Exact solutions of the one-dimension Coulomb potential

A case of non-Hermiticity with a real spectrum

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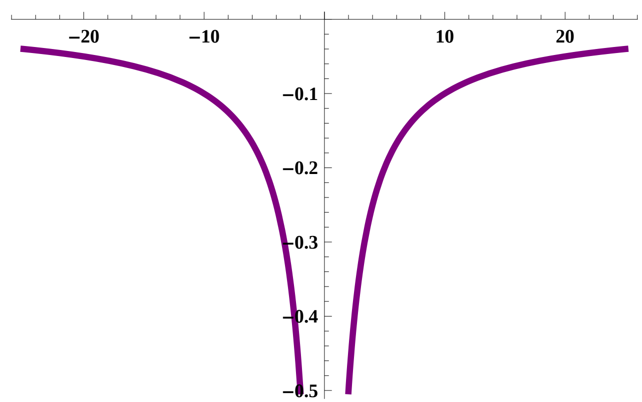
1-d Coulomb problem

- Coulomb potental $V(x) = \frac{qq'}{4\pi\epsilon_o|x|}$ as in the 3d case but for a variable $x \in \mathbb{R} \implies$ the hamiltonien is $\mathcal{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V$
- We will only consider the attractive barrier $qq' < 0$



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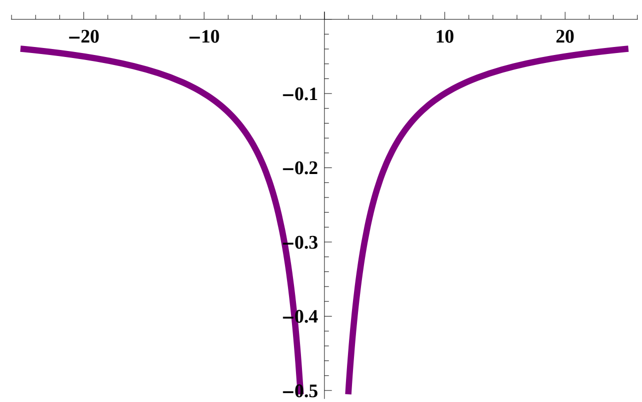


- Ordinary differential equation, but discontinuous at $x = 0$ which brings major problems, solved in G Abramovici & Y. Avishai, J. Phys. A: Math. Theor. (2009) 42285302.

Bound spectrum

One finds two kinds of wave functions :

- Régular states, which write

$$\psi_n(x) = -\left(\frac{|\lambda|}{2}\right)^{\frac{3}{2}} \frac{x}{n^3}\, \mathrm{e}^{-\frac{|\lambda x|}{2n}} L'_n\left(\frac{|\lambda x|}{n}\right)$$

($n \in \mathbb{N}^*$, L Laguerre polynomial, $\lambda = \frac{2mqq'}{4\pi\epsilon_o\hbar^2}$), with energy

$$E_n = -\frac{\hbar^2\lambda^2}{8m\, n^2}$$

- When $q = q' = q_e$, it is exactly Rydberg'energy $-E_I/n^2$.

Bound spectrum

One finds two kinds of wave functions :

- Anomalous states, which write

$$\psi_{n+\frac{1}{2}}(x) = \left(\frac{|\lambda|}{2n+1}\right)^{\frac{3}{2}} \frac{|x|}{r_n} \left(p_n\left(\frac{\lambda x}{2n+1}\right)K_0\left(\frac{\lambda x}{2n+1}\right) + q_n\left(\frac{\lambda x}{2n+1}\right)K_1\left(\frac{\lambda x}{2n+1}\right)\right)$$

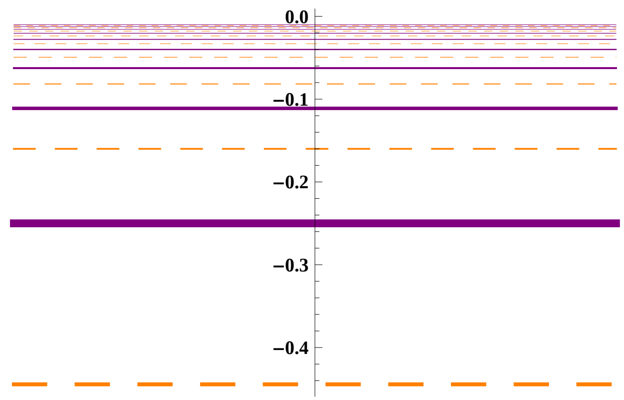
(p_n and q_n integer polynomials of degree n, K_i second kind Bessel functions), with energy

$$E_{n+\frac{1}{2}} = -\frac{\hbar^2\lambda^2}{8m(n+\frac{1}{2})^2}$$

Bound spectrum

One finds two kinds of wave functions :

- Regular and anomalous spectra intertwin and give a new Rydberg spectrum, with $E_I \rightarrow 4E_I$



Regular states

- Regular states exactly correspond to s hydrogen states ($r\psi_n(r)$, $r > 0$).
- They are continuously continued on the whole real line (with odd symmetry).
- Normalization is changed by a factor 2 (radial wave functions of hydrogen atom are only summed over the half-line).

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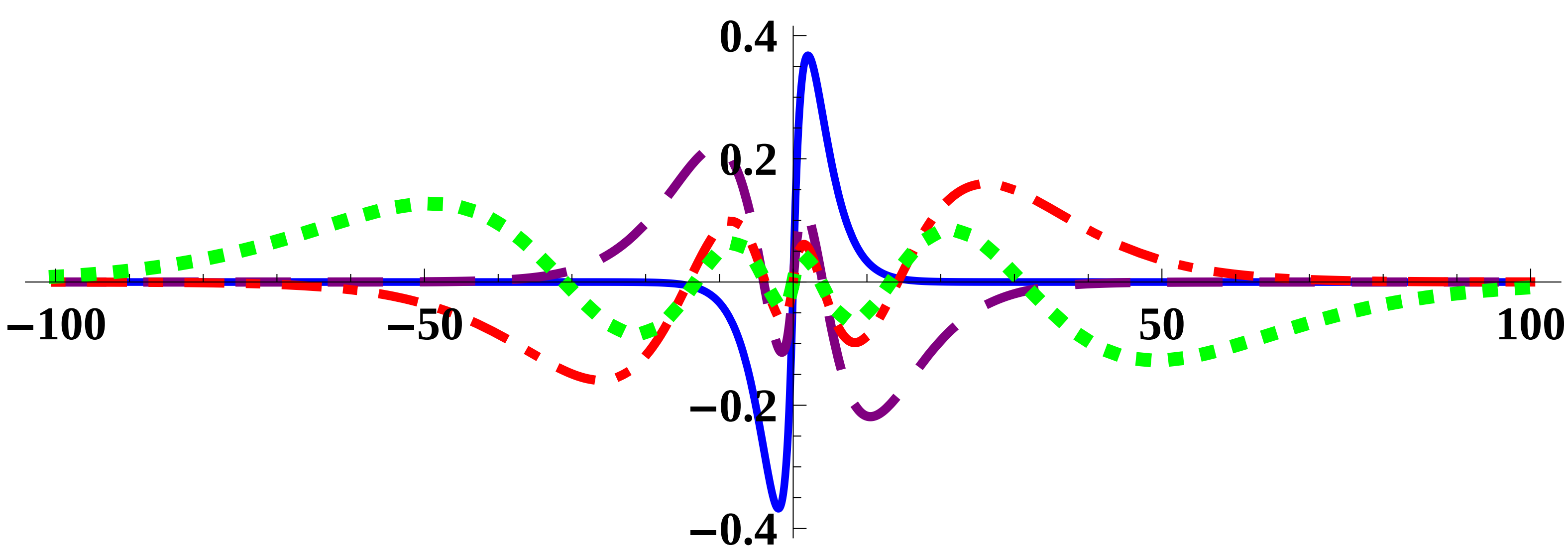

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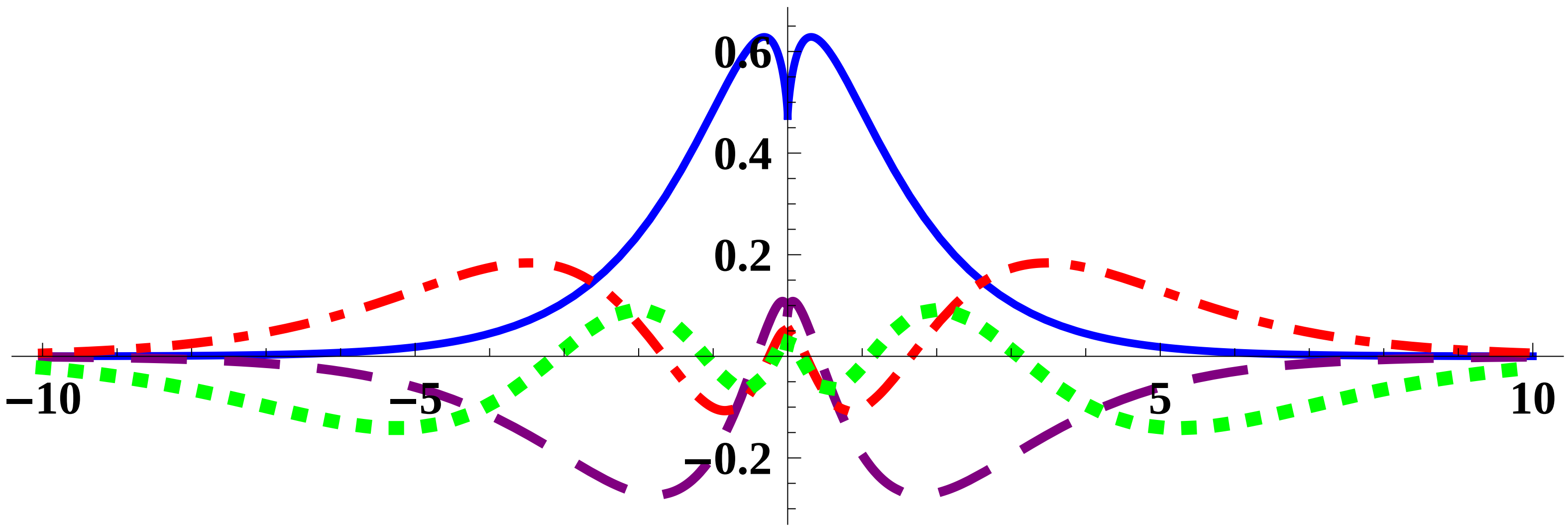
- They are continuously continued on the whole real line (with odd symmetry).
- Normalization is changed by a factor 2 (radial wave functions of hydrogen atom are only summed over the half-line).
- The free spectrum states also correspond to free hydrogen states, with $l = 0$.
- But normalization is unchanged.

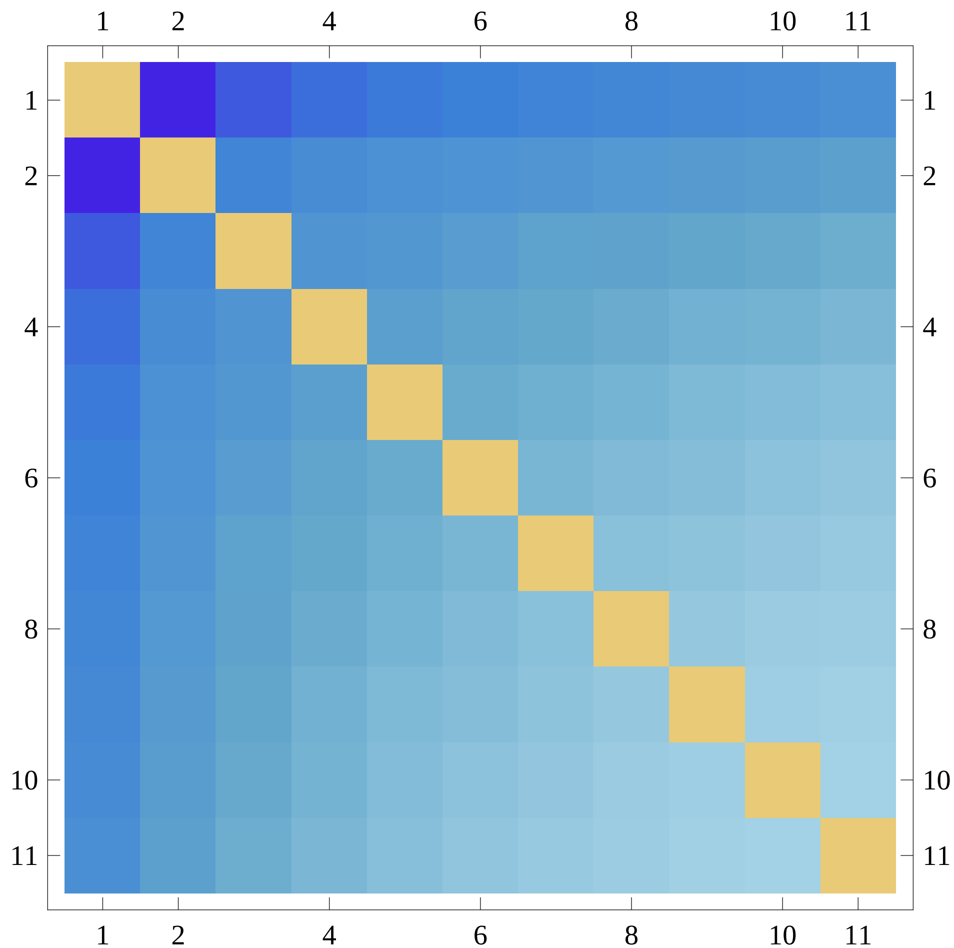
Anomalous states

- Anomalous states have no corresponding hydrogen states.
- They are even (opposite symmetry to regular states).



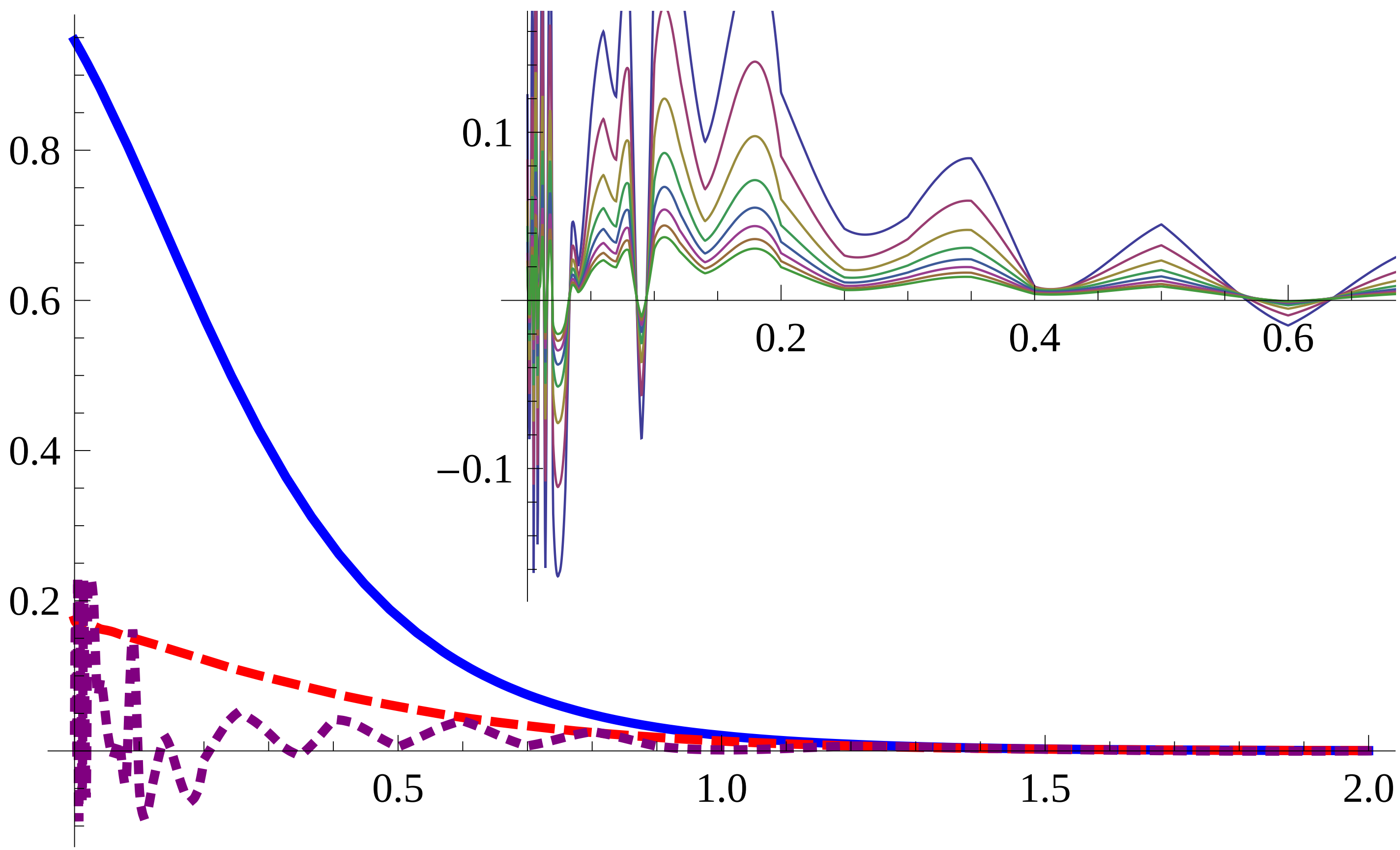
Anomalous states

- **They overlap each over (i.e. they are not orthogonal together!**



Anomalous states

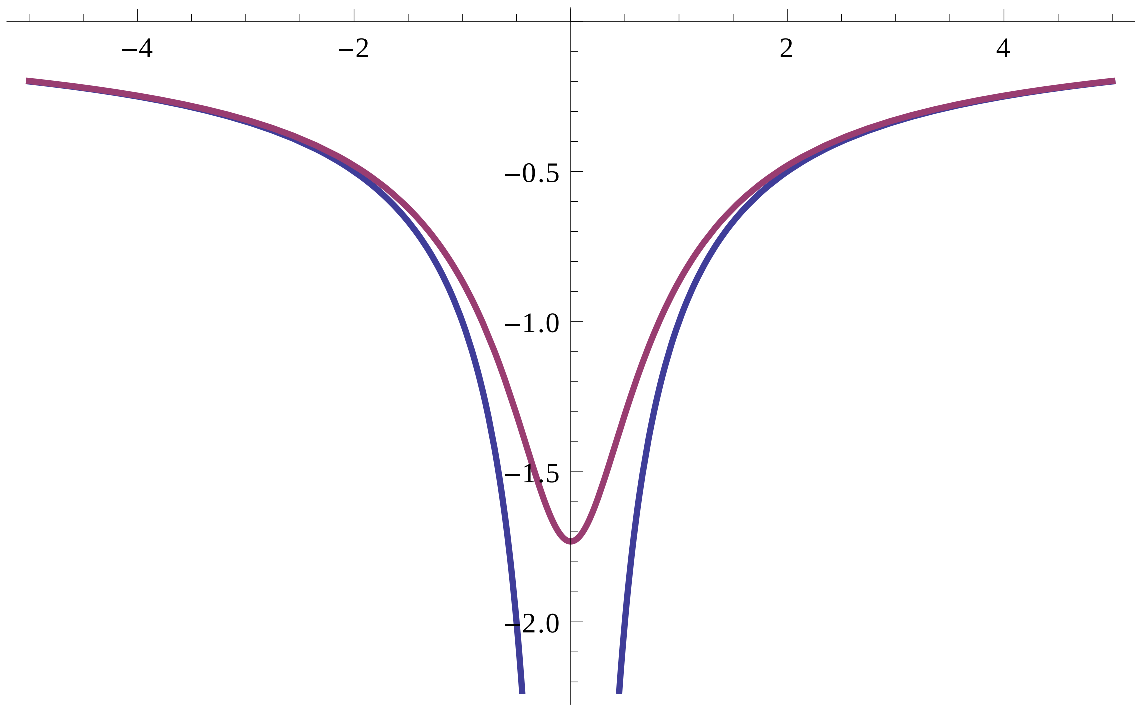
- They also overlap with free states (i.e. anomalous and free states are not orthogonal).



$\langle \psi_{p+\frac{1}{2}} | \psi_\eta \rangle$ as a function of η.

Regularized potential

- We replace the Coulomb potential V by $V_\varepsilon = \frac{qq'}{4\pi\epsilon_o\sqrt{x^2+\varepsilon^2}}$.

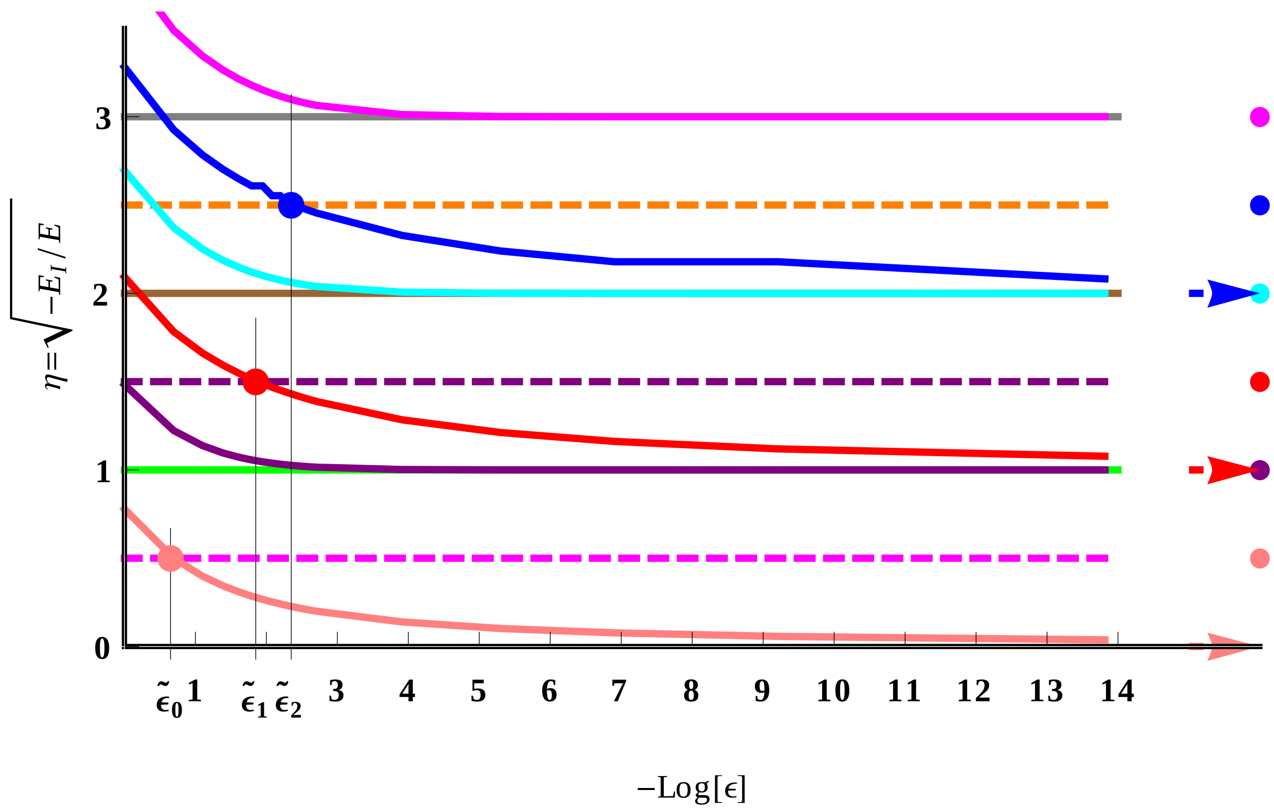


Regularized potential

- We replace the Coulomb potential V by $V_\varepsilon = \frac{qq'}{4\pi\epsilon_o\sqrt{x^2+\varepsilon^2}}$.
- The modified hamiltonian has again odd solutions χ_{2p}^{ε} and even solutions $\chi_{2p+1}^{\varepsilon}$ ($p \in \mathbb{N}$).
- $\chi_{2p}^{\varepsilon} \to \chi_{2p}^{0} = \psi_p$ when $\varepsilon \to 0$.
- $\chi_{2p+1}^{\varepsilon} \to \chi_{2p+1}^{0}$ when $\varepsilon \to 0$, but χ_{2p+1}^{0} **is not a Coulomb state**.
- They may be *associated* functions.

Regularized potential

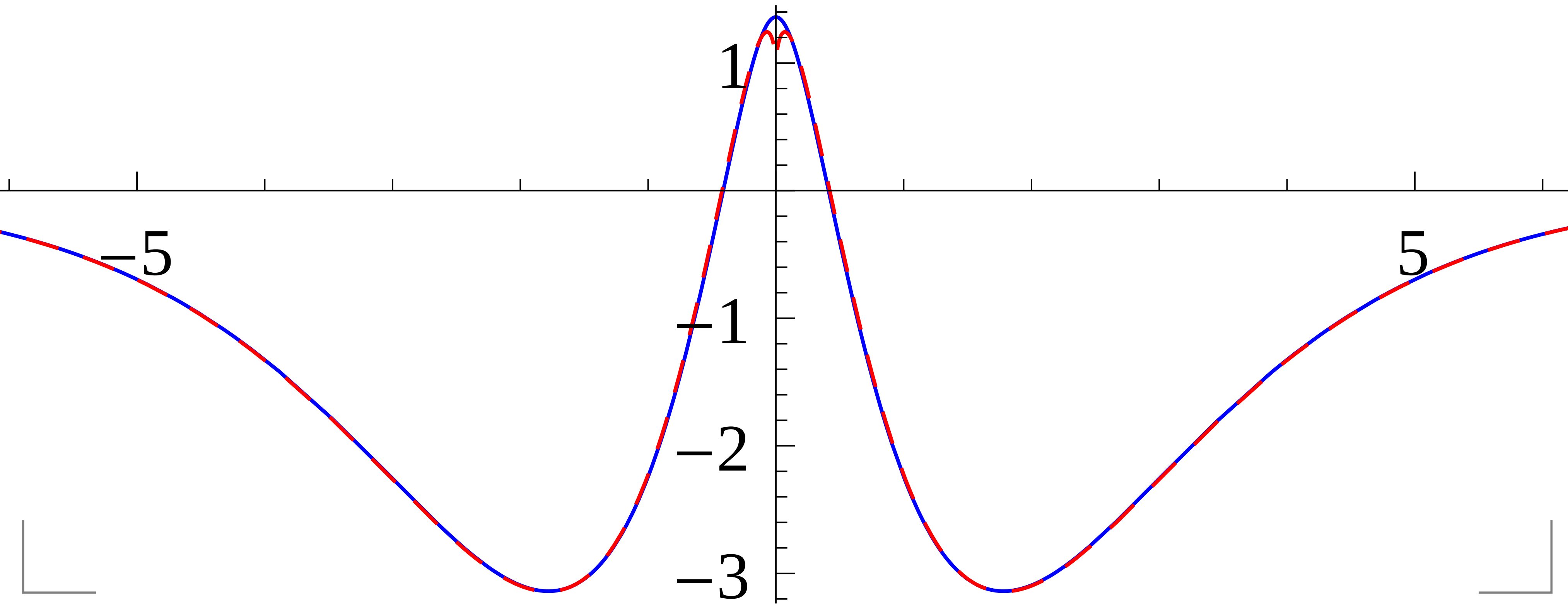
- The corresponding energies converge to E_n, therefore there is a discontinuity at $\varepsilon = 0$.



Regularized spectra versus $1/\varepsilon$.

Regularized potential

- $E^{\varepsilon}_{p+\frac{1}{2}} = E_{p+\frac{1}{2}}$, for $\varepsilon = \tilde{\varepsilon}_p$.
- The corresponding function is a *regularized* anomalous function which only differs arround $x = 0$.



Alternative

- Two possibilities, either $E^0_{p+\frac{1}{2}} = E_{p+\frac{1}{2}} \neq \lim_{\varepsilon \to 0} E^\varepsilon_{p+\frac{1}{2}}$
- Or $E^0_{p+\frac{1}{2}} = \lim_{\varepsilon \to 0} E^\varepsilon_{p+\frac{1}{2}}$ (continuous spectrum).
- In the first case, the complete basis of states exactly includes all free states ($|\psi_\eta\rangle$ and ($|\check{\psi}_\eta\rangle$), regular (odd) and anomalous (even) bound states.
- In the second case, the complete basis includes all free states, regular bound states $|\psi_p\rangle$ (odd) and $|\,|\psi_p|\rangle$ (even).
- We discriminate the two case and thus solve the alternative by calculating the corresponding completeness relations.

Completeness relation

- The completeness relation needs to use the metric matrix g and writes

$$\mathcal{I} = \sum_i |\phi_i\rangle g_{ij}^{-1} \langle \phi_j|$$

(cf G. Abramovici, Solid State Commun. **109** (1998), p. 253)

Completeness relation

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- In basis $\{|\psi_\eta\rangle$ free states in $\mathbb{R}_+$, $|\check{\psi}_\eta\rangle$ free states in $\mathbb{R}_-$, $|\psi_{n+\frac{1}{2}}\rangle$ anomalous bound states, $|\psi_n\rangle$ regular ones$\}$, the metric writes

$$g = \begin{pmatrix} I & 0 & R & 0 \\ 0 & I & R & 0 \\ R^\dagger & R^\dagger & S & 0 \\ 0 & 0 & 0 & I \end{pmatrix}$$

(R is the overlapping between anomalous and free states, S the overlapping between anomalous states).

Completeness relation

- In the same basis, its inverse writes

$$g^{-1} = \begin{pmatrix} I + RBR^{\dagger} & RBR^{\dagger} & -RB & 0 \\ RBR^{\dagger} & I + RBR^{\dagger} & -RB & 0 \\ -BR^{\dagger} & -BR^{\dagger} & B & 0 \\ 0 & 0 & 0 & I \end{pmatrix}$$

where $B = (S - 2R^{\dagger}R)^{-1}$.

Completeness relation

- The completeness relation then writes

$$
\begin{aligned}
\mathcal{I} \;=\; & \int dk|\psi_\eta\rangle\langle\psi_\eta| + \int dk|\check{\psi}_\eta\rangle\langle\check{\psi}_\eta| + \\
& \sum_{\substack{m\in\mathbb{N}\\ n\in\mathbb{N}}} \int_{\mathbb{R}_+\times\mathbb{R}_+} dk\; dk' \left(|\psi_\eta\rangle + |\check{\psi}_\eta\rangle\right) \alpha_m(\eta) B_{mn} \alpha_n(\eta') \left(\langle\psi_{\eta'}| + \langle\check{\psi}_{\eta'}|\right) \\
& - \sum_{\substack{m\in\mathbb{N}\\ n\in\mathbb{N}}} \int_{\mathbb{R}_+} dk \left(|\psi_\eta\rangle + |\check{\psi}_\eta\rangle\right) \alpha_m(\eta) B_{mn} \langle\psi_{n+\frac{1}{2}}| \\
& - \sum_{\substack{m\in\mathbb{N}\\ n\in\mathbb{N}}} \int_{\mathbb{R}_+} dk |\psi_{m+\frac{1}{2}}\rangle B_{mn} \alpha_n(\eta) \left(\langle\psi_\eta| + \langle\check{\psi}_\eta|\right) \\
& + \sum_{\substack{m\in\mathbb{N}\\ n\in\mathbb{N}}} |\psi_{m+\frac{1}{2}}\rangle B_{mn} \langle\psi_{n+\frac{1}{2}}| + \sum_{p\in\mathbb{N}^*} |\psi_p\rangle\langle\psi_p|
\end{aligned}
$$

Completeness relation

- If one discards all anomalous states, there is a degeneracy between solutions ψ_n (even) and $|\psi_n|$ (odd), these last are absent of the other basis.
- The completeness relation then writes

$$
\begin{aligned}
&\sum_{p\in\mathbb{N}*}\varphi_p(\frac{u}{2p})\varphi_p(\frac{u'}{2p}) + \sum_{p\in\mathbb{N}*}|\varphi_p(\frac{u}{2p})|\,|\varphi_p(\frac{u'}{2p})| + \\
&\int_0^\infty f_\eta(-\frac{u}{2\eta})f_\eta(-\frac{u'}{2\eta})dk + \int_0^\infty f_\eta(\frac{u}{2\eta})f_\eta(\frac{u'}{2\eta})dk \quad = \quad \lambda\delta(u-u')
\end{aligned}
$$

- This relation proves wrong, which indicates that anomalous states should not be discarded.

Completeness relation

- The spaning of $|\psi_{n+\frac{1}{2}}\rangle$ writes

$$|\psi_{n+\frac{1}{2}}\rangle = \sum_{p\in\mathbb{N}^*} b_{pn}|\,|\psi_p|\rangle + \int_0^{\infty} \alpha_n(\eta)(|\psi_\eta\rangle + |\check{\psi}_\eta\rangle)dk$$

- We apply $\mathcal{H}$ on the left and get

$$E_{n+\frac{1}{2}}|\psi_{n+\frac{1}{2}}\rangle = \sum_{p\in\mathbb{N}^*} b_{pn}E_p|\,|\psi_p|\rangle + \int_0^{\infty} \alpha_n(\eta)E_\eta(|\psi_\eta\rangle + |\check{\psi}_\eta\rangle)dk$$

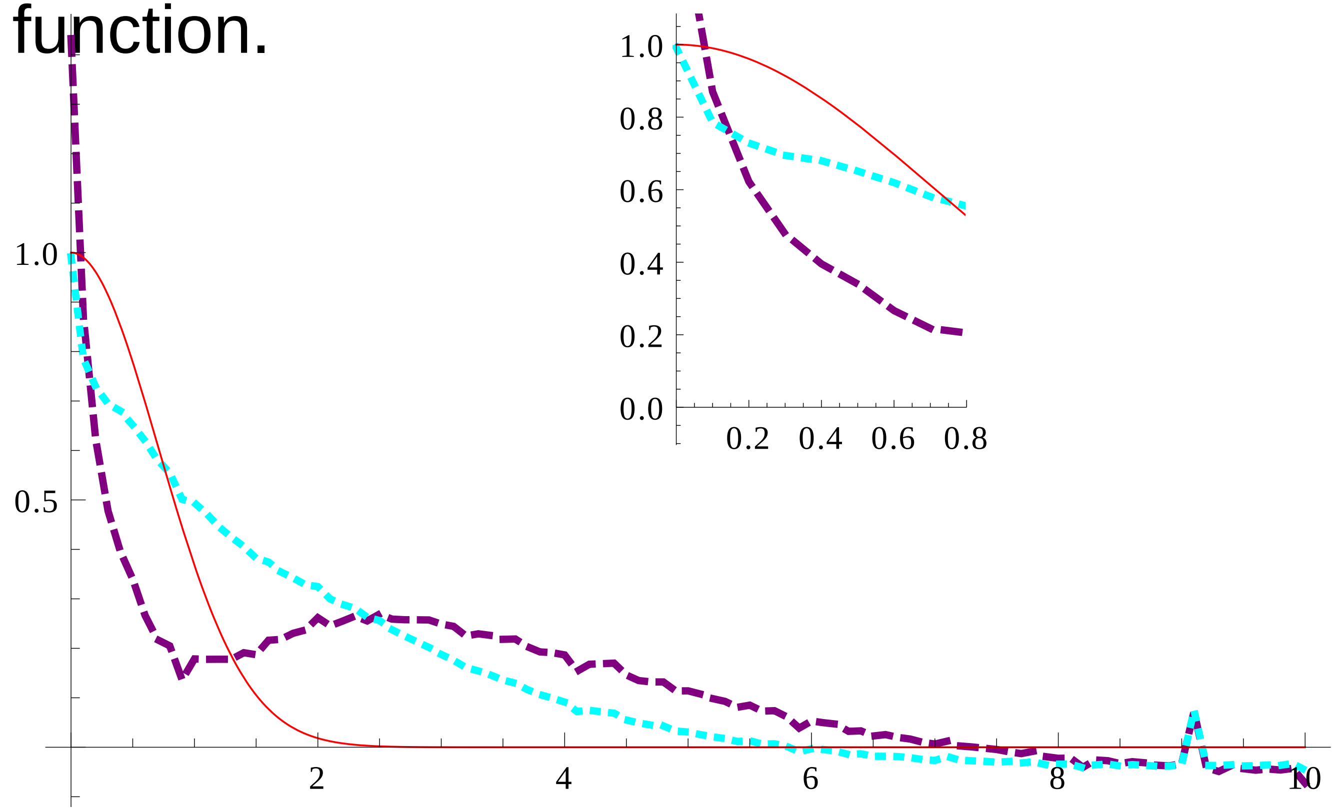
- Substituting in the completeness relation (2^{nd} case),

$$\sum_{p\in\mathbb{N}^*} b_{pn}(E_p - E_{n+\frac{1}{2}})|\,|\psi_p|\rangle + \int_0^{\infty} \alpha_n(\eta)(E_\eta - E_{n+\frac{1}{2}})(|\psi_\eta\rangle + |\check{\psi}_\eta\rangle)dk = 0$$

$$\iff b_{pn} = 0\ \forall p \in \mathbb{N}^* \text{ and } \alpha_n(\eta) = 0\ \forall \eta \in \mathbb{R}_+ \text{ impossible}$$

Numerical proof

- We test the two completeness relations on a centered gaussian function.



In red, the test function, in blue dotted line its decomposition through the basis including anomalous functions, in red dashed line its decomposition through the basis including only regular functions.

Numerical proof

- This test is not concluding, however one should not forget that the curves are calculated with several approximations.
- In particular, I take $p = 1$ up to 30, for ψ_p, calculations seem to be converging within this limit.
- Also, I take $q = 0, 10$ for $\psi_{q+\frac{1}{2}}$, calculations seem to be converging within this limit.
- I tried to include anomalous *free* states, but it seems not the right idea.

Non-hermiticity of $\mathcal{H}$

- Here, hermiticity writes, in detail,

$$\int dx \overline{\psi(x,E_1)}\left[-\frac{\partial^2\psi}{\partial x^2}(x,E_2)+\frac{\lambda}{|x|}\psi(x,E_2)\right] =$$
$$\int dx\left[-\overline{\frac{\partial^2\psi}{\partial x^2}(x,E_1)}+\frac{\lambda}{|x|}\overline{\psi(x,E_1)}\right]\psi(x,E_2)$$

- Its violation comes from the discontinuity at $x=0$ of

$$\left[-\overline{\psi(x,E_1)}\frac{\partial\psi}{\partial x}(x,E_2)+\overline{\frac{\partial\psi}{\partial x}(x,E_1)}\psi(x,E_2)\right]$$

- This term is zero when you calculate it with only regular states.

Regularized hamiltonian

- We introduce a point-like correction to $\mathcal{H}$:

$$\delta\mathcal{H} = \theta(\mathcal{H})(\delta \times \mathcal{H})\theta(\mathcal{H}^\dagger) - \theta(\mathcal{H})(\mathcal{H} \times \delta)\theta(\mathcal{H}^\dagger) \ ,$$

  where $\forall n \in \mathbb{N}$, $\theta(E_{n+\frac{1}{2}}) = \frac{1}{\varphi_{n+\frac{1}{2}}(0)}$, $\quad \delta(x)|\chi\rangle = \chi(0)|\chi\rangle \ \forall \chi$.

- θ is analytical.
- Regular free and bound states are still eigenfunctions of $\mathcal{H} + \delta\mathcal{H}$.
- Anomalous states are modified: $\varphi_{n+\frac{1}{2}} \longrightarrow \tilde{\varphi}_{n+\frac{1}{2}}$, the new eigenfunctions of $\mathcal{H} + \delta\mathcal{H}$.

Regularized hamiltonian

- $\tilde{\varphi}_{n+\frac{1}{2}}$ are solutions of $g^{-1}(H+H^\dagger)_{\mathrm{reduced}}$

$$= \begin{pmatrix} H + RBR^\dagger H - RBHR^\dagger & HR/2 + RBR^\dagger HR - RBHS/2 \\ -BR^\dagger H + BHR^\dagger & H/2 - BR^\dagger HR + BHS/2 \end{pmatrix}$$

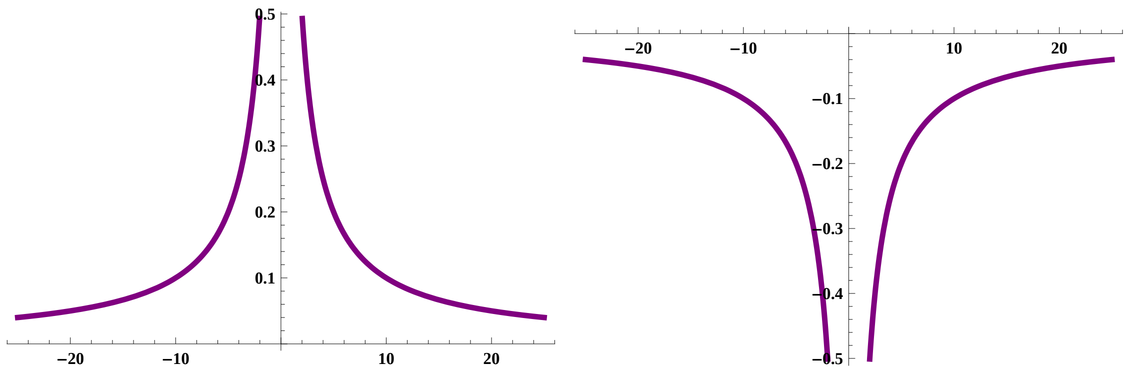
- Should the hamiltonian **be** corrected ?
  If yes, these corrected states are valid.
  If no, uncorrected anomalous states are the valid solutions.

Conclusion

- Anomalous states are (slightly) interacting one with another.
- The Coulomb potential is non-hermitian.
- It is corrected by adding pointlike terms, which can be interpretated as self-interacting terms.
- The spectrum could not be complete if anomalous states were removed.

Free states

- One can use repulsive or attractiv Coulomb potential



- In both cases, one finds (non-trivially) that transmission is zero, $t = 0$.
- $\Longrightarrow$ free states have the **same** normalization than radial 3-d solutions of hydrogen atom, while bound states have a modified normalization.

Transmission

- The transmission is 0.
- It was first claimed by M. Andrews, Am. J. Phys. **44**, 1064 (1976) (no complete demonstration).
- A wrong solution is given in V. S. Mineev, Theor. Math. Phys. **140** 1157 (2004).

Overlappings

Here are the first overlappings (matrix S)

$$\begin{pmatrix} 1 & -0.0108486 & -0.00510692 & -0.00309526 \\ -0.0108486 & 1 & -0.0011072 & -0.000672455 \\ -0.00510692 & -0.0011072 & 1 & -0.000319168 \\ -0.00309526 & -0.000672455 & -0.000319168 & 1 \end{pmatrix}$$

Integer polynomials p_n, q_n

$$
\begin{aligned}
p_0 &= 1\,, \\
q_0 &= 1\,, \\
p_n(x) &= (2n+1)p_{n-1}(x) + 2x(p'_{n-1}(x) - p_{n-1}(x) - q_{n-1}(x))\,, \\
q_n(x) &= (2n-1)q_{n-1}(x) + 2x(q'_{n-1}(x) - p_{n-1}(x) - q_{n-1}(x))\,,
\end{aligned}
$$

and normalization factor writes

$$
r_n = (2s_n + \frac{\pi^2((2n+1)!!)^2}{4})(2n+1)\,,
$$

where

$$
\begin{aligned}
s_0 &= 1\,, \\
s_1 &= 11\,, \\
s_{n+1} &= s_n(2n+3)^2 + 2((2n-1)!!)^2\,.
\end{aligned}
$$

Calculation of $\tilde{\varphi}_{n+\frac{1}{2}}$

- We define matrix representation $M = \langle \phi_i | \mathcal{M} | \phi_j \rangle$.
- Be careful that eigenvectors are that of $g^{-1}M$, with this definition.
-

$$H = \begin{pmatrix} E_\eta \delta(\eta - \eta') & 0 & E_{n+\frac{1}{2}} R_{\eta,n} & 0 \\ 0 & E_\eta \delta(\eta - \eta') & E_{n+\frac{1}{2}} R_{\eta,n} & 0 \\ E_{\eta'} R_{m,\eta'} & E_{\eta'} R_{m,\eta'} & E_{n+\frac{1}{2}} S_{mn} & 0 \\ 0 & 0 & 0 & E_p \delta_{pq} \end{pmatrix}$$

$$H^\dagger = \begin{pmatrix} E_\eta \delta(\eta - \eta') & 0 & E_\eta R_{\eta,n} & 0 \\ 0 & E_\eta \delta(\eta - \eta') & E_\eta R_{\eta,n} & 0 \\ E_{m+\frac{1}{2}} R_{m,\eta'} & E_{m+\frac{1}{2}} R_{m,\eta'} & E_{m+\frac{1}{2}} S_{mn} & 0 \\ 0 & 0 & 0 & E_p \delta_{pq} \end{pmatrix}$$

Calculation of $\tilde{\varphi}_{n+\frac{1}{2}}$

- We get rid of state $|\psi_\eta\rangle - |\check{\psi}_\eta\rangle$ by $(|\psi_\eta\rangle, |\check{\psi}_\eta\rangle) \rightarrow (|\psi\eta\rangle + |\check{\psi}\eta\rangle, \frac{|\psi\eta\rangle - |\check{\psi}\eta\rangle}{2})$