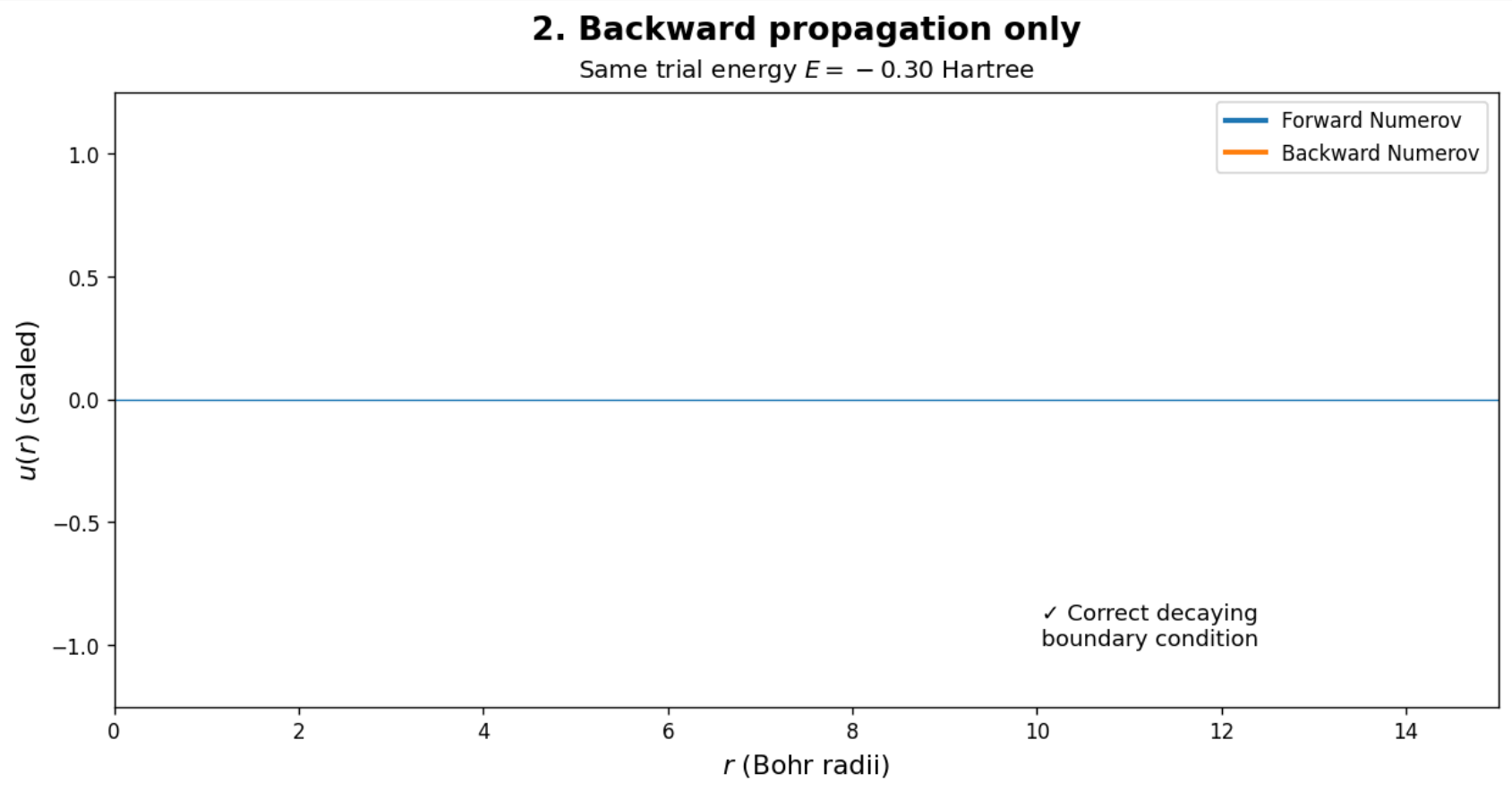

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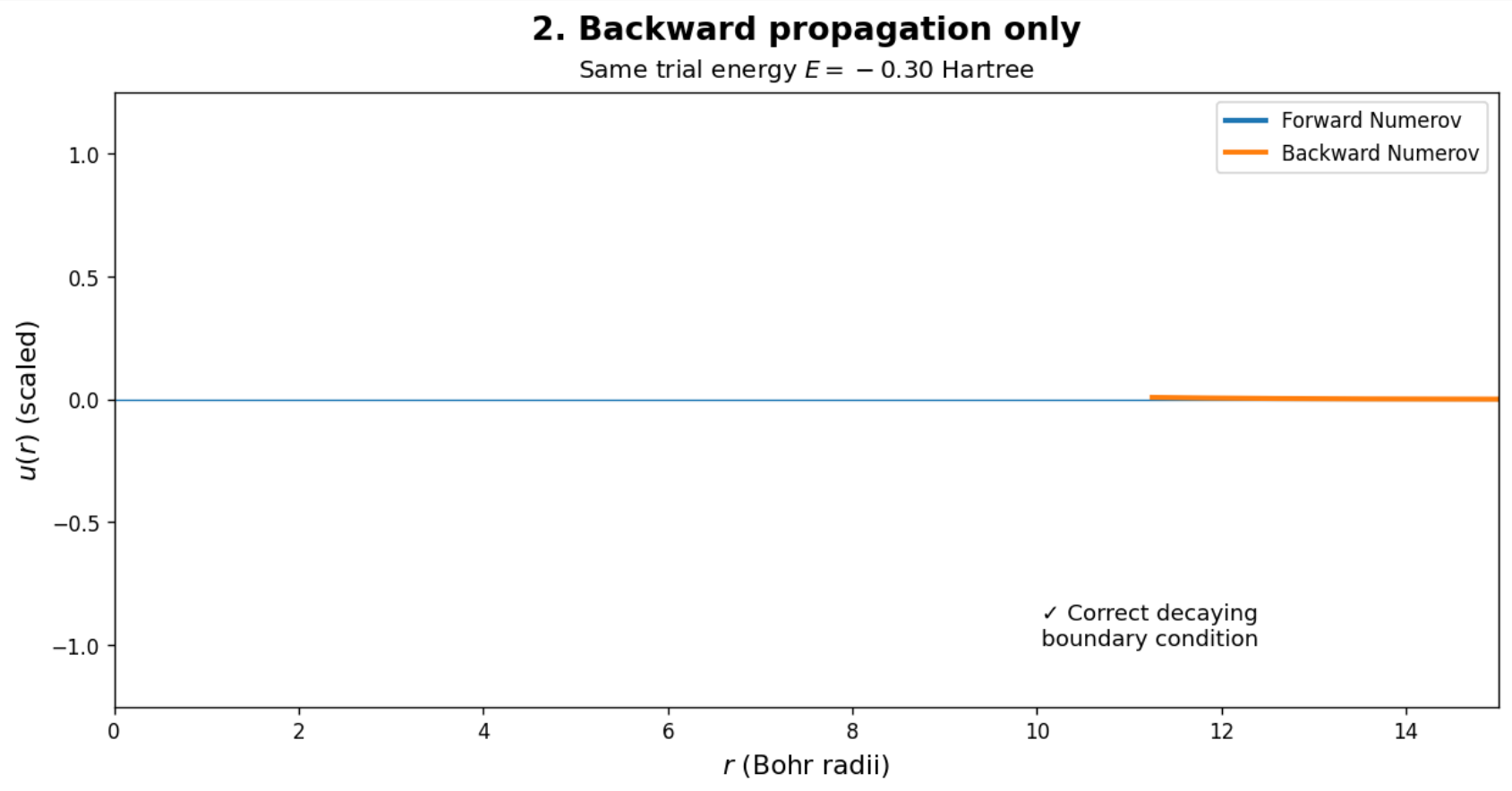

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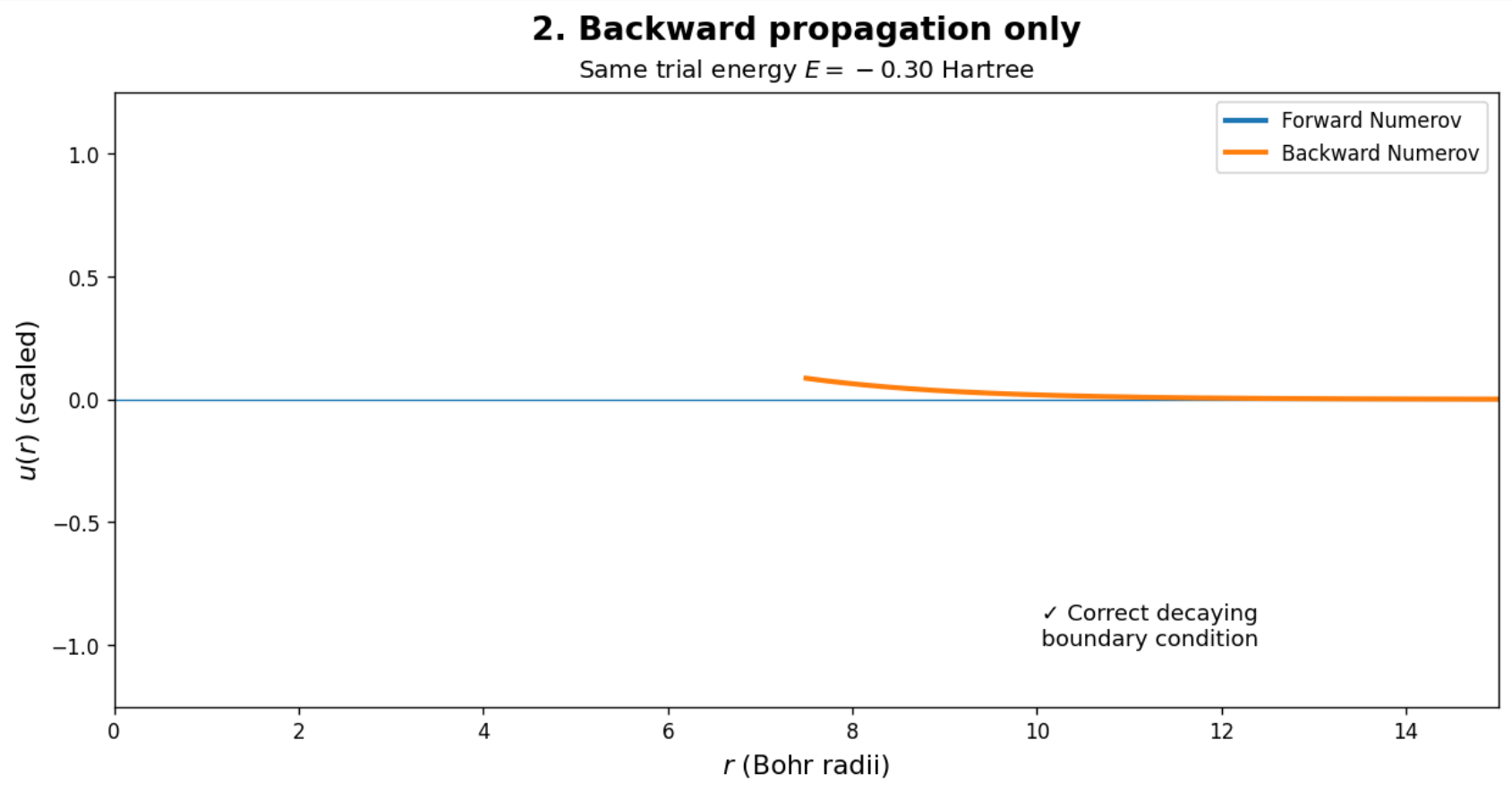

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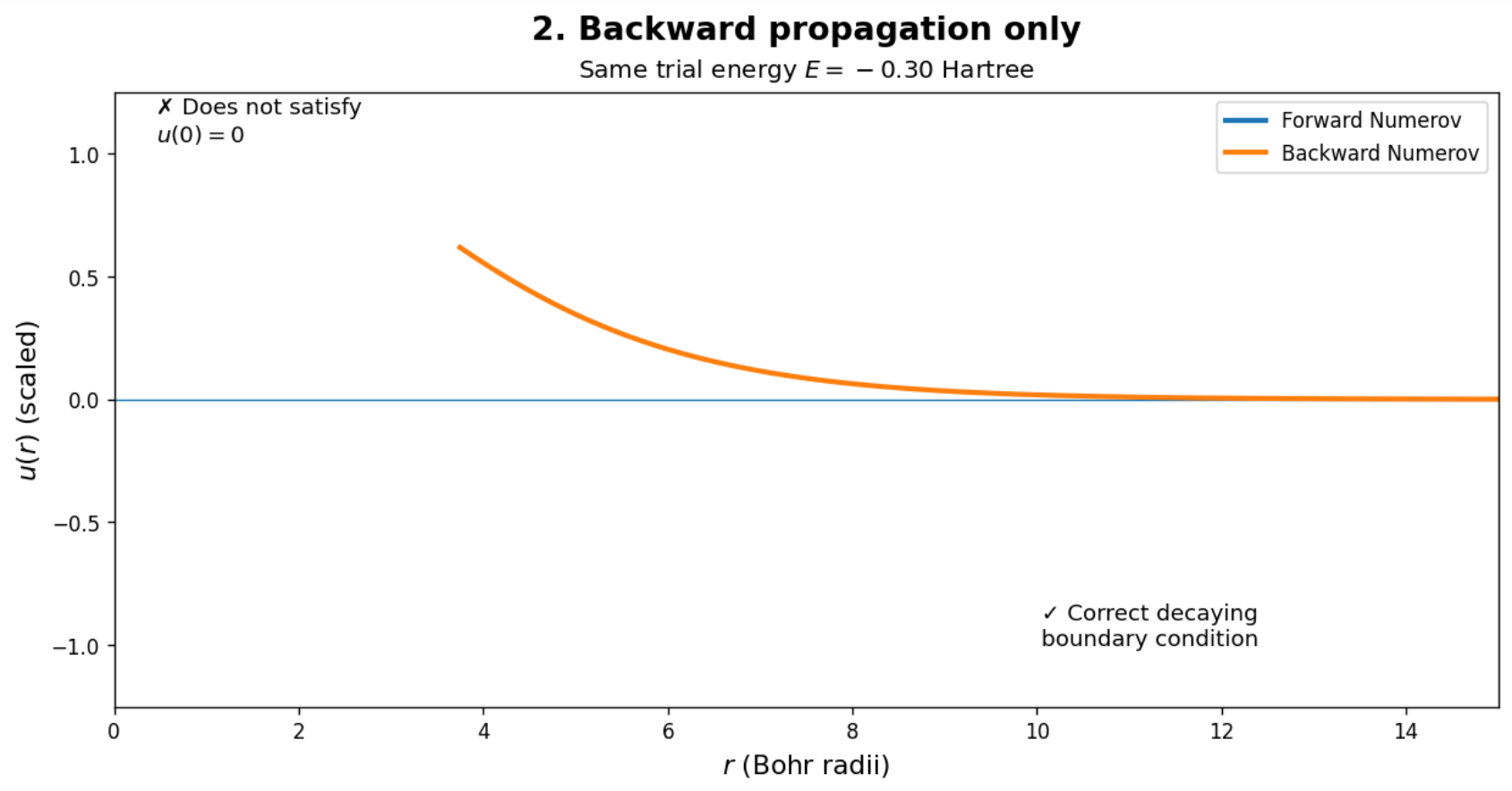

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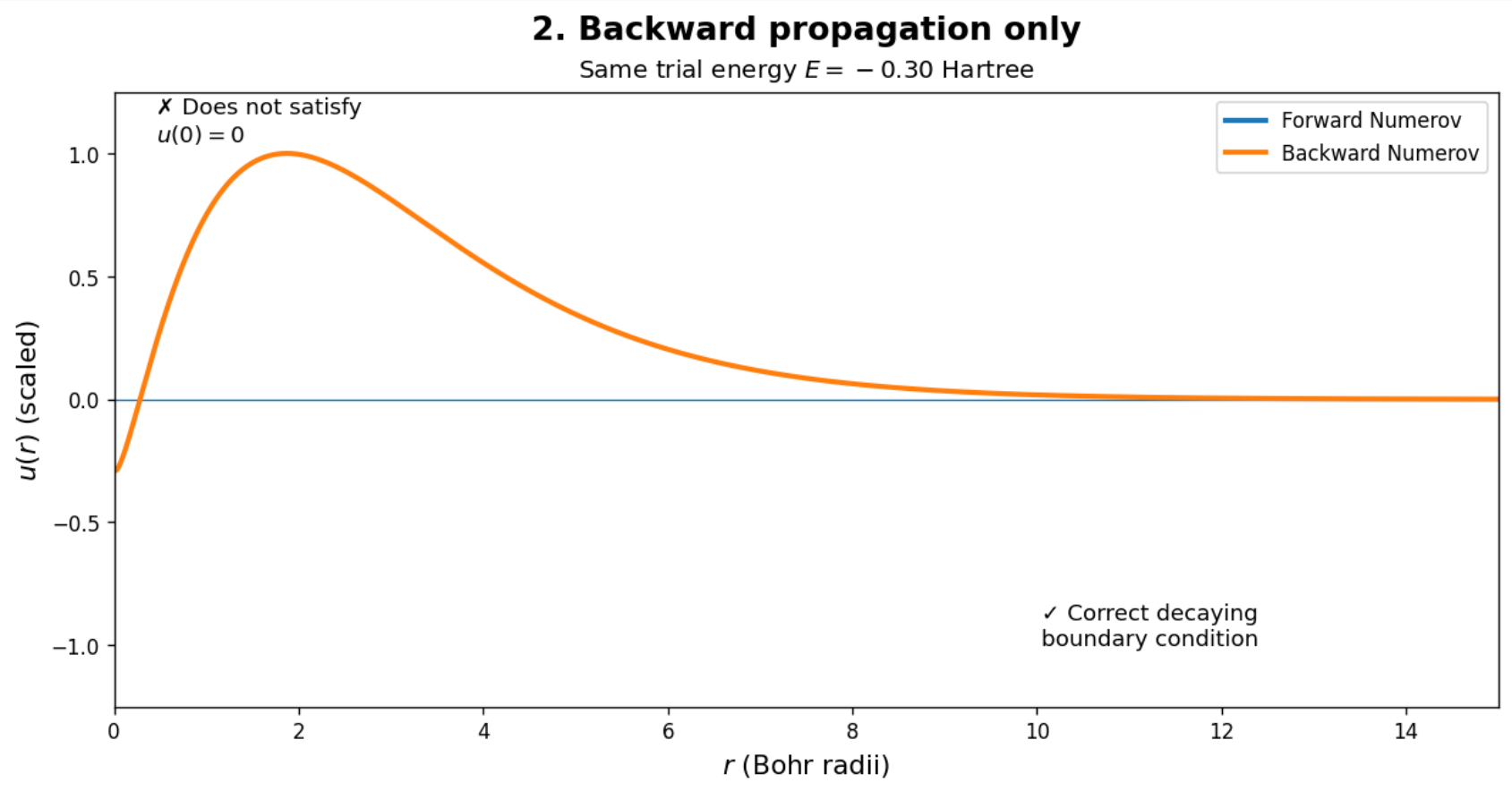

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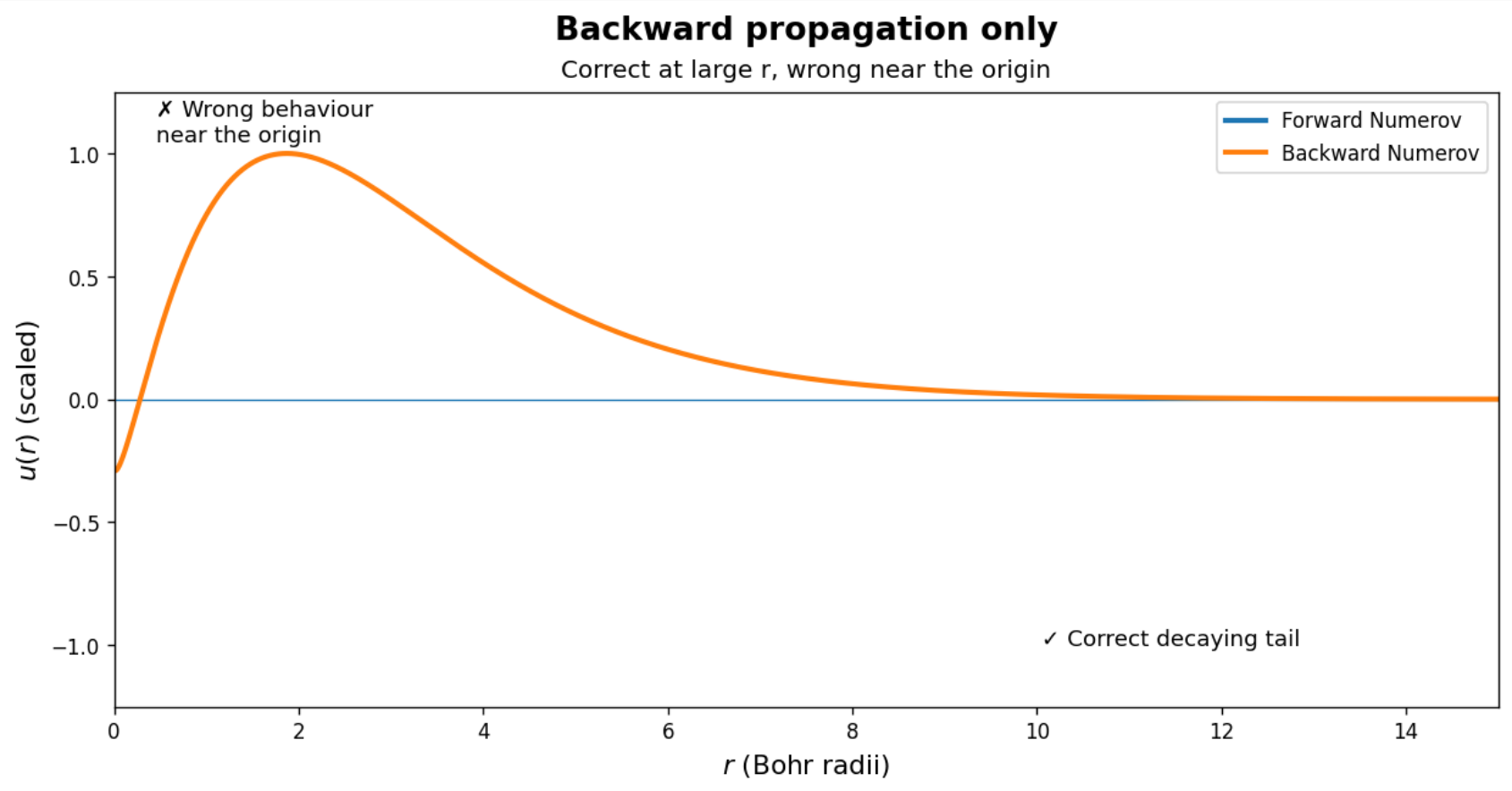

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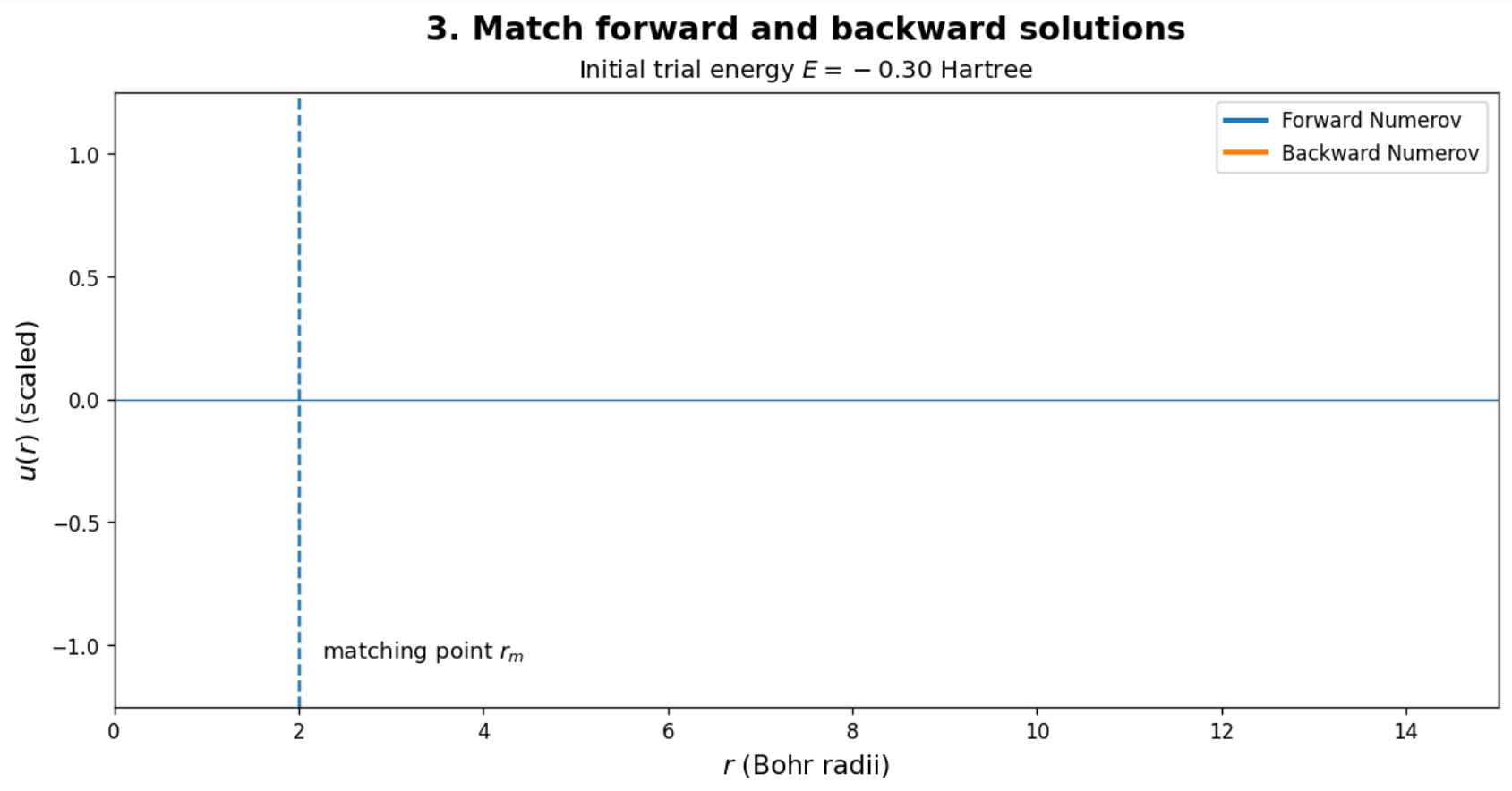

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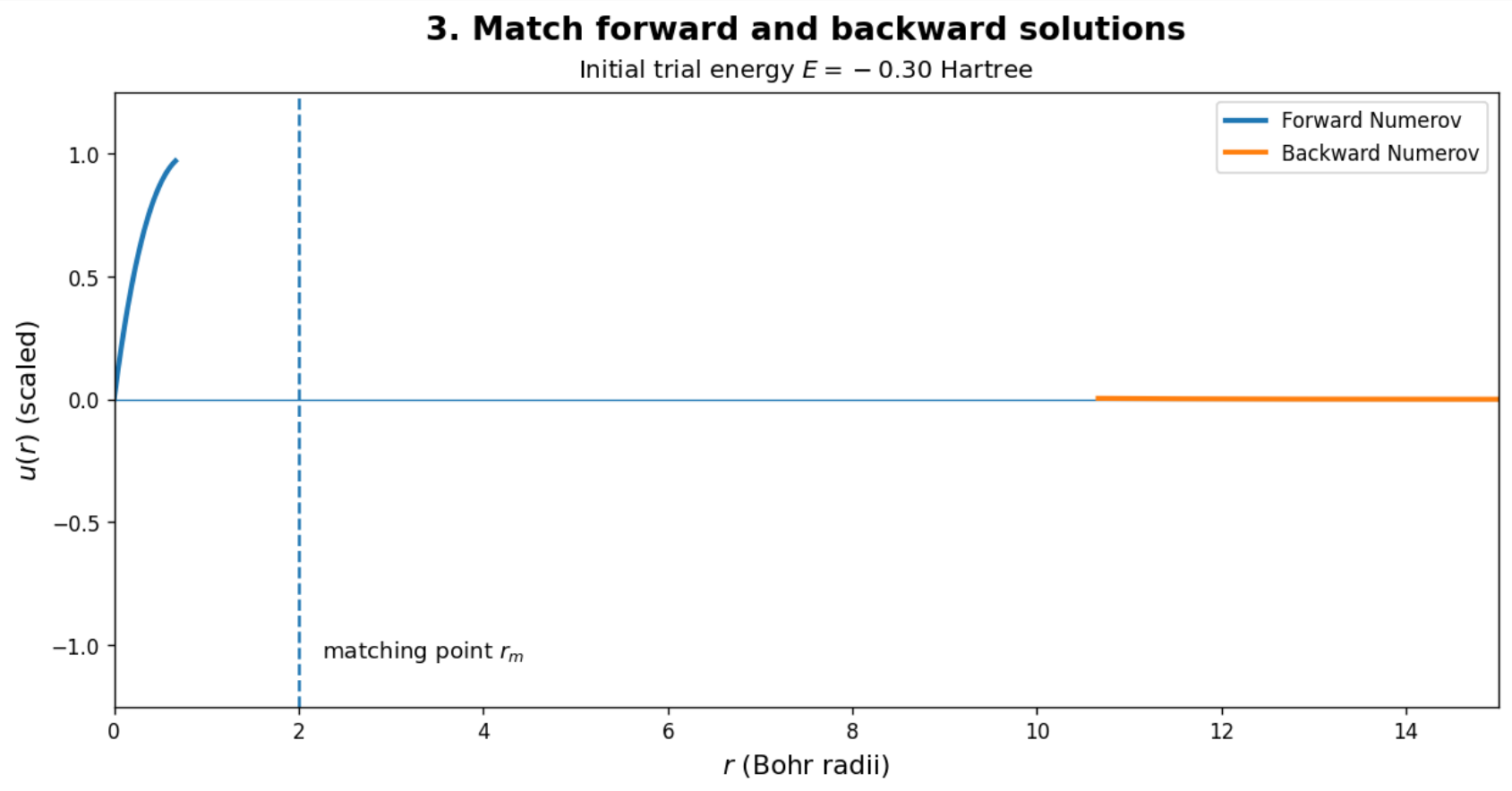

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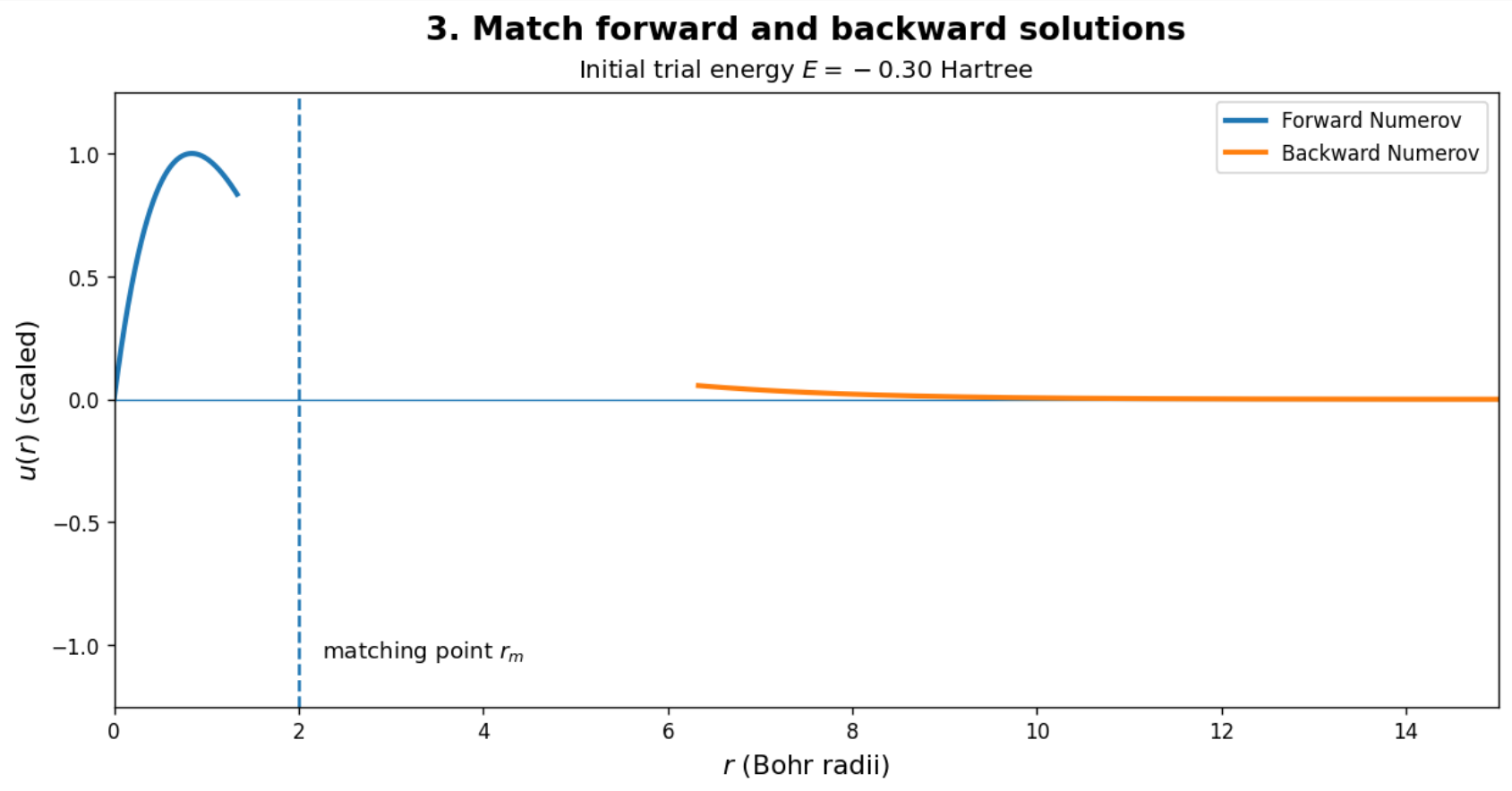

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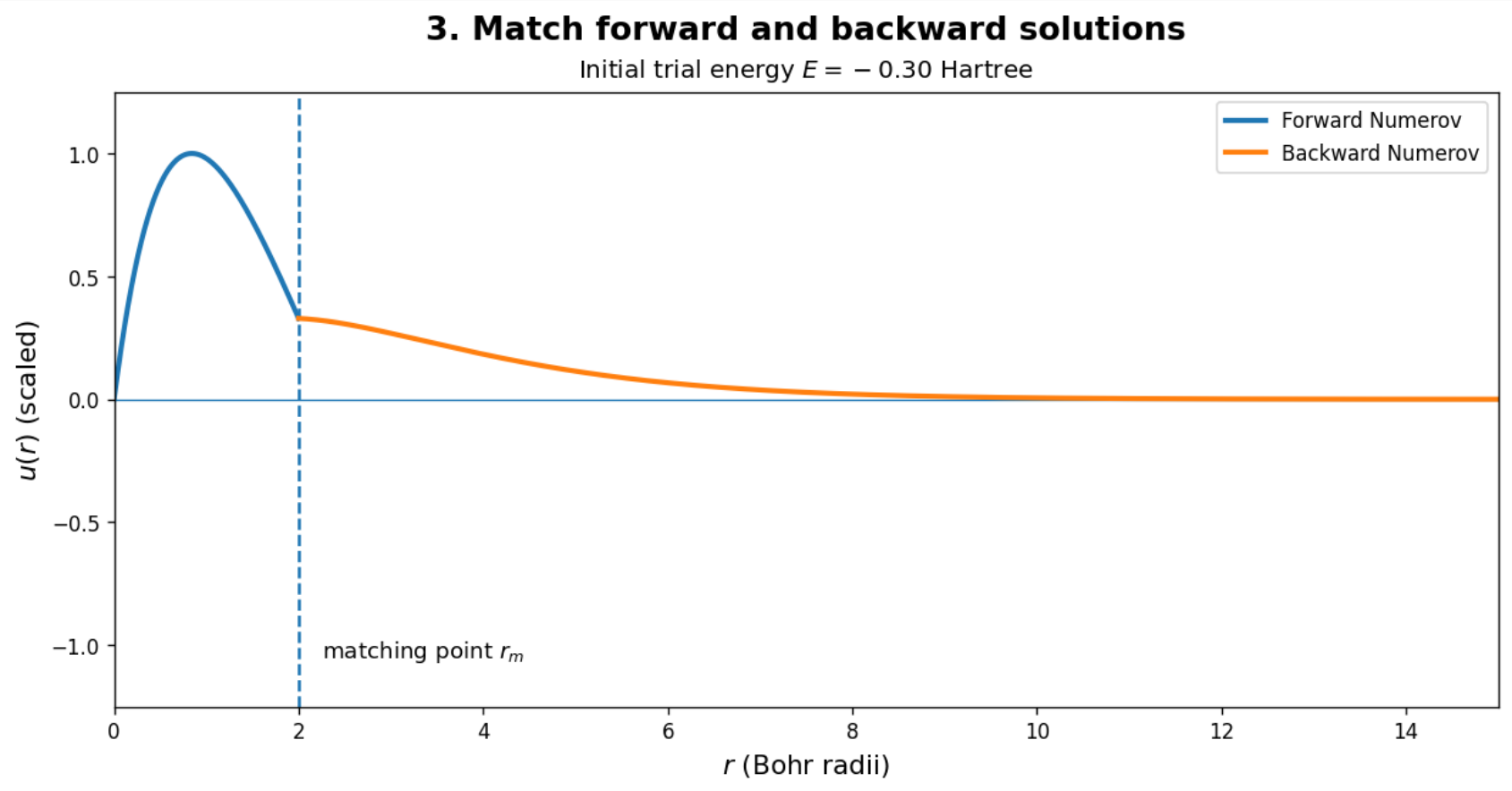

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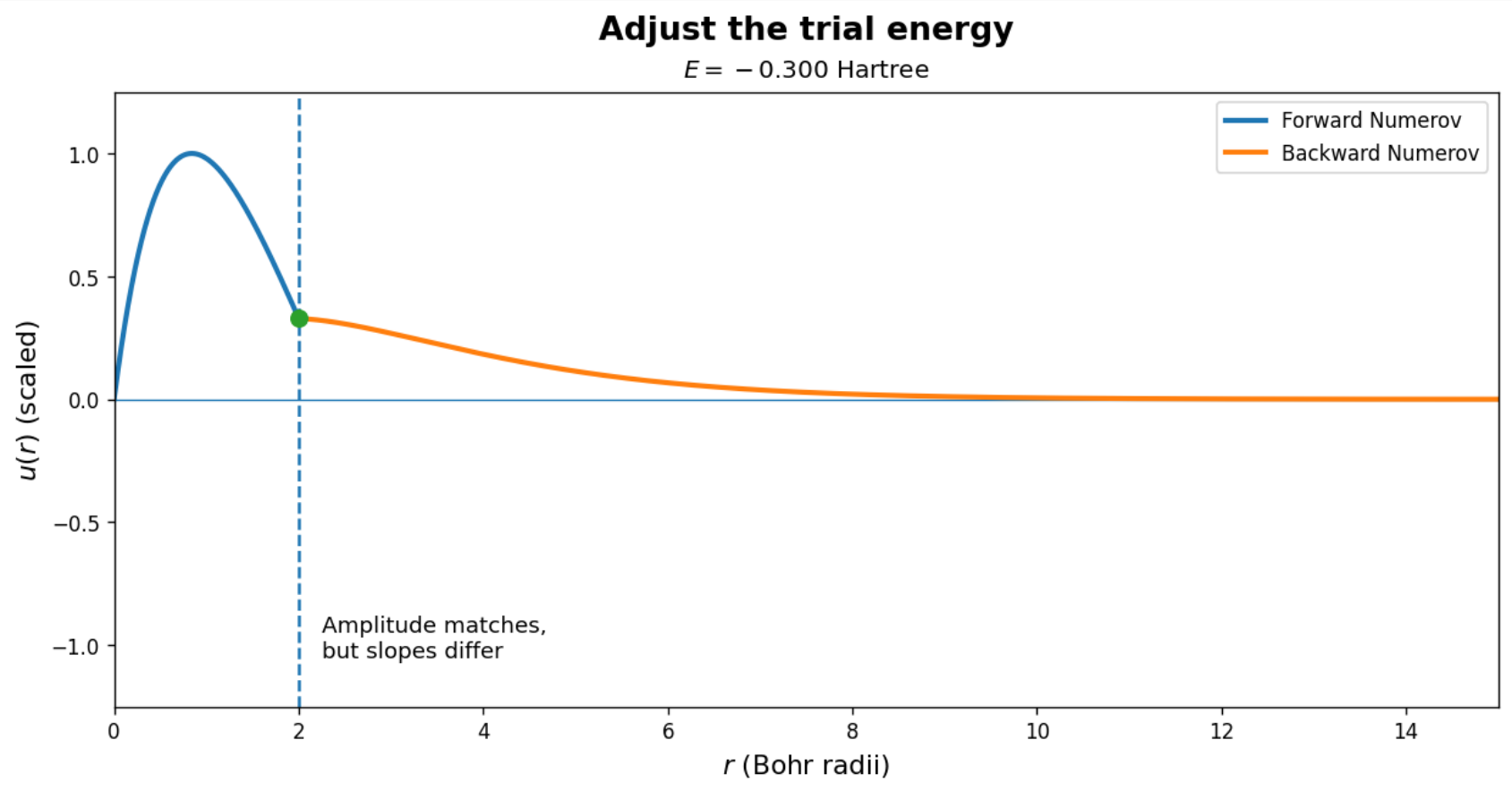

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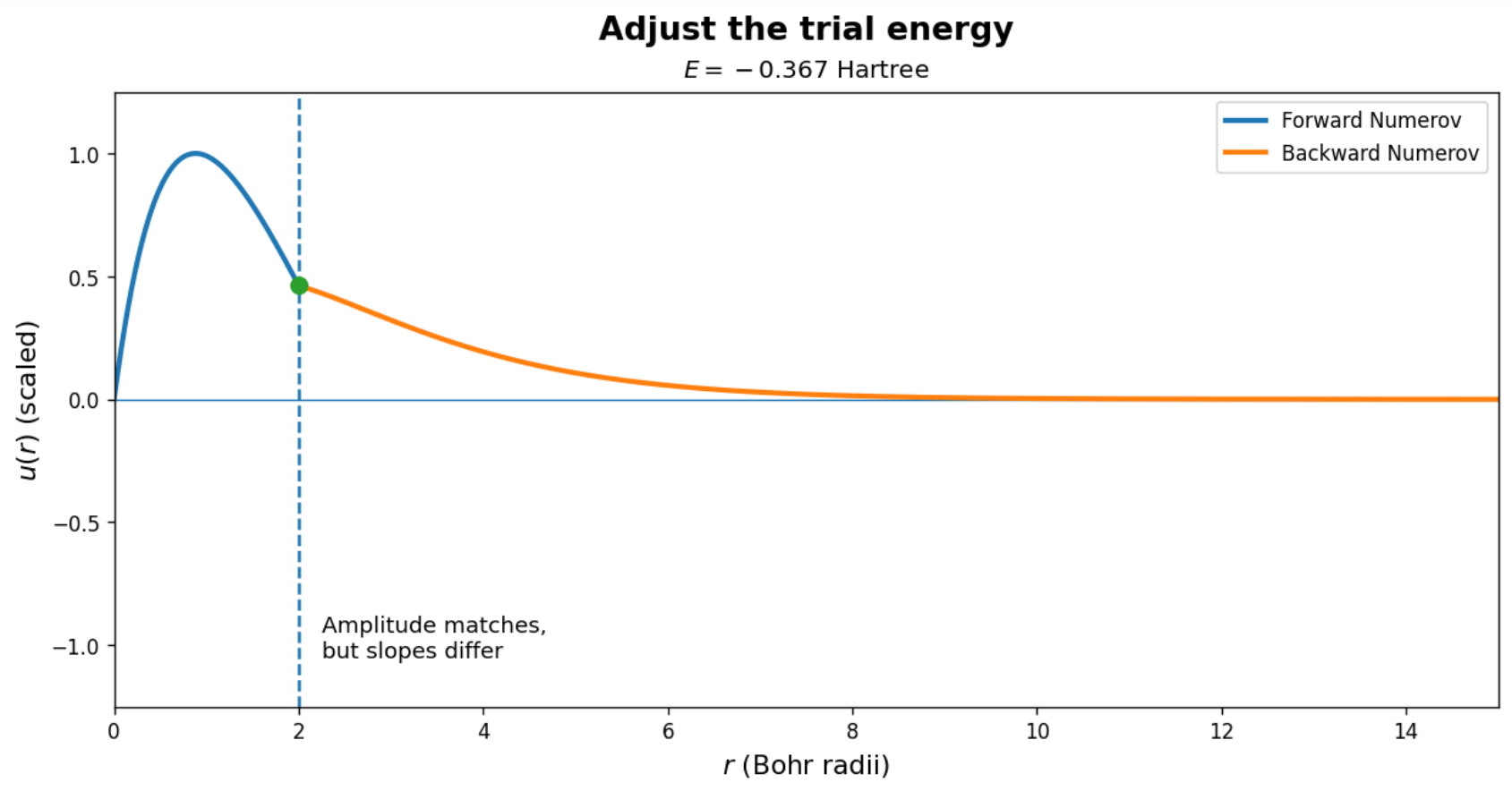

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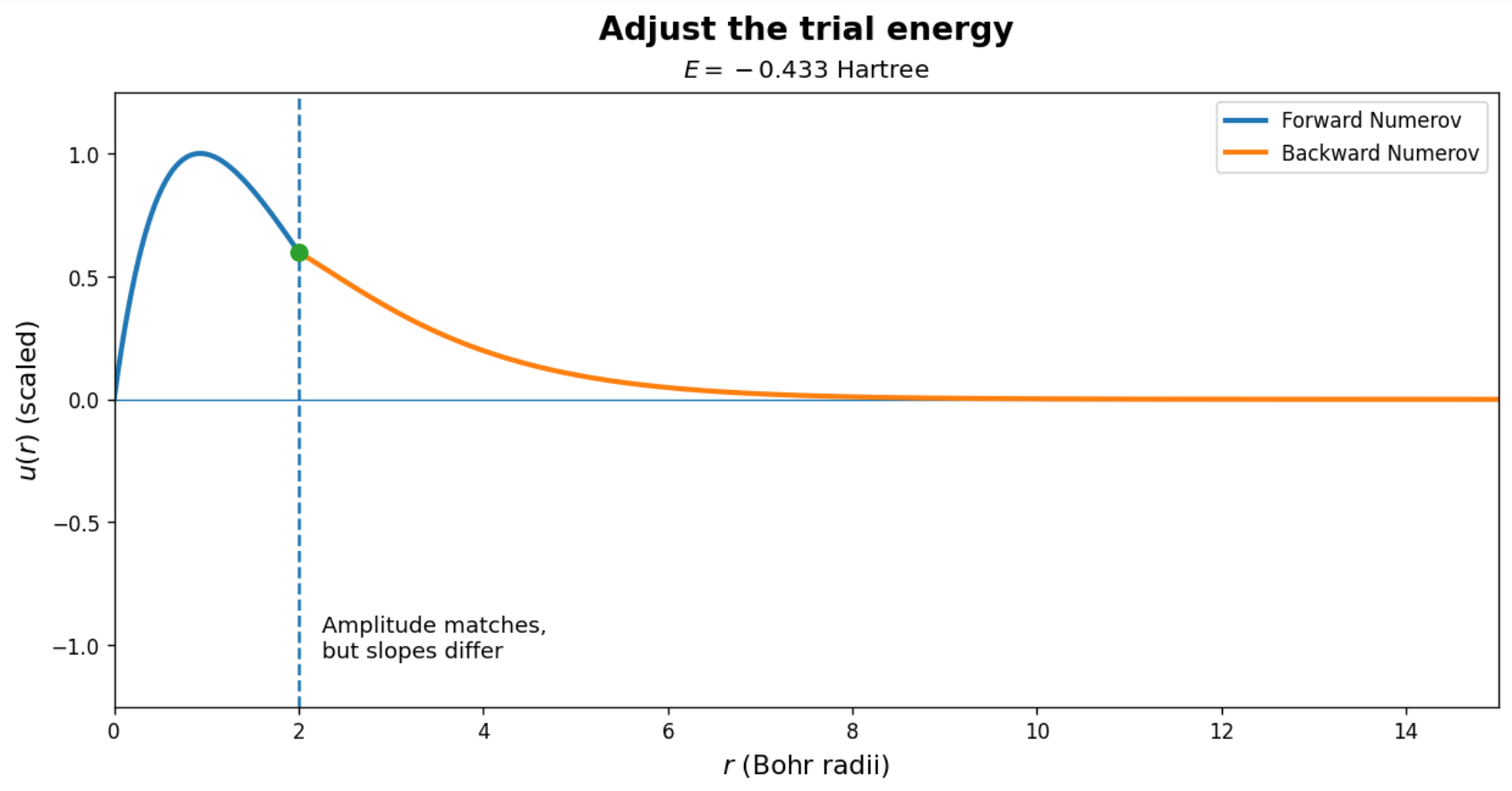

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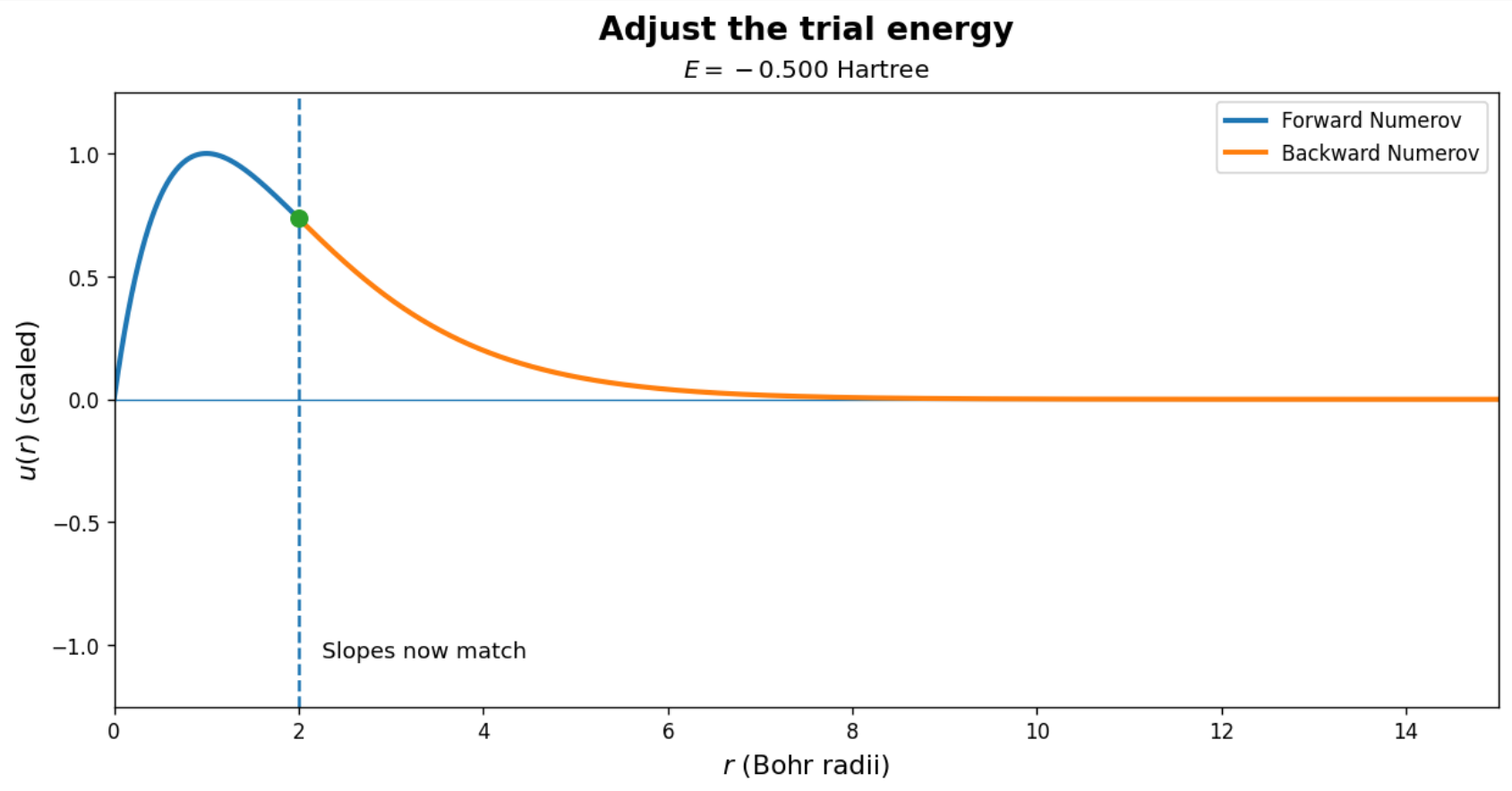

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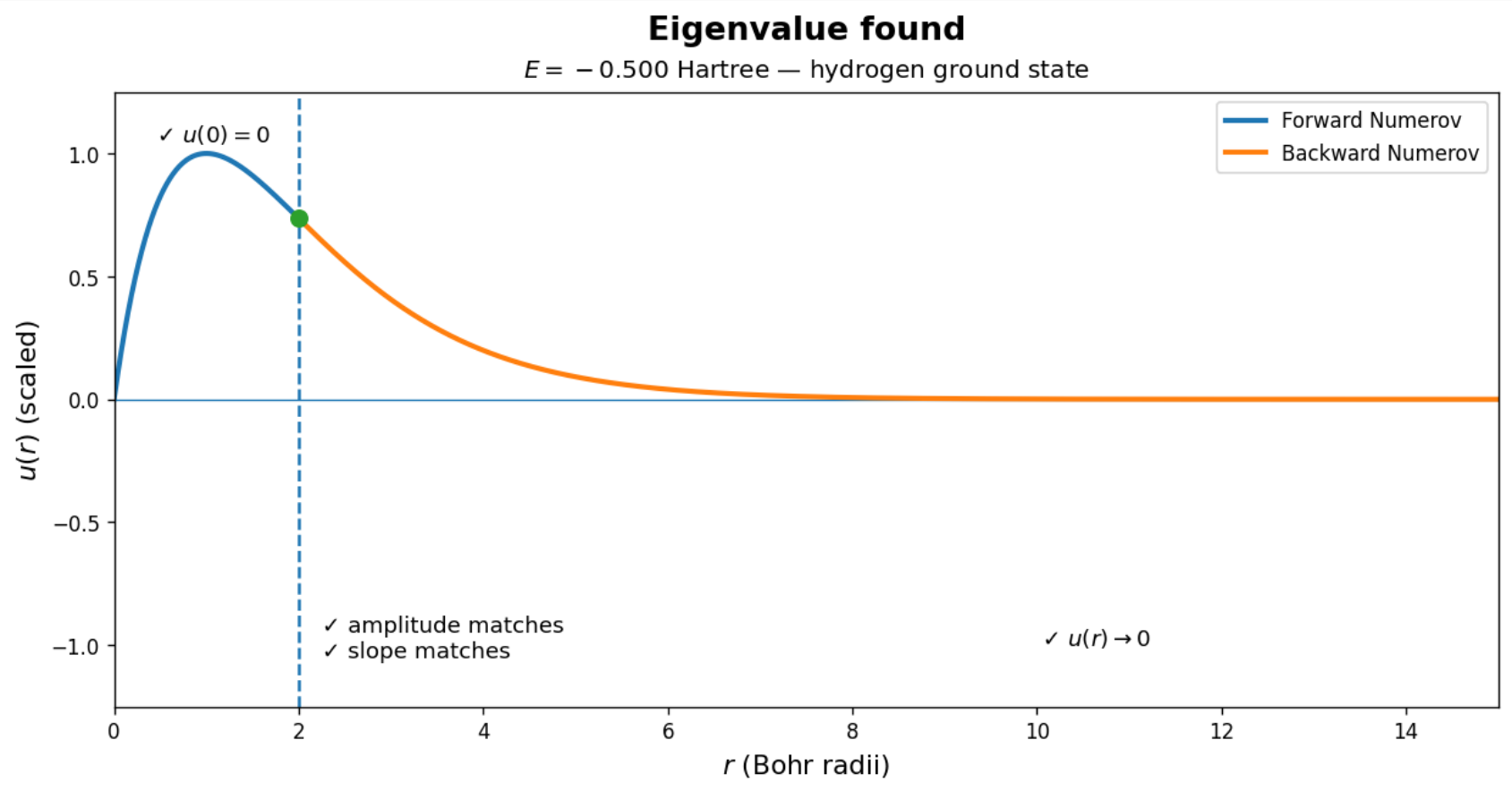

Matching point

How to choose a reasonable matching point?

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Classical turning point

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Schrödinger equation looks roughly like $u'' = -k^2 u \rightarrow$ oscillatory

Matching point

How to choose a reasonable matching point?

Classical turning point $V_{eff}(r) = E$

Look at the sign of $g(r) = \frac{2\mu}{\hbar^2}(V_{eff} - E)$

In the classically *allowed* region, $E > V_{eff}$, so $g(r) < 0$
Schrödinger equation looks roughly like $u'' = -k^2 u \rightarrow$ oscillatory

In the classically *forbidden* region, $E < V_{eff}$

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Schrödinger equation looks roughly like $u'' = -k^2 u \rightarrow$ oscillatory

In the classically *forbidden* region, $E < V_{eff}$, so $g(r) > 0$
Schrödinger equation looks roughly like $u'' = k^2 u \rightarrow$ exponential

Matching point

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Classical turning point $V_{eff}(r) = E$

Implementation in the code

Matching point

How to choose a reasonable matching point?

Classical turning point $V_{eff}(r) = E$

Implementation in the code

$$(V_{eff,i} - E)(V_{eff,i-1} - E) \leq 0$$

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$$u_f(r_{\min}) \to u_f(r_m) \qquad u_b(r_{\max}) \to u_b(r_m)$$

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$$\text{scale} = A = \frac{u_f(r_m)}{u_b(r_m)} \Rightarrow u_f(r_m) = A u_b(r_m)$$

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$$\text{scale} = A = \frac{u_f(r_m)}{u_b(r_m)} \Rightarrow u_f(r_m) = A u_b(r_m)$$

Derivatives calculated using centred differences:

$$u_f'(r_m) \approx \frac{u_f(r_{m+1}) - u_f(r_{m-1})}{2h}, \quad u_b'(r_m) \approx A\frac{u_b(r_{m+1}) - u_b(r_{m-1})}{2h}$$

Matching point

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Implementation in the code

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$$\text{scale} = A = \frac{u_f(r_m)}{u_b(r_m)} \Rightarrow u_f(r_m) = A u_b(r_m)$$

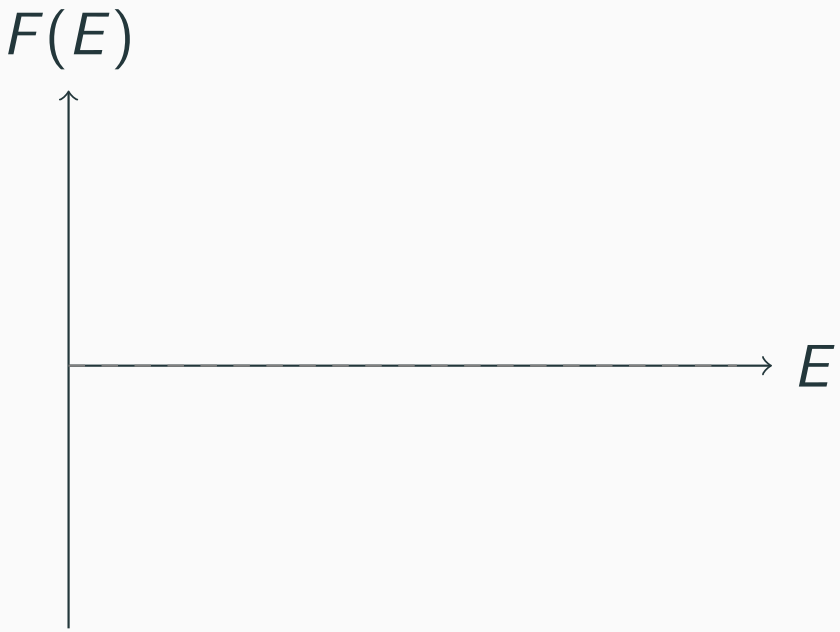
Derivatives calculated using centred differences:

$$u'_f(r_m) \approx \frac{u_f(r_{m+1}) - u_f(r_{m-1})}{2h}, \quad u'_b(r_m) \approx A\frac{u_b(r_{m+1}) - u_b(r_{m-1})}{2h}$$

Shooting function: $\boxed{F(E) = u'_f(r_m) - u'_b(r_m)}$

Scanning the energy range

$$\boxed{F(E) = u_f'(r_m) - u_b'(r_m)}$$



Scanning the energy range

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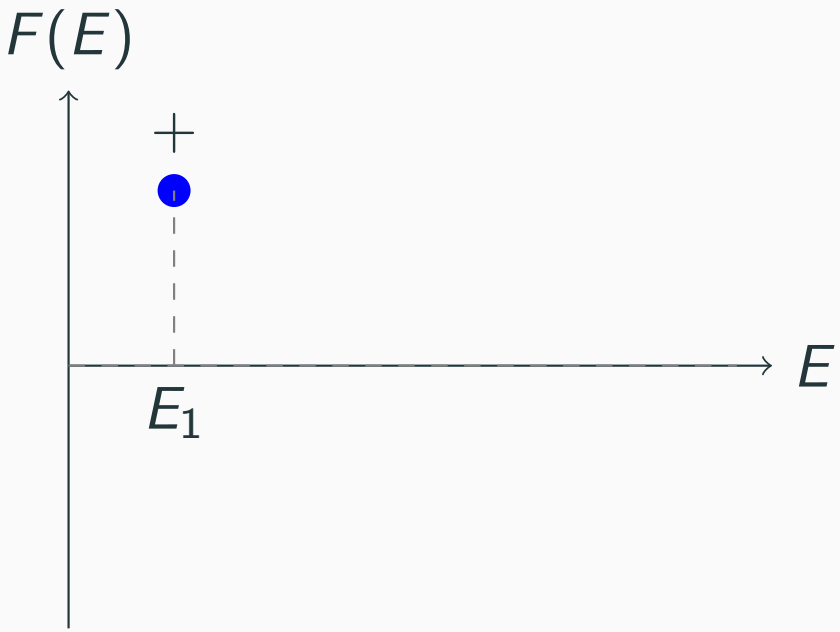

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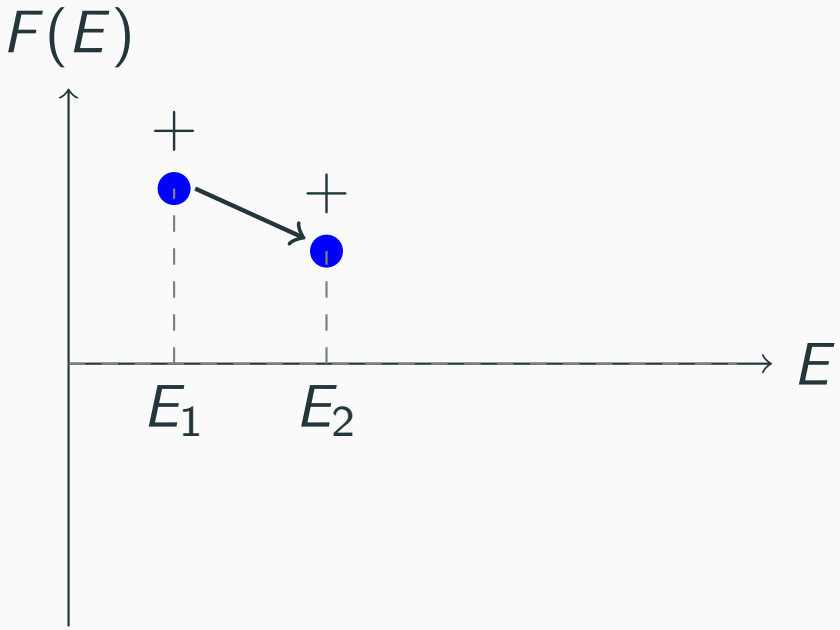
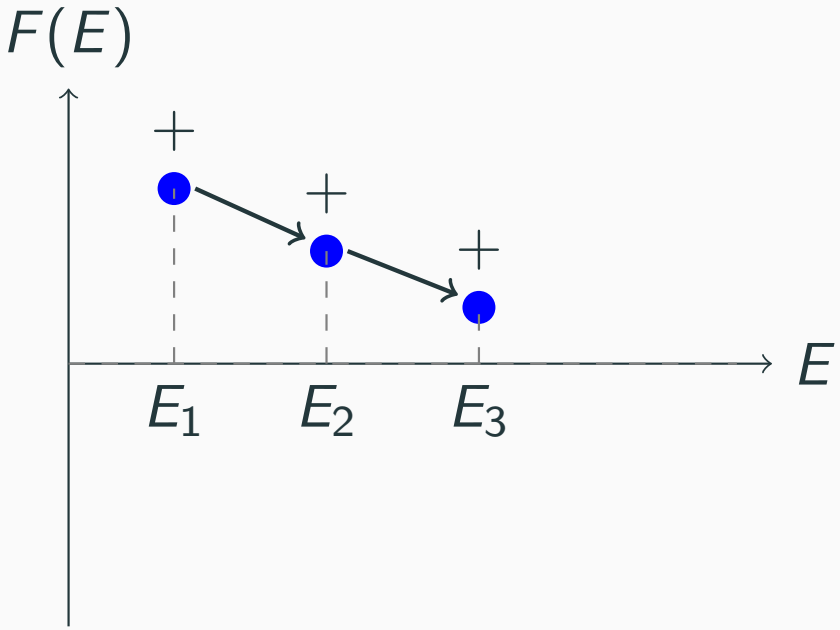


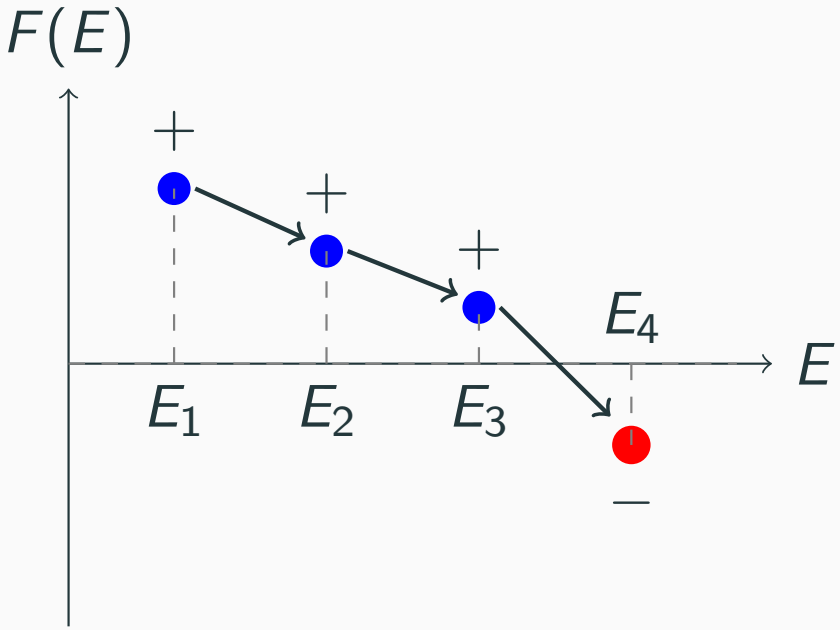
Scanning the energy range

$$F(E) = u'_f(r_m) - u'_b(r_m)$$



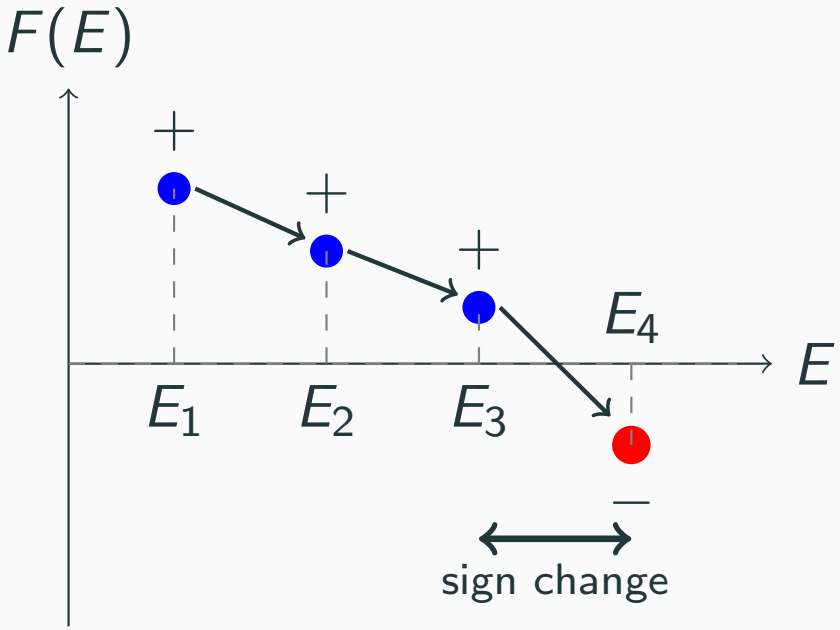
Scanning the energy range

$$F(E) = u'_f(r_m) - u'_b(r_m)$$



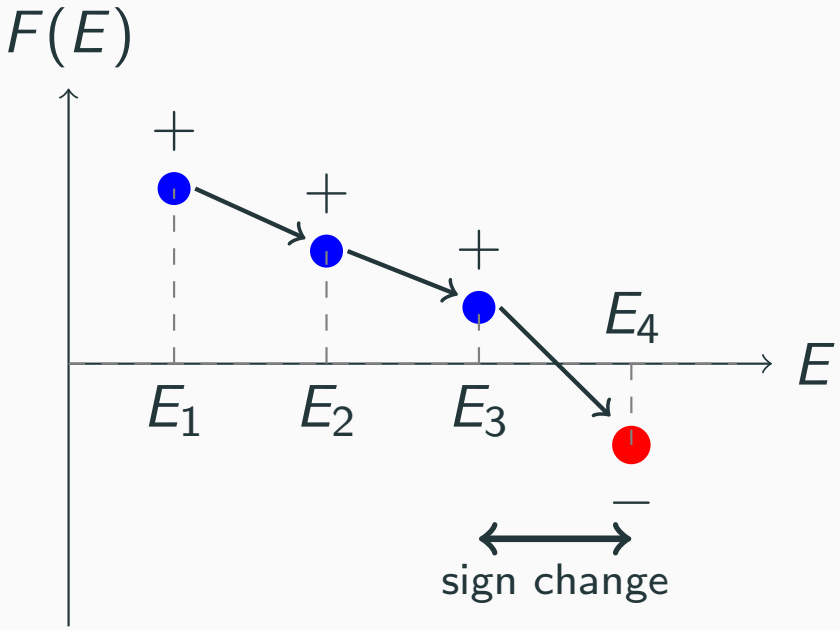
Scanning the energy range

$$F(E) = u_f'(r_m) - u_b'(r_m)$$



Scanning the energy range

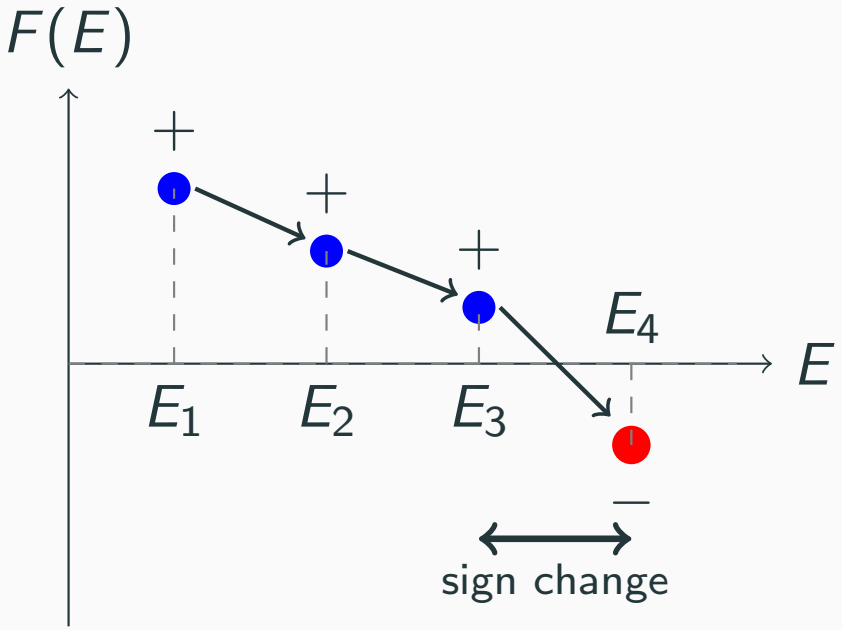
$$\boxed{F(E) = u_f'(r_m) - u_b'(r_m)}$$



$F(E_3) > 0, \qquad F(E_4) < 0$

Scanning the energy range

$$\boxed{F(E) = u_f'(r_m) - u_b'(r_m)}$$

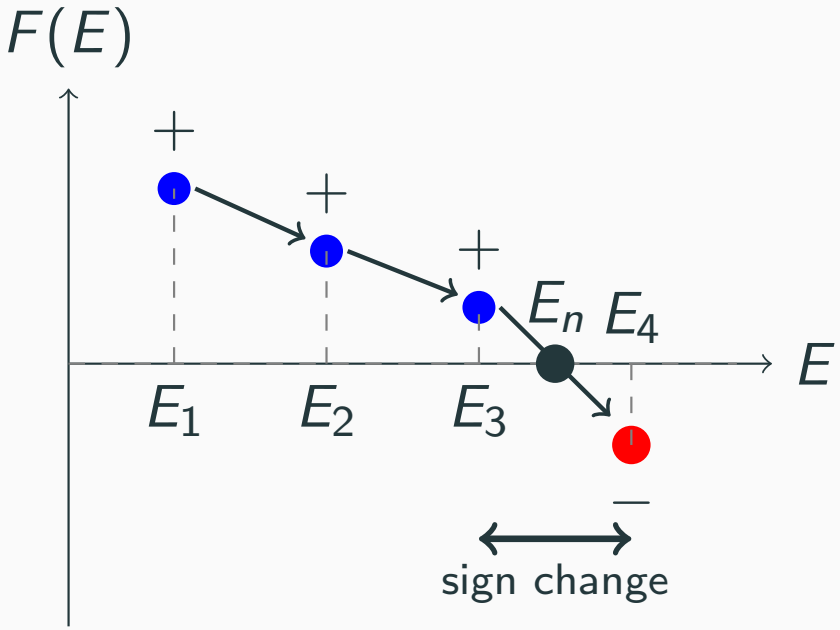


$$F(E_3) > 0, \qquad F(E_4) < 0$$

$$F(E_3)F(E_4) < 0$$

Scanning the energy range

$$\boxed{F(E) = u_f'(r_m) - u_b'(r_m)}$$

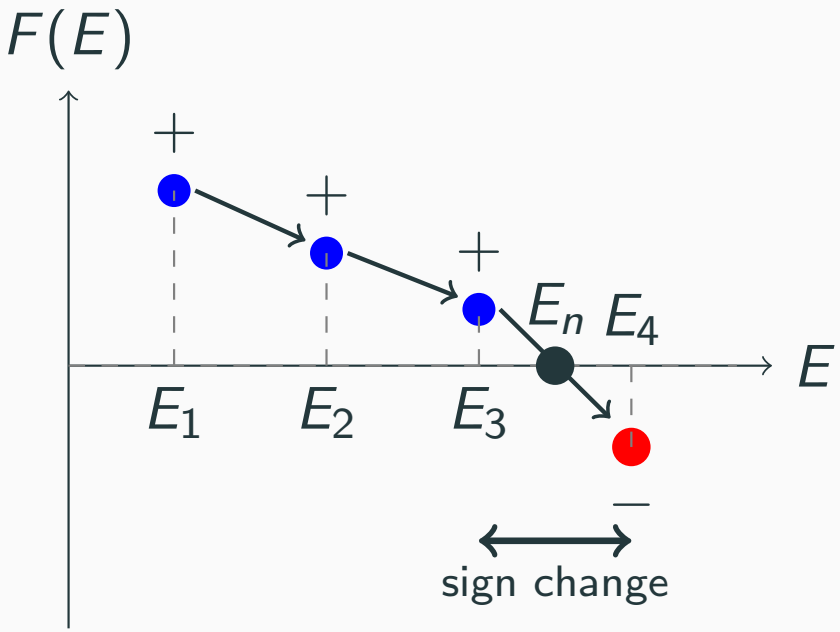


$$F(E_3) > 0, \qquad F(E_4) < 0$$

$$F(E_3)F(E_4) < 0$$

$$E_3 < E_n < E_4$$

Scanning the energy range



$$\boxed{F(E) = u_f'(r_m) - u_b'(r_m)}$$

$$F(E_3) > 0, \qquad F(E_4) < 0$$

$$F(E_3)F(E_4) < 0$$

$$E_3 < E_n < E_4$$

$$\boxed{F(E_n) = 0}$$

Regularization of the potentials

Regularized vector (one-gluon-exchange) potential:

$$V_V^{\text{reg}}(r) = -\alpha_s \frac{1 - e^{-\Lambda_g r}}{r}\,, \tag{7}$$

As $r \to \infty$, $V_V^{\text{reg}}(r) \to -\dfrac{\alpha_s}{r}$ and as $r \to 0$, $V_V^{\text{reg}}(r) \to -\alpha_s \Lambda_g$.

Regularized scalar (confinement) potential:

$$V_S^{\text{reg}}(r) = \sigma r \left[1 - \frac{\sqrt{2}}{r\Lambda_L} + \frac{2}{(r\Lambda_L)^2} e^{-\frac{r\Lambda_L}{\sqrt{2}}} \sin\left(\frac{r\Lambda_L}{\sqrt{2}}\right)\right], \tag{8}$$

As $r \to \infty$, $V_S^{\text{reg}}(r) \to \sigma r - \sqrt{2}\,\sigma/\Lambda_L$, recovering the linear confining behaviour up to a constant shift.

Spin–spin interaction

For equal-mass constituents ($m_1 = m_2 = m$), the spin-spin term is given by:

$$H_{SS} = \frac{2}{3m^2}\,\mathbf{S}_1 \cdot \mathbf{S}_2\,\Delta V_V(r)\,, \tag{9}$$

Expectation value of $\mathbf{S_1} \cdot \mathbf{S_2}$:
Writing the total spin as $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ and squaring,

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \tfrac{1}{2}\left(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2\right)\,, \tag{10}$$

so that, in general,

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = \tfrac{1}{2}\left[S(S+1) - S_1(S_1+1) - S_2(S_2+1)\right], \tag{11}$$

subject to the triangle rule $|S_1 - S_2| \le S \le S_1 + S_2$ in integer steps.

Spin-spin interaction

For two spin-1/2 constituents this reduces to the two values:

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = \begin{cases} -\dfrac{3}{4} & S = 0 \text{ (singlet)}\,, \\ +\dfrac{1}{4} & S = 1 \text{ (triplet)}\,. \end{cases} \tag{12}$$

Spin–orbit interaction

For equal-mass constituents ($m_1 = m_2 = m$), the spin-orbit term is given by:

$$H_{LS} = \frac{1}{2m^2 r}\,\mathbf{L}\cdot\mathbf{S}\left[3\,\frac{d}{dr}V_V(r) - \frac{d}{dr}V_S(r)\right], \tag{13}$$

where $\mathbf{L} \equiv \mathbf{x} \times \mathbf{p}$ is the relative orbital angular momentum and $\mathbf{S} \equiv \mathbf{S}_1 + \mathbf{S}_2$ is the total spin.

Spin–orbit interaction

Expectation value of $\mathbf{L}\cdot\mathbf{S}$:

Writing the total angular momentum as $\mathbf{J}=\mathbf{L}+\mathbf{S}$ and squaring:

$$\mathbf{L}\cdot\mathbf{S}=\tfrac{1}{2}\left(\mathbf{J}^2-\mathbf{L}^2-\mathbf{S}^2\right), \tag{14}$$

so that, in general:

$$\langle\mathbf{L}\cdot\mathbf{S}\rangle=\tfrac{1}{2}\left[j(j+1)-\ell(\ell+1)-S(S+1)\right], \tag{15}$$

where ℓ, S, j denote the quantum numbers of $\mathbf{L}$, $\mathbf{S}$, $\mathbf{J}$, respectively.

For two spin-1/2 constituents, this yields:

$$\langle\mathbf{L}\cdot\mathbf{S}\rangle=\begin{cases}\ell & j=\ell+1\,,\\ -1 & j=\ell\,,\\ -(\ell+1) & j=\ell-1\,.\end{cases} \tag{16}$$

Tensor interaction

For equal-mass constituents, the tensor term is given by:

$$H_T = \frac{1}{12\,m^2}\,S_{12}\left[\frac{1}{r}\frac{d}{dr}V_V(r) - \frac{d^2}{dr^2}V_V(r)\right] \tag{17}$$

with the abbreviation of the spin-dependent factor (tensor operator):

$$S_{12} \equiv 12\left[\frac{(\mathbf{S}_1\cdot\mathbf{x})(\mathbf{S}_2\cdot\mathbf{x})}{r^2} - \frac{1}{3}\,\mathbf{S}_1\cdot\mathbf{S}_2\right] \tag{18}$$

Tensor interaction

The diagonal matrix elements follow from

$$\langle S_{12}\rangle = \frac{4}{(2\ell+3)(2\ell-1)}\left[\langle \mathbf{S}^2\rangle\langle \mathbf{L}^2\rangle - \tfrac{3}{2}\langle \mathbf{L}\cdot\mathbf{S}\rangle - 3\big(\langle \mathbf{L}\cdot\mathbf{S}\rangle\big)^2\right], \tag{19}$$

yielding the three nonvanishing diagonal values:

$$\langle S_{12}\rangle = \begin{cases} -\dfrac{2\ell}{2\ell+3} & j=\ell+1\,, \\ 2 & j=\ell\,, \\ -\dfrac{2(\ell+1)}{2\ell-1} & j=\ell-1\,. \end{cases} \tag{20}$$

Tensor interaction: L-mixing

For spin-triplet states ($S = 1$), the tensor interaction couples different orbital angular momenta at fixed J:

$$\boxed{L = J - 1 \;\longleftrightarrow\; L = J + 1}$$

The tensor operator has the matrix structure:

$$S_{12} = \begin{pmatrix} -\dfrac{2(J-1)}{2J+1} & 0 & \dfrac{6\sqrt{J(J+1)}}{2J+1} \\ 0 & 2 & 0 \\ \dfrac{6\sqrt{J(J+1)}}{2J+1} & 0 & -\dfrac{2(J+2)}{2J+1} \end{pmatrix}$$

- Diagonal terms $\rightarrow$ energy shifts.
- Off-diagonal terms $\rightarrow$ L-mixing.
- The coupled channels must be solved simultaneously.

Plots: Nodes of the Radial Wavefunction

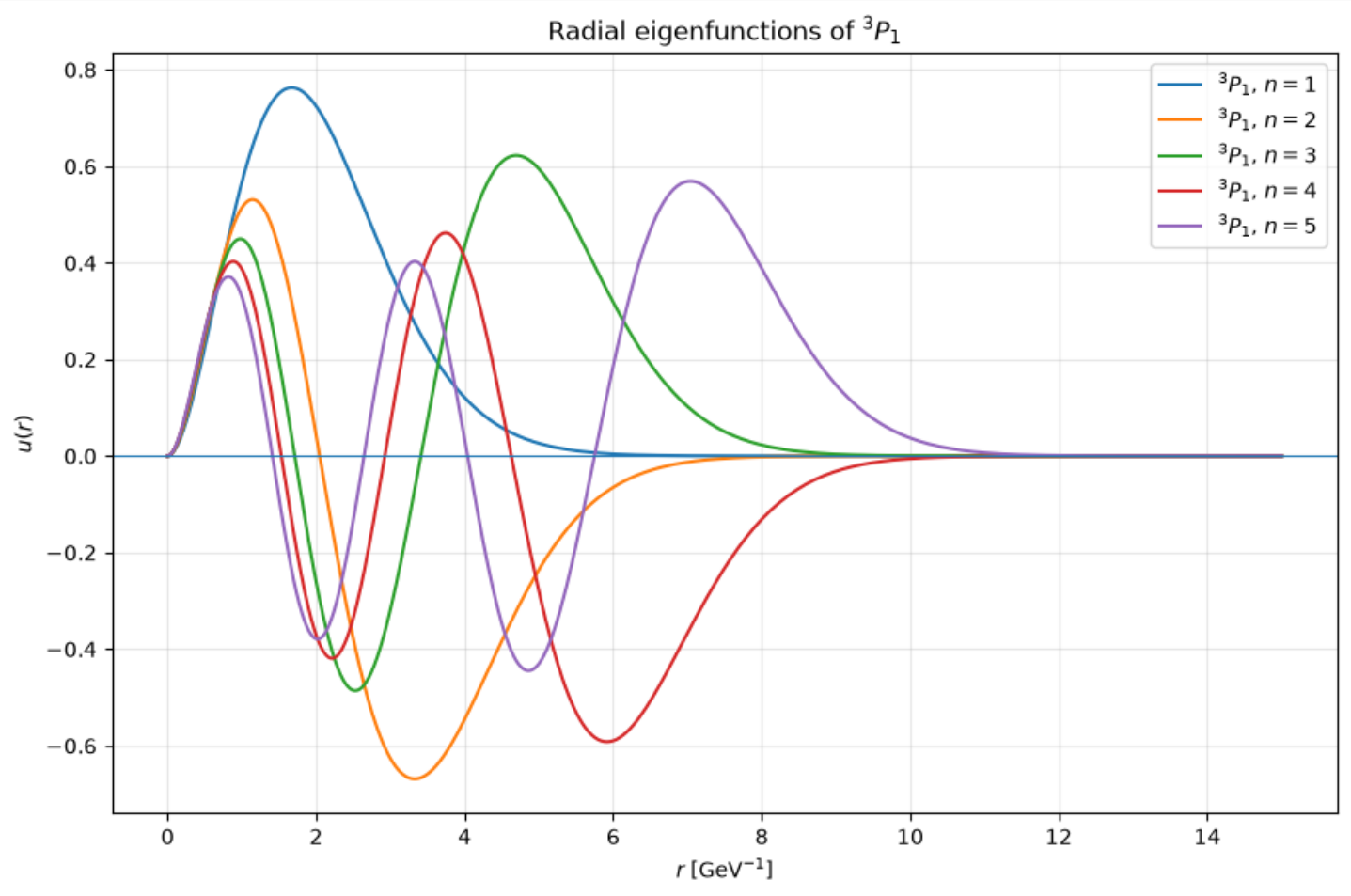


Figure 1: Radial wavefunction and their nodes (J=1, S=1, L=1)

Plots: Bottomonium and Charmonium comparision

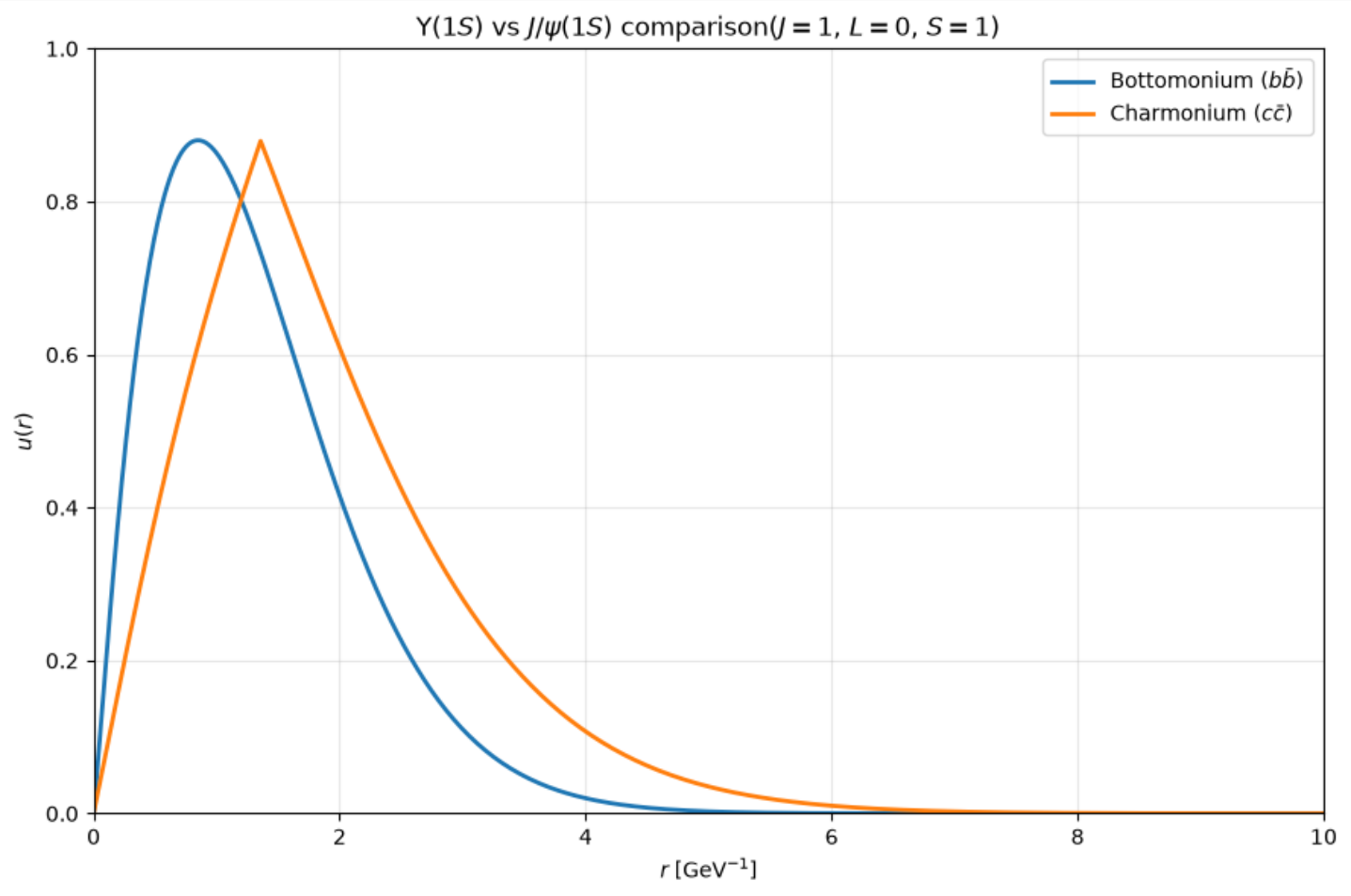


Figure 2: Radial wavefunction for bottomonium and charmonium (J=1, L=0, S=1)

Plots: Radial wavefunction (J=0)

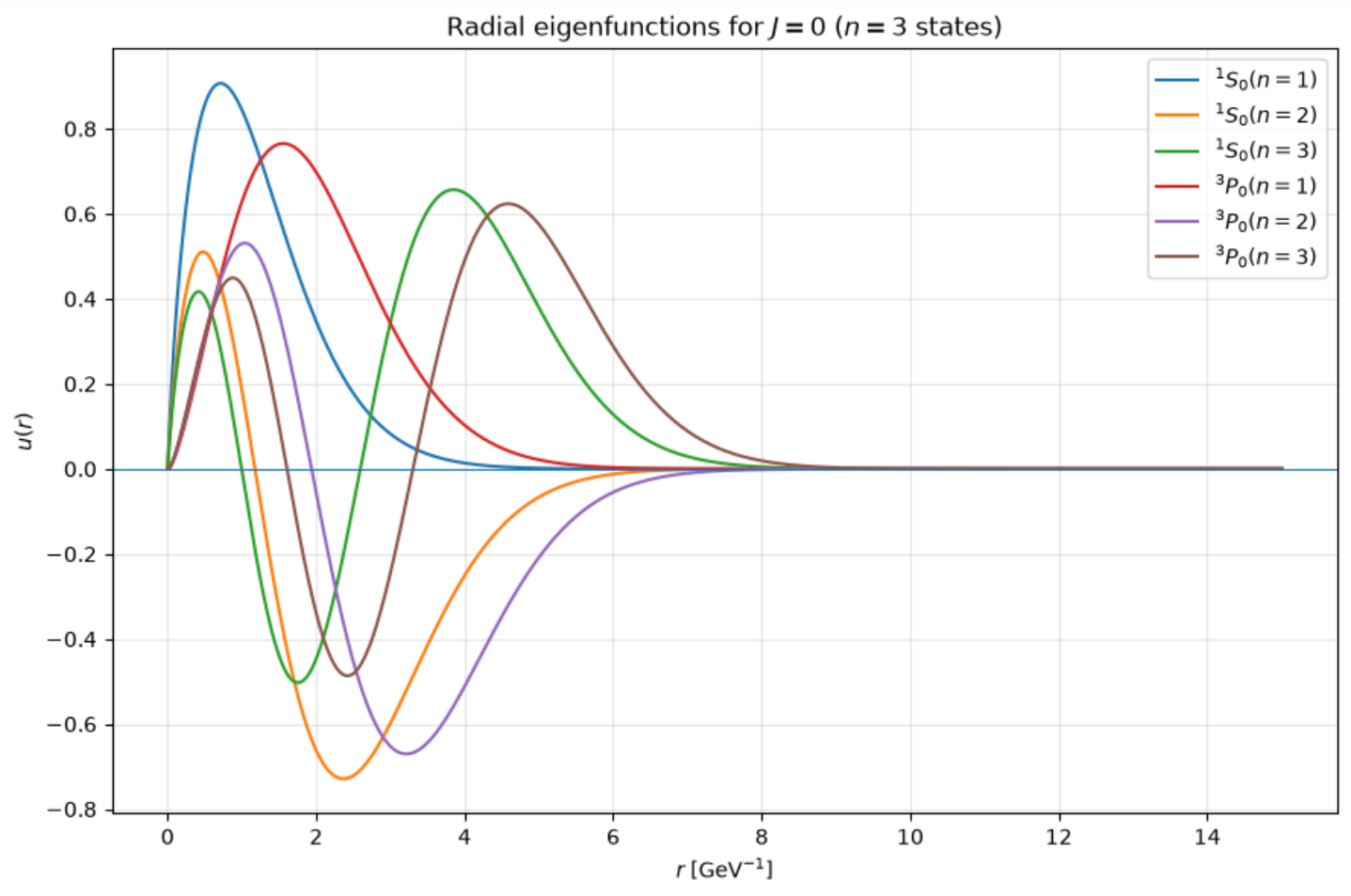


Figure 3: Radial wavefunction for bottomonium (J=0)

Near the origin, the radial wavefunction satisfies $u(r) \sim r^{\ell+1}$.

Numerical Results: Bottomonium

J	L	S	n		E [GeV]	M [GeV]
0	0	0	0		−0.00809402	9.48470598
0	0	0	1		0.55956918	10.05236918
0	0	0	2		0.93036074	10.42316074
1	1	0	0		0.45716631	9.94996631
1	1	0	1		0.83697325	10.32977325
1	1	0	2		1.15010795	10.64290795
2	2	0	0		0.71018270	10.20298270
2	2	0	1		1.03508440	10.52788440
2	2	0	2		1.31975697	10.81255697
3	3	0	0		0.91514240	10.40794240
3	3	0	1		1.20870397	10.70150397
3	3	0	2		1.47387302	10.96667302
0	1	1	0		0.42320016	9.91600016
0	1	1	1		0.80677547	10.29957547
0	1	1	2		1.12179821	10.61459821

Numerical Results: Bottomonium

J	L	S	n		E [GeV]	M [GeV]
1	0/2 (mixed)	1	0		0.06002555	9.55282555
1	0/2 (mixed)	1	1		0.59459300	10.08739300
1	0/2 (mixed)	1	2		0.70558641	10.19838641
1	1	1	0		0.45195207	9.94475207
1	1	1	1		0.83224808	10.32504808
1	1	1	2		1.14561381	10.63841381
2	1/3 (mixed)	1	0		0.46530646	9.95810646
2	1/3 (mixed)	1	1		0.84439038	10.33719038
2	1/3 (mixed)	1	2		0.91574369	10.40854369
2	2	1	0		0.71016365	10.20296365
2	2	1	1		1.03481196	10.52761196
2	2	1	2		1.31932627	10.81212627
3	2/4 (mixed)	1	0		0.71192645	10.20472645
3	2/4 (mixed)	1	1		1.03722464	10.53002464
3	2/4 (mixed)	1	2		1.09843802	10.59123802
3	3	1	0		0.91587221	10.40867221
3	3	1	1		1.20923889	10.70203889
3	3	1	2		1.47427284	10.96707284

Numerical Results: Charmonium

J	L	S	n		E [GeV]	M [GeV]
0	0	0	0		0.32627737	3.11187737
0	0	0	1		0.98945368	3.77505368
0	0	0	2		1.49207123	4.27767123
1	1	0	0		0.79897477	3.58457477
1	1	0	1		1.32446243	4.11006243
1	1	0	2		1.77156766	4.55716766
2	2	0	0		1.12423055	3.90983055
2	2	0	1		1.59016957	4.37576957
2	2	0	2		2.00410010	4.78970010
3	3	0	0		1.40503931	4.19063931
3	3	0	1		1.83248603	4.61808603
3	3	0	2		2.22156900	5.00716900
0	1	1	0		0.75594503	3.54154503
0	1	1	1		1.28268329	4.06828329
0	1	1	2		1.73141515	4.51701515

Numerical Results: Charmonium

J	L	S	n		E [GeV]	M [GeV]
1	0/2 (mixed)	1	0		0.39778392	3.18338392
1	0/2 (mixed)	1	1		1.04028114	3.82588114
1	0/2 (mixed)	1	2		1.13982159	3.92542159
1	1	1	0		0.80251357	3.58811357
1	1	1	1		1.32584161	4.11144161
1	1	1	2		1.77192898	4.55752898
2	1/3 (mixed)	1	0		0.80474725	3.59034725
2	1/3 (mixed)	1	1		1.33283158	4.11843158
2	1/3 (mixed)	1	2		1.43656925	4.22216925
2	2	1	0		1.13369733	3.91929733
2	2	1	1		1.59743253	4.38303253
2	2	1	2		2.00998612	4.79558612
3	2/4 (mixed)	1	0		1.11047200	3.89607200
3	2/4 (mixed)	1	1		1.58079882	4.36639882
3	2/4 (mixed)	1	2		1.69956956	4.48516956
3	3	1	0		1.41465619	4.20025619
3	3	1	1		1.84060912	4.62620912
3	3	1	2		2.22864028	5.01424028

Results: Bottomonium Mass Spectrum

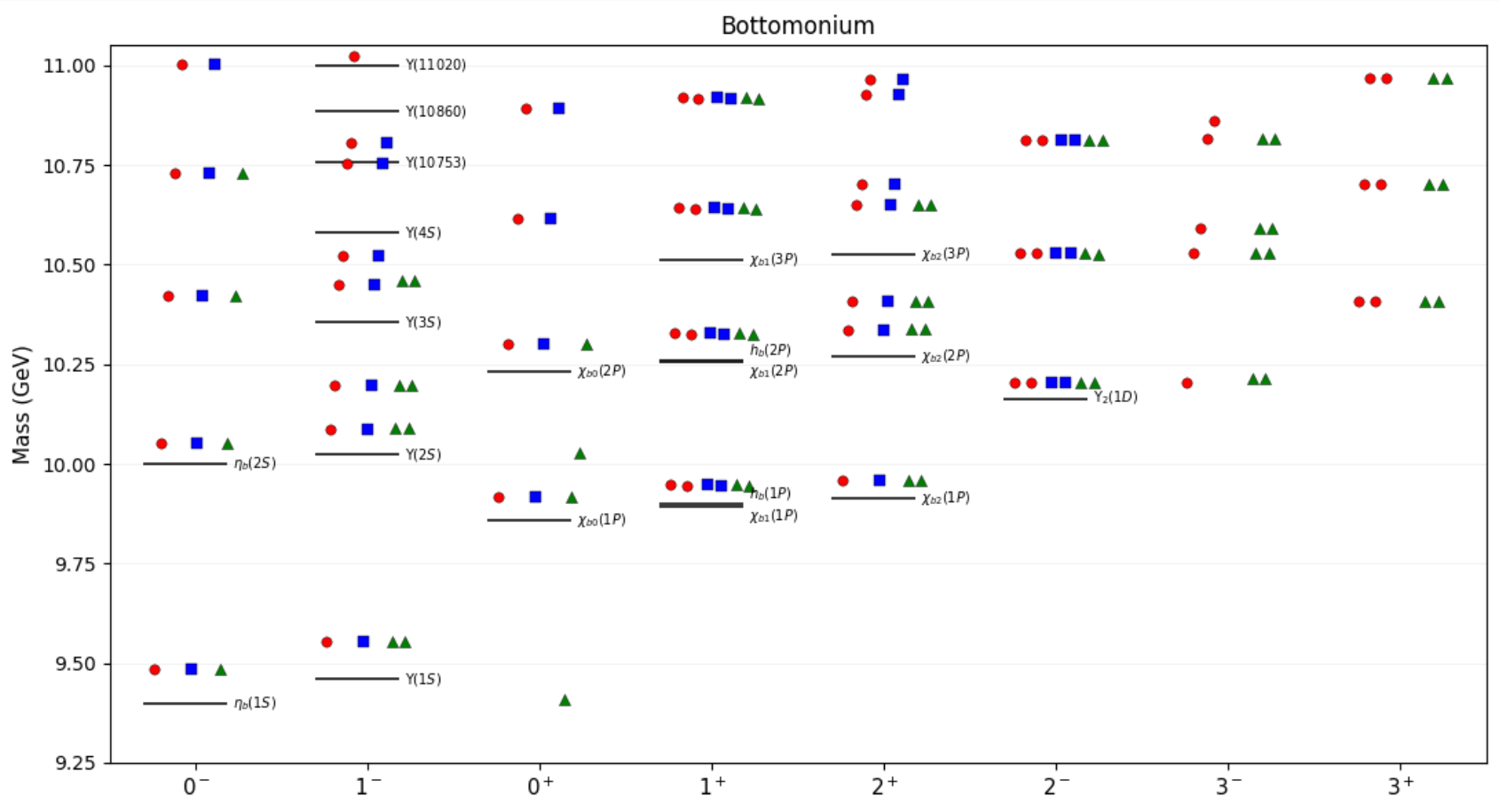


Figure 4: Bottomonium Mass Spectrum

Results: Charmonium Mass Spectrum

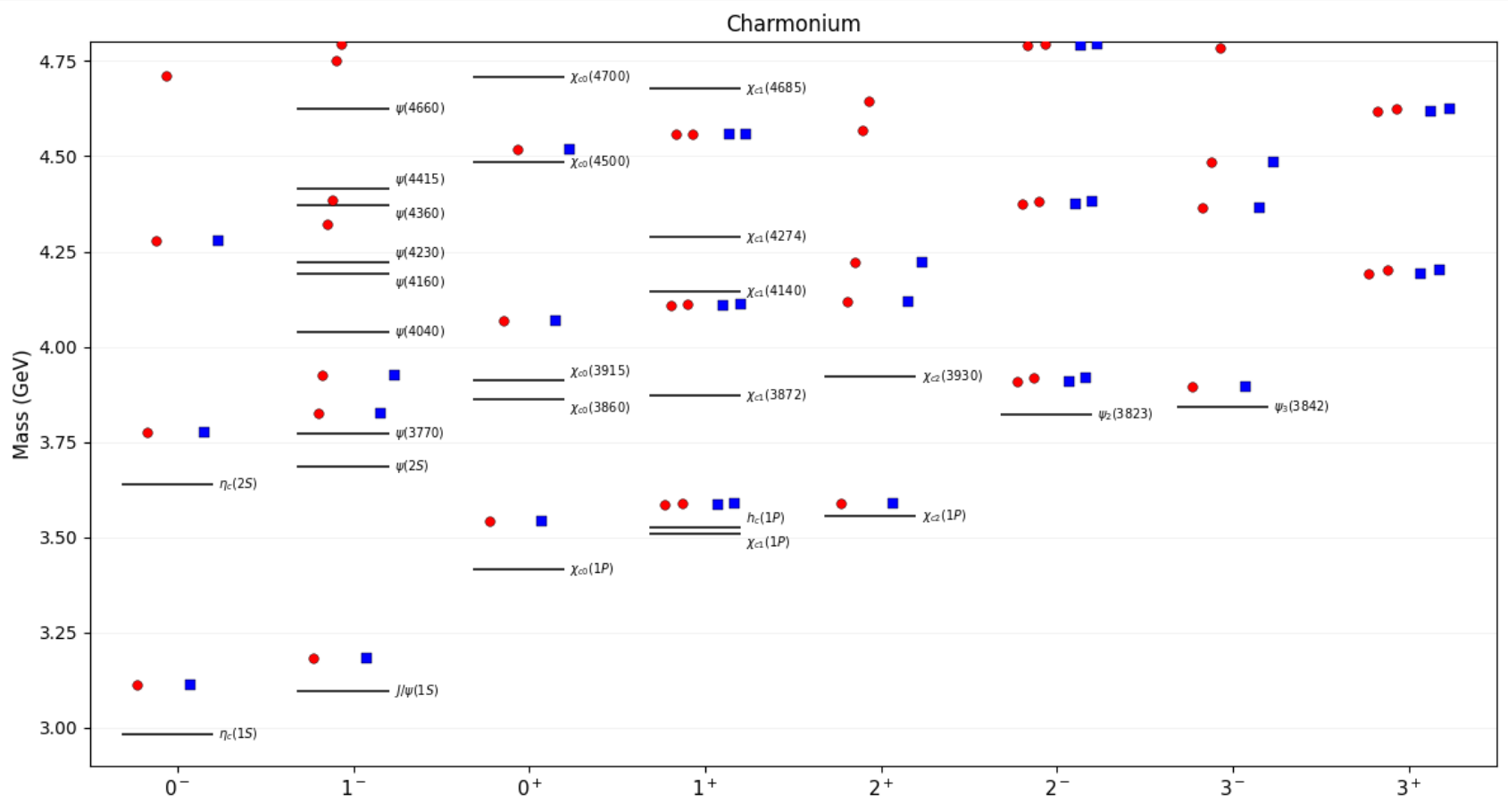


Figure 5: Charmonium Mass Spectrum

Conclusion

- The **Numerov method** provides an efficient and accurate numerical approach to solving the radial Schrödinger equation for heavy quarkonia in coordinate space.
- The implemented **regularized potentials** provide a consistent description of the interaction in both momentum and coordinate space.
- The model reproduces the expected **physical structure of the bound states**, including:
  - the nodal structure of radial excitations;
  - the dependence of the radius on the quark mass;
  - the effects of orbital and spin-dependent interactions.
- The framework provides a consistent description of **bottomonium and charmonium spectra and wavefunctions**.

What is left to do?

- **Extend the model to the B_c meson**
  - Unequal quark masses: $m_b \neq m_c$
  - Implement the corresponding reduced mass and mass-dependent terms
  - Solve the $b\bar{c}$ spectrum and obtain the corresponding wavefunctions

- **Finalize the analysis**
  - Compare radius and wavefunctions across $c\bar{c}$, $b\bar{b}$, and $b\bar{c}$
  - Analyze the effect of spin-dependent interactions and tensor mixing

Extra: Tensor coupling: coupled-channel structure

Expanding the eigenstate $|\Psi\rangle$ in the partial-wave basis $|(\ell S)JM\rangle$ (with J, M fixed) and projecting the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ onto this basis gives

$$\sum_{\ell' S'} \Big\{ \langle (\ell S)JM|\, T\, |(\ell' S')JM\rangle + \langle (\ell S)JM|\, V\, |(\ell' S')JM\rangle \Big\}\, \psi^{JM}_{\ell' S'} = E\, \psi^{JM}_{\ell S}\,. \tag{21}$$

The kinetic term is diagonal in ℓ and S,

$$\langle (\ell S)JM|\, T\, |(\ell' S')JM\rangle = \delta_{\ell\ell'}\, \delta_{SS'}\; T_\ell\,, \tag{22}$$

so that the radial equation for each channel reads

$$T_\ell\, \psi^{JM}_{\ell S} + \sum_{\ell' S'} V^{JM}_{\ell S,\, \ell' S'}\, \psi^{JM}_{\ell' S'} = E\, \psi^{JM}_{\ell S}\,. \tag{23}$$

Since the tensor operator S_{12} does *not* commute with $\mathbf{L}^2$, V is in general **off-diagonal** in ℓ — it couples different orbital angular momenta at fixed J.

Extra: Off-diagonal terms: coupling of $\ell = J \mp 1$ (S = S' = 1)

For fixed J and spin triplet $S = S' = 1$, the tensor operator couples *only* the two channels $\ell = J - 1$ and $\ell = J + 1$. Equation (23) then reduces to a system of two coupled radial equations:

$$T_{J-1}\,\psi_{J-1} + V_{J-1,\,J-1}\,\psi_{J-1} + V_{J-1,\,J+1}\,\psi_{J+1} = E\,\psi_{J-1}\,, \quad (24)$$

$$T_{J+1}\,\psi_{J+1} + V_{J+1,\,J-1}\,\psi_{J-1} + V_{J+1,\,J+1}\,\psi_{J+1} = E\,\psi_{J+1}\,, \quad (25)$$

which must be solved **simultaneously**. The kinetic operator includes the centrifugal barrier and thus itself depends on ℓ:

$$T_\ell = -\frac{\hbar^2}{2m_R}\nabla^2 + \frac{\hbar^2\,\ell(\ell+1)}{2m_R\,r^2}\,. \quad (26)$$

If $S = S' = 0$, the tensor matrix elements vanish identically, $V_{\ell 0,\,\ell' 0} = 0$: the off-diagonal coupling is present only in the spin-triplet channel.

Extra: Unequal masses

For unequal masses, the spin-spin term generalizes to:

$$H_{SS} = \frac{2}{3\, m_1 m_2}\, \mathbf{S}_1 \cdot \mathbf{S}_2\, \Delta V_V(r)\,. \tag{27}$$

Extra: Unequal masses

For unequal masses, the spin-orbit term generalizes to:

$$H_{LS} = \frac{1}{4m_1^2 m_2^2}\frac{1}{r}\Big\{\Big[\left((m_1+m_2)^2 + 2m_1 m_2\right)\mathbf{L}\cdot\mathbf{S}_+ + \left(m_2^2 - m_1^2\right)\mathbf{L}\cdot\mathbf{S}_-\Big]\frac{d}{dr}V_V(r) - \Big[\left(m_1^2+m_2^2\right)\mathbf{L}\cdot\mathbf{S}_+ + \left(m_2^2 - m_1^2\right)\mathbf{L}\cdot\mathbf{S}_-\Big]\frac{d}{dr}V_S(r)\Big\} \tag{28}$$

with $\mathbf{S}_+ \equiv \mathbf{S}_1 + \mathbf{S}_2$ and $\mathbf{S}_- \equiv \mathbf{S}_1 - \mathbf{S}_2$.

Extra: Unequal masses

For unequal masses, the tensor term generalizes to:

$$H_T = \frac{1}{12\, m_1 m_2}\, S_{12} \left[\frac{1}{r}\frac{d}{dr} V_V(r) - \frac{d^2}{dr^2} V_V(r) \right] . \qquad (29)$$

Extra: Tensor interaction

Expectation value of S_{12}. For two spin-1/2 constituents, the spin-dependent factor may be rewritten as

$$S_{12} = 2\left[3\,\frac{(\mathbf{S}\cdot\mathbf{x})^2}{r^2} - \mathbf{S}^2\right], \tag{30}$$

which vanishes identically for $S = 0$ or $\ell = 0$ (the latter by rotational symmetry, $\langle x_i x_j/r^2\rangle = \frac{1}{3}\delta_{ij}$), contributing only for $\ell \neq 0$ and $S = 1$. The diagonal matrix elements follow from

$$\langle S_{12}\rangle = \frac{4}{(2\ell+3)(2\ell-1)}\left[\langle\mathbf{S}^2\rangle\langle\mathbf{L}^2\rangle - \tfrac{3}{2}\langle\mathbf{L}\cdot\mathbf{S}\rangle - 3\big(\langle\mathbf{L}\cdot\mathbf{S}\rangle\big)^2\right], \tag{31}$$

Extra: Derivatives of the regularized vector potential

The spin-dependent operators H_{LS}, H_{SS}, H_T require the first and second derivatives of $V_V(r)$. Differentiating Eq. (7) gives

$$\frac{d}{dr} V_V^{\text{reg}}(r) = \alpha_s \frac{1 - e^{-\lambda_g r}(1 + \lambda_g r)}{r^2}, \tag{32}$$

$$\frac{d^2}{dr^2} V_V^{\text{reg}}(r) = -\alpha_s \frac{2 - e^{-\lambda_g r}\left[2 + 2\lambda_g r + (\lambda_g r)^2\right]}{r^3}. \tag{33}$$

Regularity at the origin

Expanding Eqs. (32)–(33) for small r shows that both derivatives remain **finite** as $r \to 0$ (the leading singular terms cancel exactly). In particular, the Laplacian $\Delta V_V^{\text{reg}}(r)$ no longer produces the contact term $\delta^{(3)}(\mathbf{x})$ present in the Coulomb case, making H_{SS} and H_T well-defined at short distance.

Extra: Regularized scalar (confining) potential

Although $V_S(r) = \sigma r$ itself is finite, its contribution to the spin-orbit term via dV_S/dr needs to be regularized. It is controlled by a scale Λ_L:

$$V_S^{\text{reg}}(r) = \sigma r \left[1 - \frac{\sqrt{2}}{r\Lambda_L} + \frac{2}{(r\Lambda_L)^2} e^{-\frac{r\Lambda_L}{\sqrt{2}}} \sin\left(\frac{r\Lambda_L}{\sqrt{2}}\right)\right], \tag{34}$$

with derivative

$$\frac{d}{dr} V_S^{\text{reg}}(r) =$$

$$\sigma + \frac{e^{-r\Lambda_L/\sqrt{2}}\left[\sqrt{2}\, r\Lambda_L\, \sigma \cos\left(\frac{r\Lambda_L}{\sqrt{2}}\right) - (2+\sqrt{2}\, r\Lambda_L)\, \sigma \sin\left(\frac{r\Lambda_L}{\sqrt{2}}\right)\right]}{r^2\Lambda_L^2} \tag{35}$$

As $r \to \infty$, $V_S^{\text{reg}}(r) \to \sigma r - \sqrt{2}\,\sigma/\Lambda_L$, recovering the linear confining behaviour up to a constant shift.