ON THE APPLICATION OF THE EXTERIOR COMPLEX SCALING METHOD TO PURE COULOMB POTENTIALS

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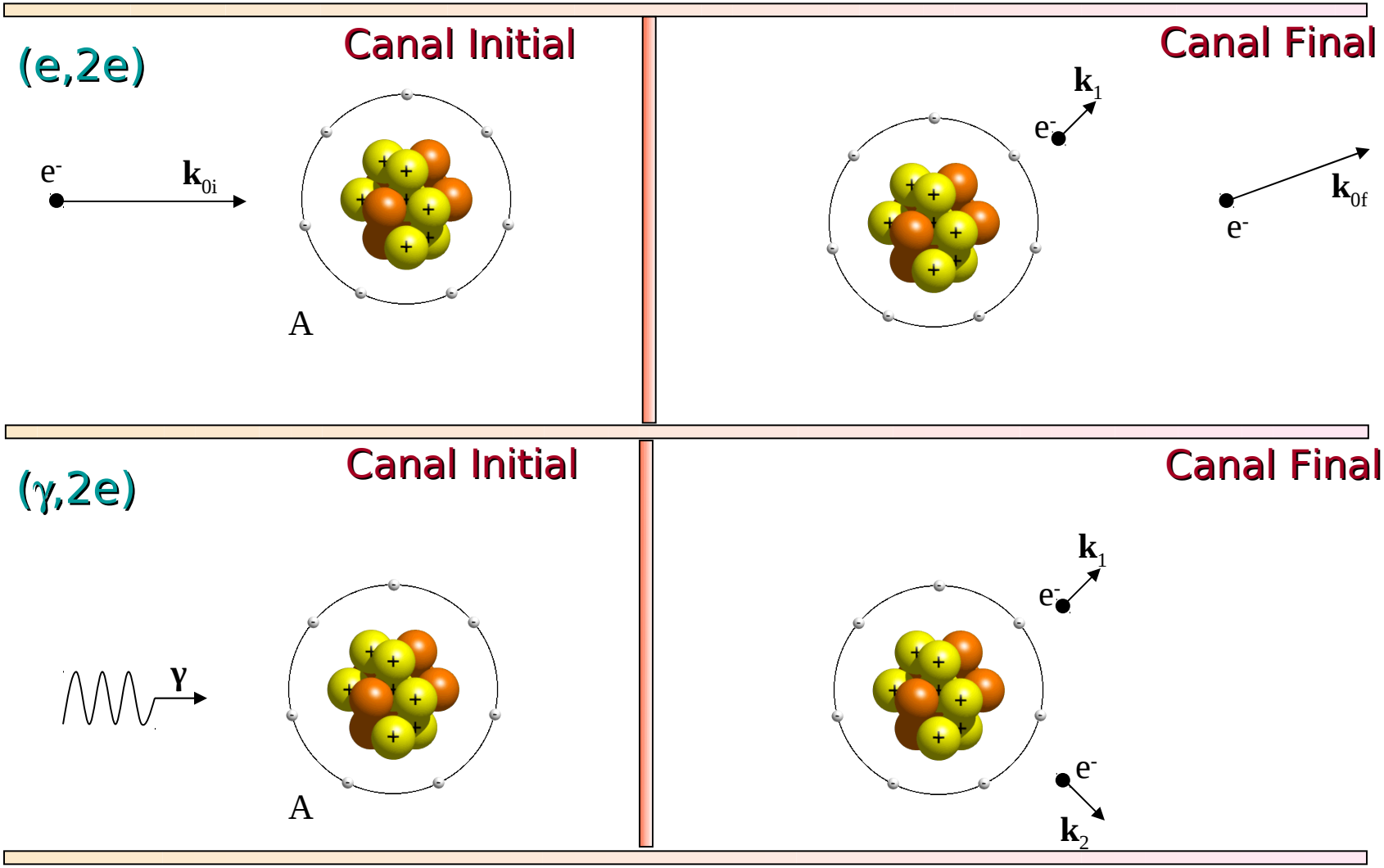
OUTLINE

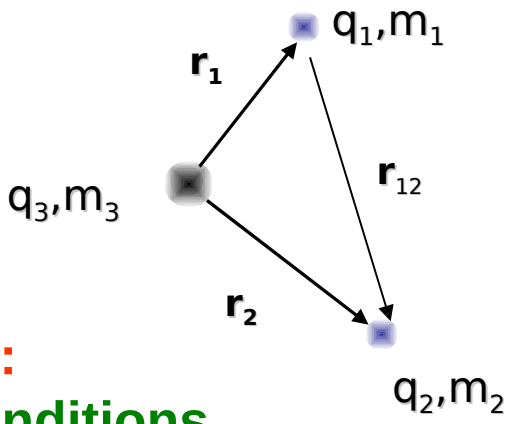
- Why ?
- Main ingredients of the Exterior Complex Scaling (ECS)
- Questions?
- Short-range and long-range Coulombic potentials
- Pure Coulomb potential
- Summary
- Use of Complex basis (Sturmian functions)

Example: Single ionization : (e,2e) and (γ,2e) TDCS



WHY?

$$\frac{q_1 q_3}{r_1} + \frac{q_2 q_3}{r_2} + \frac{q_1 q_2}{r_{12}}$$



Three-body Coulomb break-up processes (e.g. e⁻-H):
VERY difficult to enforce asymptotic conditions

Peterkop-type asymptotic behavior (all particles far from each other)

$$\Psi^{+}_{sc}(\rho, \omega_5) \propto \rho^{-5/2} e^{iK\rho + i\frac{C(\omega_5)}{K}\ln(2K\rho)}$$

$$\rho = \sqrt{r_1^2 + r_2^2} \qquad \alpha = \arctan(r_1/r_2)$$

$$V(\rho, \omega_5) = \frac{q_1 q_3}{\rho \cos\alpha} + \frac{q_2 q_3}{\rho \sin\alpha} + \frac{q_1 q_2}{\rho\sqrt{1 - \sin(2\alpha)\cos\theta_{12}}} = \frac{C(\omega_5)}{\rho}$$

No one has yet applied it to the numerical resolution of S.E. for the ionization problem

WHY?

Methods without explicit use of any asymptotic boundary conditions
→ VERY PRACTICAL

→ Exterior Complex scaling (ECS)

Complex Scaling method: $r \rightarrow r\, e^{i\eta}$

(since Nuttal and Cohen, PR, 1969)

Initially: structure of atomic systems + resonance scattering

Exterior Complex scaling (ECS): (Simon, Phys Lett. A, 1979)

Extension to scattering problems including long-range potentials (Rescigno et al, PRA, 1997)

Since then, very successful method for the study of a variety of (ionization) processes

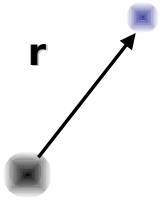
EXAMPLES:
- e^--H ionization (Rescigno et al, Science, 1999)
- Photo Double Ionization of He (McCurdy et al, PRA, 2004)
- PhotoIonization of molecules (Vanroose et al, PRA, 2006 – Yip et al, PRA, 2008 – Fernandez et al, PRA, 2009)
- Two-slit type experiments (Tao et al, PRA, 2010)

WHY?

We do not question the ECS capabilities or computation technique but

- Why does it work numerically?
- Understand and reinforce the foundations of the ECS
- Raise and answer some questions.
- Can the ECS be applied to pure Coulomb potentials?

TWO-BODY V(r)



Ingredients of the ECS approach

1) Formulation of the scattering problem
2) Exterior Complex Scaling
3) Numerical evaluation of scattering w.f.
4) Artificial cut-off of the potential
5) Amplitude extraction

For details, see for example review paper:
McCurdy, Baertschy and Rescigno, JPB, **37**, R137, (2004)

ECS ingredients (1)

TWO-BODY CASE

Consider the scattering between two particles interacting via a spherically symmetric potential $V(r)$. The radial two–body Schrödinger equation describing the dynamics of the problem is

$$[\mathcal{T}_l + V(r) - E]\,\Psi(r) = 0.$$

where $\mathcal{T}_l = -\frac{1}{2\mu}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right)$ represents the reduced kinetic energy operator, μ is the reduced mass, l the angular momentum eigenvalue and the energy $E = k^2/(2\mu)$ assumed positive.

Simplified problem (without potential) $\quad [\mathcal{T}_l - E]\,\Psi_0(r) = 0$

$\rightarrow$ free–particle solution (Riccati-Bessel function)

$$\Psi_0(r) = kr j_l(kr) \;\rightarrow \sin\left(kr - \frac{\pi}{2}l\right).$$

The solution of the scattering problem can be separated into two terms (ANSATZ)

$$\Psi(r) = \Psi_0(r) + \Psi_{\rm sc}(r)$$

– $\Psi_0(r)$ is taken as **initial – asymptotic – state**, corresponding to no scattering;
– $\Psi_{\rm sc}(r)$ is the **scattering term** describing the dynamics of the collision process. In principle, $\Psi_{sc}(r)$ should have **pure outgoing behavior** , noted $\Psi^+_{sc}(r)$; the corresponding wave function is noted $\Psi^+(r)$.

With the decomposition we get the following **driven Schrödinger equation for** $\Psi_{\rm sc}(r)$

$$[\mathcal{T}_l + V(r) - E]\,\Psi_{\rm sc}(r) = -V(r)\Psi_0(r).$$

THREE-BODY CASE (similar driven eq.)

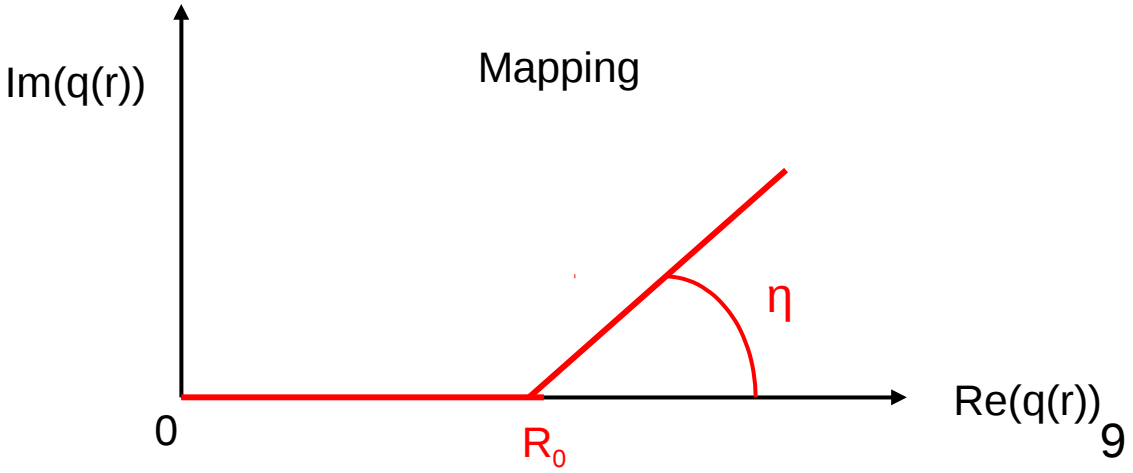
ECS ingredients (2)

EXTERIOR COMPLEX SCALING (rotation) of the radial coordinate:

$$r = q(r) = \begin{cases} r & r \leq R_0 \\ R_0 + (r - R_0)e^{i\eta} & r > R_0 \end{cases}$$

where R_0 defines the radius within which the wavefunction will be the usual function of real valued coordinates, and $\eta > 0$ represents the scaling rotation angle on the complex plane.

$\rightarrow$ imposition of the asymptotic conditions is avoided. This is associated to the fact that, when the exterior complex rotation is performed, $\Psi^+(r) \rightarrow 0$ **for** $r > R_0$**, and a *numerical zero* can be assumed** in, e.g., a numerical grid.



ECS ingredients (3)

1) …
2) …
3) Numerical evaluation of scattering w.f. on a finite region of space ($r<R_0$) with different techniques: finite elements, finite differences, L^2 basis, B-splines, direct numerical integration, …)
4) …
5) …

ECS ingredients (3)

HOWEVER for values of $r > R_0$

– $\Psi_{sc}(r)$ with pure outgoing behavior: the rotation gives an exponentially decreasing asymptotic behavior:

$$exp(ikr) \rightarrow exp(ikre^{i\eta}) \rightarrow 0$$

– $\Psi_0(r)$ has a standing wave behavior and becomes exponentially divergent

$$\Psi_0(r) \sim \sin\left(kre^{i\eta} - \frac{\pi}{2}l\right)$$
$$\simeq \frac{1}{2i}\left[e^{ikr(\cos(\eta)+i\sin(\eta))} - e^{-ikr(\cos(\eta)+i\sin(\eta))}\right] \simeq -\frac{1}{2i}e^{-ikr\cos(\eta)}e^{kr\sin(\eta)}.$$

$\rightarrow$ for $r > R_0$, the full wave function $\Psi(r) = \Psi_0(r) + \Psi_{sc}(r)$ will be **exponentially divergent.**

The non-homogeneity $V(r)\Psi_0(r)$ of the driven equation will be divergent unless the potential $V(r)$ on the RHS decreases fast enough to make it well defined and bound: this condition is met *only* for **short–range potentials** decreasing exponentially or faster [Baumer et al, PRA, 1975)].

Need a vanishing RHS!
What to do?

ECS ingredients (4)

AN ARTIFICIAL SHARP CUT-OFF of the potential $V(r)$ at the value $r = R_0$

$$V_{R_0}(r) = \begin{cases} V(r) & r \leq R_0 \\ 0 & r > R_0, \end{cases}$$

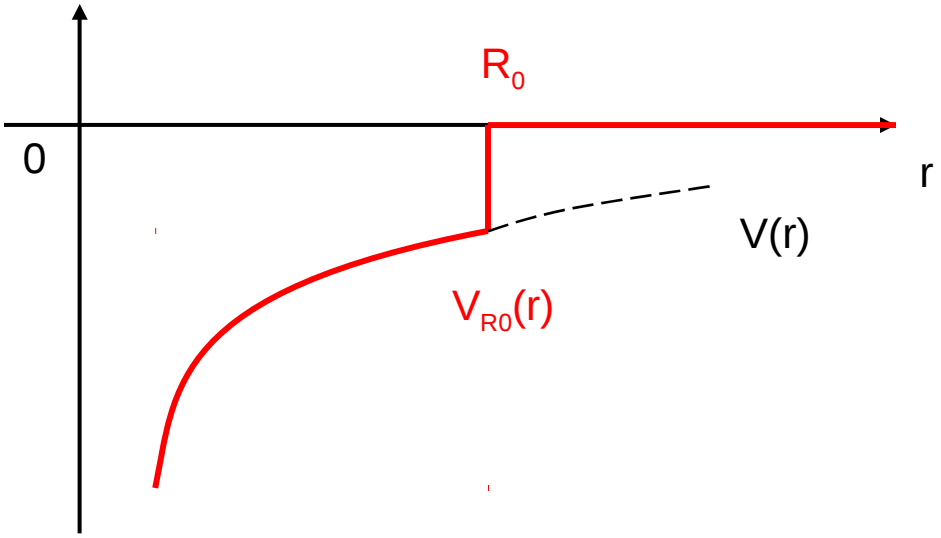
for every potential excluding those decreasing exponentially or faster.

Cut–off **ONLY on RHS** of the driven equation

$$[\mathcal{T}_l + V(r) - E]\,\Psi_{sc}(r) = -V_{R_0}(r)\Psi_0(r)\,.$$

→ **UNBALANCED TREATMENT !**

Making R_0 large enough we can guarantee that $V_{R_0}(r)$ differs negligibly from the physical potential $V(r)$.



Extraction of the transition amplitude

The amplitude A_l can be extracted using the definition

$$A_l = -2\mu\langle\frac{\Psi_0(r)}{r}|V(r)|\frac{\Psi^+(r)}{r}\rangle$$

Using the Schrödinger equations and assuming a vanishing contribution for $r > R_0$:

$$A_l = 2\mu\langle\frac{\Psi_0(r)}{r}|\mathcal{T} - E|\frac{\Psi^+_{sc}(r)}{r}\rangle_{R_0},$$

where the subscript R_0 denotes **the integration limited to the domain** $0 \leq r \leq R_0$.

The amplitude is obtained from the function defined in the inner region ($r < R_0$),
by taking **the limit of the function for large** r **but smaller than** R_0 .

PHYSICAL REVIEW A, VOLUME 63, 022712

2001

Electron-impact ionization of atomic hydrogen

M. Baertschy,[1] T. N. Rescigno,[2,3] W. A. Isaacs,[2] X. Li,[2] and C. W. McCurdy[2,4]

Technical reasons connected with the use of complex scaling require us to truncate the interaction potentials on the complex portions of the grid [20]. The physically correct results are then recovered by extrapolating the computed values to infinite box size. Because we cannot offer a strict mathematical proof that this extrapolation yields the exact value, we have carried out a number of numerical tests to show that the procedures employed are in fact producing the correct result. For instance, we will show that the radial wave

Ultimately, however, the fundamental correctness of our procedure relies on the empirical observation that the computed results are in perfect agreement with absolute experimental measurements that probe the most intimate details of the collision dynamics at energies where long-range correlation effects are very important.

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problems with long-range interactions. The key to applying the ECS procedure to long-range potential problems is to truncate the interaction potential at the boundary of the hypersphere and to either carry out calculations with R_0 large enough that the truncation of the potential is of no physical consequence or, if this is impractical, to carry out calculations for different values of R_0 and perform a numerical extrapolation of $R_0 \rightarrow \infty$ to obtain the physically correct results.

plex part of the contour, making it necessary to truncate the long-range Coulomb potentials at R_0 in the inhomogeneous terms $\chi^L_{l_1 l_2}$ [20]. This is the only source of systematic error in our scheme for calculating the scattered wave with exterior complex scaling. The numerical procedures we employed to

PHYSICAL REVIEW A VOLUME 55, NUMBER 6 JUNE 1997

Making complex scaling work for long-range potentials

T. N. Rescigno M. Baertschy and D. Byrum C. W. McCurdy

The purpose of this paper is to show that exterior scaling can be used to formulate a procedure for solving the full scattering problem using only square-integrable functions and that, unlike the original complex scaling method, the method is not restricted to exponentially bounded potentials.

We reiterate that by zeroing the potential on the complex portion of the contour, we eliminate any numerical difficulties associated with a less than exponential fall off of the potential at large distances, but have no measurable effect on the cross section.

PHYSICAL REVIEW A VOLUME 55, NUMBER 6 JUNE 1997

Making complex scaling work for long-range potentials

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required matrix elements. Since $V_{R_0}(r)$ is a finite-range potential, the method will converge for any value of R_0 if N is large enough. This truncation of the potential allows us to define a process that limits to the correct physical result as $R_0 \rightarrow \infty$. Thus, by choosing the *interior* region large enough, we can insure that the truncated potential differs insignificantly from the physical potential under consideration [28].

N: number of basis functions

[28] This discussion assumes that the potential falls off more rapidly than $|1/r|$ at infinity.

QUESTION: COULOMB CASE?

- Since the 1997 PRA paper, the authors carried out a series of VERY succesful calculations but do not question again the Coulomb case.

  Just make reference to that paper !

earlier to the best of our knowledge. Furthermore, its extension to the Coulomb case remained questionable. However, the definite success in applying this method to important and complicated problems (see papers [5,8] and [12] and references therein) makes a detailed study urgent.

- In 1997 PRA paper, the authors state: *« The discussion assumes that the potential falls off more rapidly than |1/r| at infinity »* .

  Is it possible to deal with the pure Coulomb potential?

QUESTION?

- What is neglected?

$$A_l = 2\mu\langle\frac{\Psi_0(r)}{r}|\mathcal{T}-E|\frac{\Psi^+_{sc}(r)}{r}\rangle_{R_0} - 2\mu\langle\frac{\Psi_0(r)}{r}|V(r)-V_{R_0}(r)|\frac{\Psi^+(r)}{r}\rangle.$$

Within the ECS framework, **only the first term is used** to evaluate the transition amplitude as the potential is assumed to be cut, and hence $V(r) - V_{R_0}(r)$ is zero.
→ **an error – which decreases as R_0 increases – is introduced in the calculation** by neglecting the external contribution of the potential.

Green's function formalism (integral representation)

$$\frac{\Psi^+(r)}{r} = \frac{\Psi_0(r)}{r} + \int_0^\infty r'^2 dr G^+(r,r')V(r')\frac{\Psi_0(r')}{r'}$$

G^+ provides correct asymptotic behavior

To avoid divergency:

$$\frac{\Psi^+(r)}{r} = \frac{\Psi_0(r)}{r} + \int_0^{R_0} r'^2 dr G^+(r,r')V(r')\frac{\Psi_0(r')}{r'}$$

→ $\Psi^+(r)$ not correct !

MORE QUESTIONS?

What are the consequences of cutting the potential ONLY on RHS?

What is the meaning of the solution in the outer region?

Is it really necessary to cut the potential?

HOW DOES THE ECS METHOD WORK?
HOW TO ADAPT IT FOR THE COULOMB POTENTIAL?

SHORT RANGE POTENTIALS

The RHS of the **driven Schrödinger equation for** $\Psi_{\rm sc}(r)$

$$[\mathcal{T}_l + V(r) - E]\,\Psi_{\rm sc}(r) = -V(r)\Psi_0(r)\,.$$

is zero at large enough distances from the origin
$\rightarrow$ **the function** $\Psi_{\rm sc}(r)$ **may have outgoing wave behavior** at large distances
as given by the Riccati–Hankel functions, $H_l^{\pm}(0,r)$, which behave asymptotically as $e^{\pm i\left(kr-\frac{\pi}{2}l\right)}$

$$\Psi^+(r) = \Psi_0(r) + \Psi^+_{\rm sc}(r) \rightarrow \frac{1}{2i}\left[-e^{-i\left(kr-\frac{\pi}{2}l\right)} + e^{i\left(kr-\frac{\pi}{2}l\right)}\right] + A_l\, e^{i\left(kr-\frac{\pi}{2}l\right)}$$
$$= e^{i\delta_l}\sin\left(kr - \frac{\pi}{2}l + \delta_l\right).$$

$\Psi^+_{\rm sc}(r)$ provides asymptotically **the transition matrix** $A_l = e^{i\delta_l}\sin(\delta_l)$ in terms of the scattering phase-shift δ_l

Explicitly excluded in 1997 PRA paper ---- note [28] !

Solution $v^{REG}(r)$ is known – it is real.

$\Psi_{sc}(r)$ needs to construct the well-known Coulomb logarithmic phase

$$H_l(\alpha,r) \rightarrow e^{i[kr-\alpha \ln(2kr)-l\pi/2]}$$

with $\alpha=z_1z_2\mu/k$ (Sommerfeld parameter).

If a standing-wave free-particle initial state $\Psi_0(r)$ is taken

→ INCOMPATIBLE with pure outgoing behavior of $\Psi_{sc}(r)$

$$\Psi^+(r) = \Psi_0(r) + \Psi^+_{sc}(r) \rightarrow \frac{1}{2i}\left[-e^{-i\left(kr-\frac{\pi}{2}l\right)} + e^{i\left(kr-\frac{\pi}{2}l\right)}\right] + A_l\, e^{i\left(kr-\alpha\ln(2kr)\frac{\pi}{2}l\right)}$$

BAD CHOICE OF $\Psi_0(r)$ FROM THE OUTSET !

COULOMB POTENTIAL $V_1(r)=z_1z_2/r$ + SHORT RANGE POTENTIALS $V_2(r)$

$$V(r)=V_1(r)+V_2(r)$$

Reformulation: (McCurdy and Martin, JPB, 2004)

The regular solution of $V_1(r)$ is taken as initial state $\Psi_0(r)$ and the scattering is associated to $V_2(r)$.

Then scattering theory is correctly recovered.

BUT WHAT ABOUT THE PURE COULOMB CASE ?

Gasaneo, Ancarani and Mitnik (submitted)

Introduce a Coulomb distorted initial state $\Psi_{0,dis}(r)$
which « diagonalizes » the Coulomb interaction at large distances.

NEW decomposition:

Instead of

$$\Psi^+(r) = \Psi_{0,dis}(r) + \bar{\Psi}^+_{sc}(r)$$

$$\Psi^+(r) = \Psi_0(r) + \Psi^+_{sc}(r)$$

TWO PROPOSALS for $\Psi_{0,dis}(r)$

$$\Psi_{0,\mathrm{dis}}(r) = \sin\left[kr - \left(\alpha \ln(2kr) + \frac{\pi}{2} l\right) g(r)\right]$$
$$\to^{r\to\infty} \frac{1}{2i}\left(-e^{-i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]} + e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}\right),$$

where $g(r)$ can be any function growing faster than r at the origin and going to one at large distances as, e.g., $g(r) = 1 - e^{-ar^2}$ (a is a positive real constant).

The function $\Psi_{0,\mathrm{dis}}(r)$ solves, asymptotically, the Schrödinger equation

$$\left[\mathcal{T}_l + V(r) - E\right]\Psi_{0,\mathrm{dis}}(r) = \mathcal{O}\left(\frac{1}{r^2}\right).$$

The standard scattering theory is recovered as we may ask $\bar{\Psi}_{\mathrm{sc}}(r)$ to have outgoing behavior :

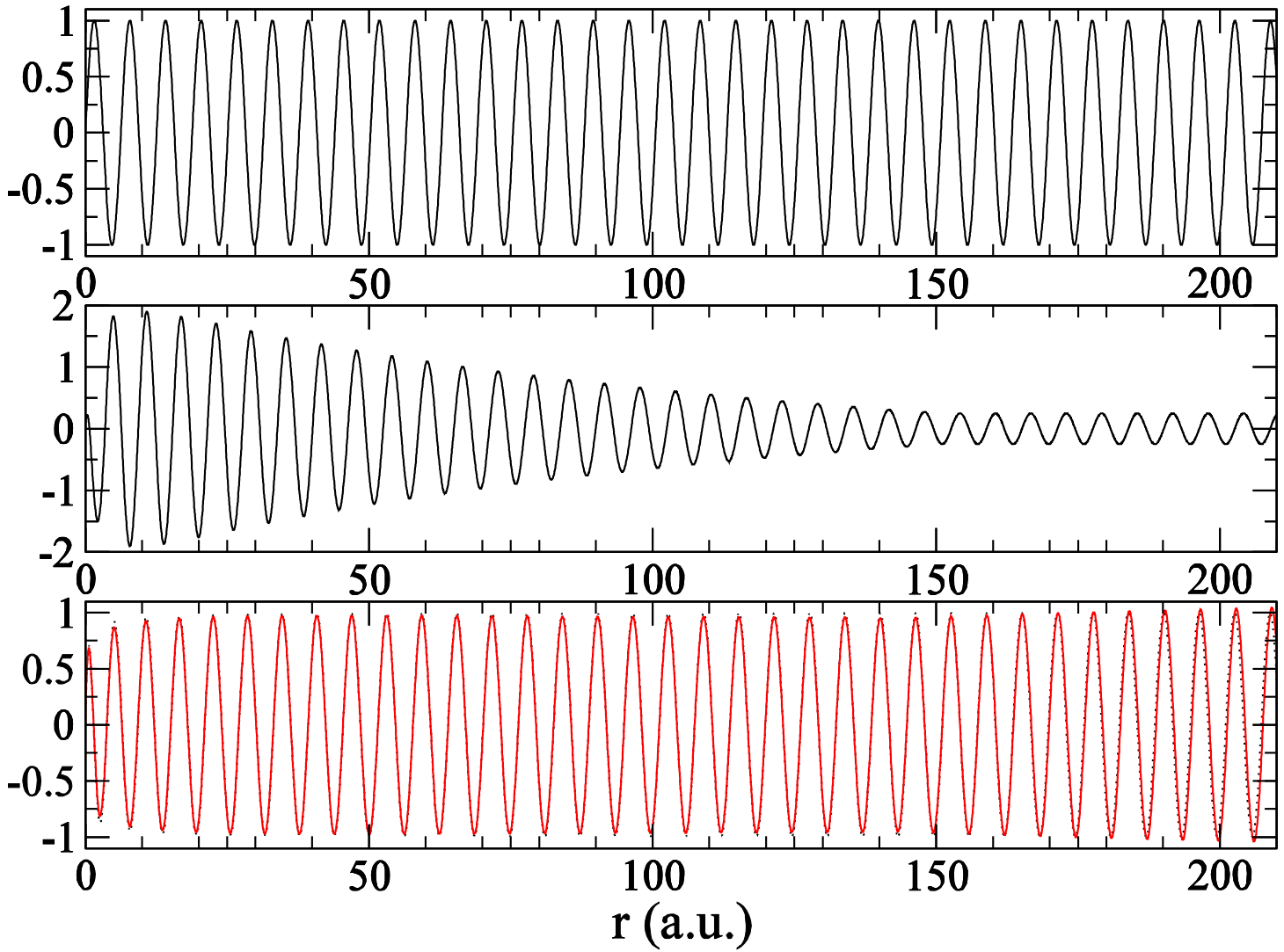
$$\Psi^{+}(r) \to \frac{1}{2i}\left(-e^{-i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]} + e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}\right) + A_l\, e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}.$$

A transition amplitude $A_l = e^{i\delta_l}\sin(\delta_l)$ is extracted.

$\Psi_{0,dis}(r)$

$\Psi_{sc}(r)$

$\Psi(r)=\Psi_{0,dis}(r)+\Psi_{sc}(r)$



Angular momentum l=0, momentum k=1 (E=0.5), μ=1, z_1z_2=-1, and a=0.5.

In the bottom panel, the Coulomb wave function $v^{Reg}(r)$ is included (dotted line) for comparison.

$$\Psi_{0,\mathrm{dis}}(r) = \begin{cases} krj_l(kr) = \Psi_0(r) & r \le R_0 \\ \frac{1}{2i}\left(e^{i\delta_{dis,l}} F_l^+(\alpha, r) - e^{-i\delta_{dis,l}} F_l^-(\alpha, r)\right) & r > R_0, \end{cases}$$

where $F_l^{\pm}(\alpha, r)$ **are solutions of the Coulomb problem from** $r = R_0$ **and up to** ∞**.**

The function $\Psi_{0,\mathrm{dis}}(r)$ solves the Schrödinger equation

$$\left[\mathcal{T}_l + V_{\mathrm{dis}}(r) - E\right] \Psi_{0,\mathrm{dis}}(r) = 0,$$

where

$$V_{\mathrm{dis}}(r) = \begin{cases} 0 & r \le R_0 \\ V(r) & r > R_0, \end{cases}$$

For $r > R_0$, the RHS is zero (as ECS recipe requires)

$$\left[\mathcal{T}_l + V(r) - E\right] \bar{\Psi}_{sc}(r) = 0,$$

$\rightarrow$ $\bar{\Psi}_{\mathrm{sc}}(r)$ may have outgoing behavior $\bar{A}_l e^{i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2}l\right]}$ and one may extract the transition amplitude.

Our second proposal is equivalent to the one discussed in the work of Elander and co–workers [Elander et al, Few Body Systems, 2009, Volkov et al, EuroPhys. Lett, 2009).

HOWEVER, this requires the knowledge of the exact asymptotic solution of the problem.

If OK for two-body, what about three-body?

QUESTION:

- In 1997 PRA paper, the authors state: « *The discussion assumes that the potential falls off more rapidly than* |*1/r*| *at infinity* » .
- Is it possible to deal with the pure Coulomb potential?

ANSWER:

YES, but need to use a Coulomb distorted initial state $\Psi_{0,dis}(r)$ rather than $\Psi_0(r)$

ALTERNATIVE CUT-OFF PROCEDURE
MORE CONSISTENT WITH SCATTERING THEORY

Gasaneo, Ancarani and Mitnik (submitted)

Valid for any potential
but illustrated here for the Coulomb case : ALL ANALYTICAL !!

DRIVEN EQUATION

$$\left[\mathcal{T}_l + V(r) - E\right]\Psi_{\rm sc}(r) = -V(r)\Psi_0(r)$$

A. UNBALANCED TREATMENT (ECS procedure)

$$\left[\mathcal{T}_l + V(r) - E\right]\Psi_{\rm sc}(r) = -V_{R_0}(r)\Psi_0(r)$$

B. BALANCED TREATMENT (our proposal)

$$\left[\mathcal{T}_l + V_{R_0}(r) - E\right]\Psi_{\rm sc}(r) = -V_{R_0}(r)\Psi_0(r)$$

- **divergency of RHS still avoided (as in ECS)**
- **scattering problem properly defined**
  (amplitude can be extracted from the asymptotic behavior)

A. UNBALANCED TREATMENT (ECS procedure) [1/2]

$$[\mathcal{T}_l + V(r) - E]\,\Psi_{sc}(r) = -V_{R_0}(r)\Psi_0(r)$$

$r < R_0$: **inner region (I)**: $\Psi^G_{sc,I}(r) = A_I v^{Reg}(r) + \Psi^P(r)$
$r > R_0$: **outer region (II)**: $\Psi^G_{sc,II}(r) = A_{II} H_l^+(\alpha, r)$ (the RHS is zero - outgoing asymptotics).
Impose continuity at $r = R_0$ of the logarithmic derivative of the wave function: A_I and A_{II} are complex.
NOTE: the ECS solution has a discontinuous derivative.
QUESTION: is our solution $\Psi^G_{sc}(r)$ equivalent to the ECS solution?

FULL SOLUTION in the inner region (I): $\Psi(r) \propto v^{Reg}(r)$
i.e. a function **PROPORTIONAL TO THE EXACT** solution of the Coulomb potential !
To obtain exactly $v^{Reg}(r)$, we can renormalize $\Psi(r)$ with a KNOWN complex constant.
This is a very important result and could be the **cornerstone of the ECS methodology** .

Any other condition applied at R_0 will lead to the same conclusion, i.e., a Coulomb wave function $v^{Reg}(r)$ multiplied by constant. **This implied no necessity of imposing any boundary condition as stated in the ECS approach.** *The problem is to find appropriately the renormalization constant.*

A. UNBALANCED TREATMENT (ECS procedure) [2/2]

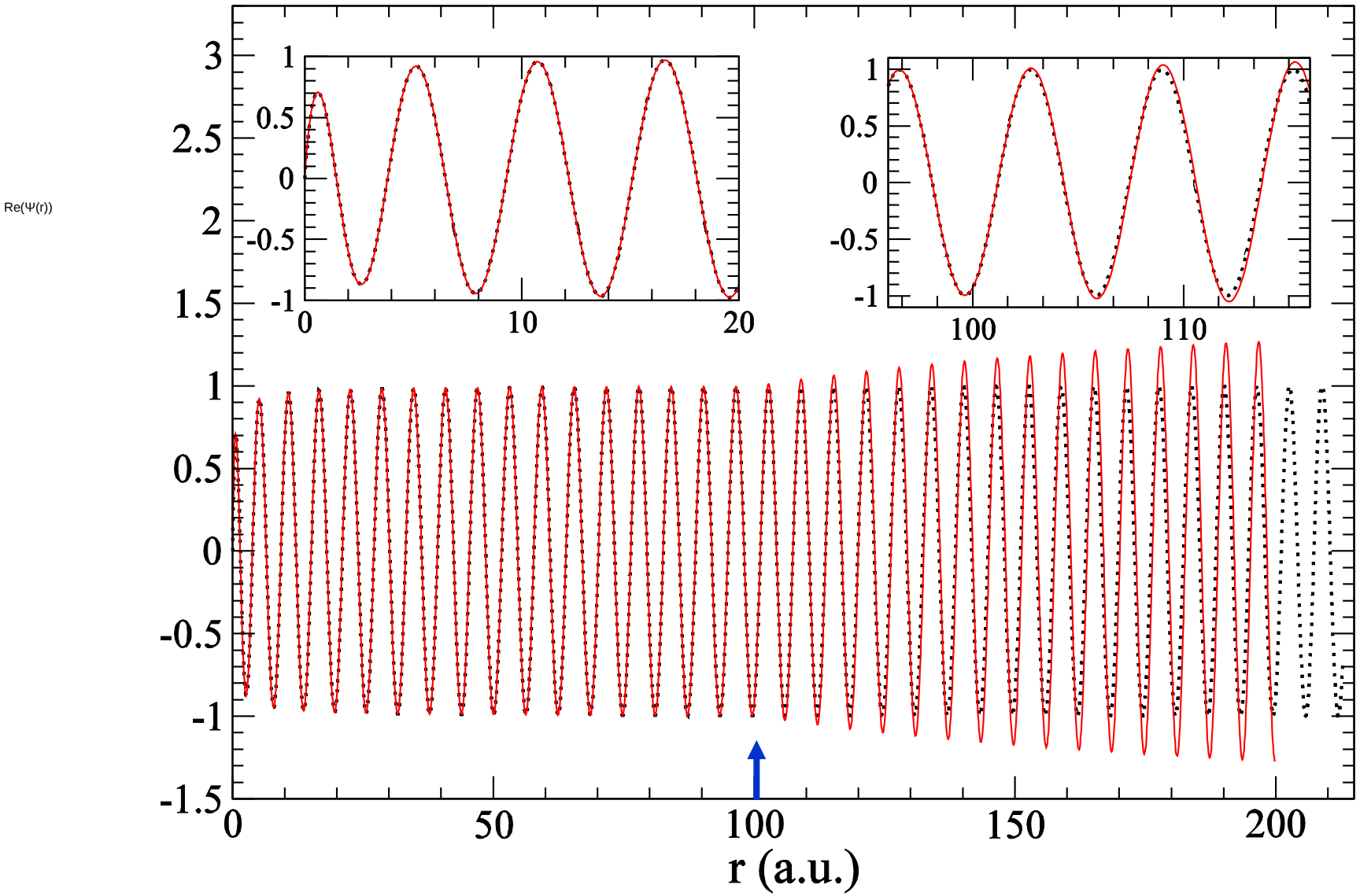
$$\left[\mathcal{T}_l + V(r) - E\right]\Psi_{sc}(r) = -V_{R_0}(r)\Psi_0(r)$$

In principle, since the potential $V_{R_0}(r)$ is of short range, we can try to extract the transition matrix from the asymptotic limit of the wave function in the region where the potential becomes negligible.
In the outer region (II) :

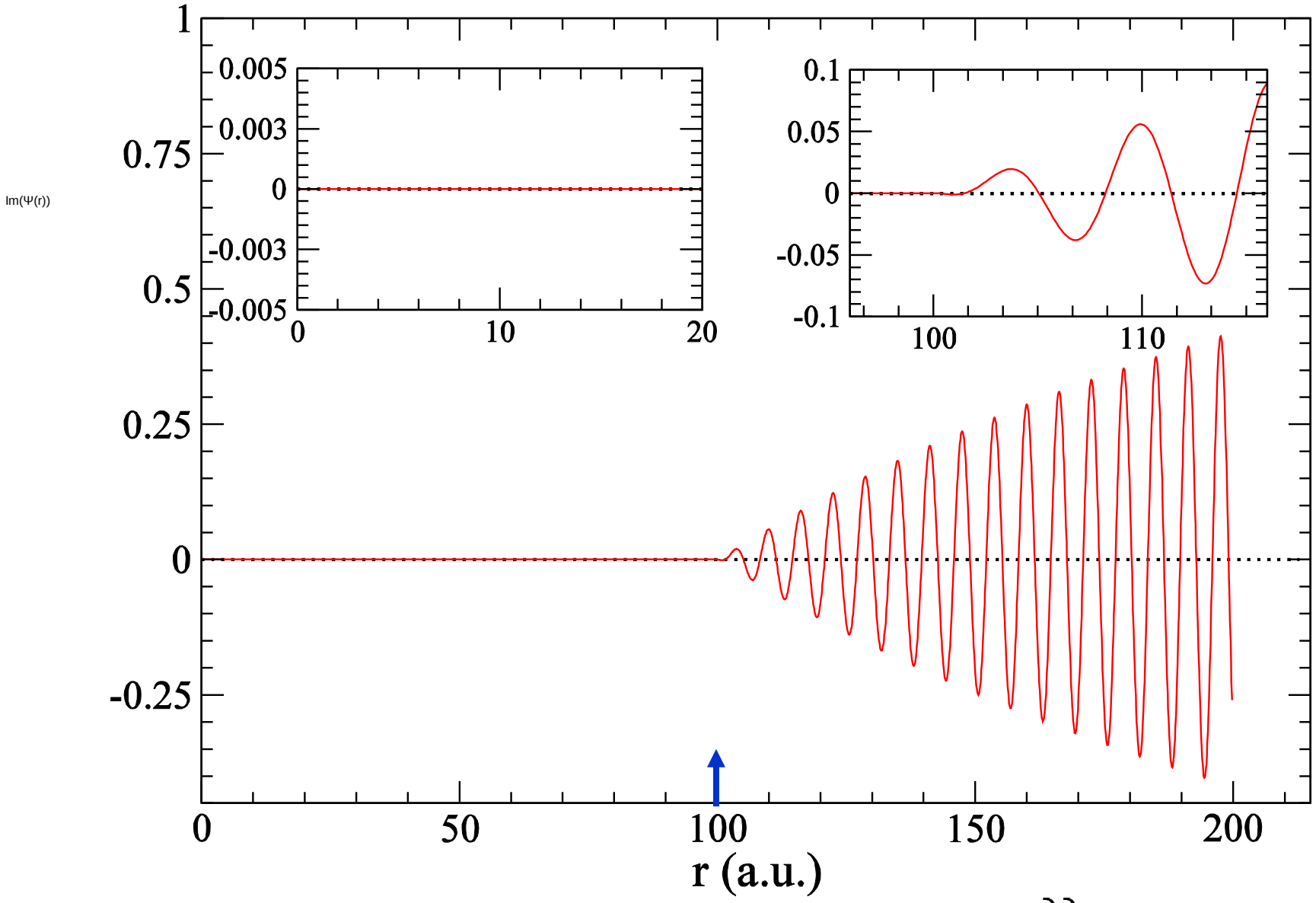
$$\begin{aligned}\Psi^+(r) &\to krj_l(kr) + A_{II}H_l^+(\alpha, r)\\ &= \frac{1}{2i}\left(-e^{-i(kr-\frac{\pi}{2}l)} + e^{i(kr-\frac{\pi}{2}l)}\right) + \frac{\Psi^G_{sc,I}(R_0)}{H_l^+(\alpha, R_0)}e^{i\left[kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right]}.\end{aligned}$$

This clearly shows that the initial state **is not compatible** with the Coulomb distorted outgoing state.
→ **need a distorted initial state,** $\Psi_{0,\mathrm{dis}}(r)$, with proper Coulombic asymptotic behavior.

A. UNBALANCED TREATMENT (ECS procedure) : ILLUSTRATION (R_0=100)



A. UNBALANCED TREATMENT (ECS procedure) : ILLUSTRATION (R_0=100)



B. BALANCED TREATMENT (our proposal)

$$\left[\mathcal{T}_l + V_{R_0}(r) - E\right]\Psi_{\rm sc}(r) = -V_{R_0}(r)\Psi_0(r)$$

In the **inner region (I)**: $\Psi^{G,cut}_{{\rm sc},I}(r) = A^{cut}_I v^{Reg}(r) + \Psi^P(r)$

In the **outer region (II)**: $\Psi^{G,cut}_{{\rm sc},II}(r) = A^{cut}_{II} H^+_l(0,r)$ (the RHS and LHS are zero)

Imposing again for logarithmic continuity at $r = R_0$: A^{cut}_I and A^{cut}_{II} are complex.

The scattering problem is now well defined.

In the limit of large distances $r > R_0$

$$\Psi(r) \to krj_l(kr) + A^{cut}_{II} H^+_l(0,r) = \frac{1}{2i}\left(-e^{-i(kr-\frac{\pi}{2}l)} + e^{i(kr-\frac{\pi}{2}l)}\right) + A_l e^{i(kr-\frac{\pi}{2}l)},$$

This can be verified by solving the scattering problem following the standard QM recipe used for short–range potentials.

As R_0 is increased, the Schrödinger equation with the truncated potential $V_{R_0}(r)$ tends to the original Coulomb one with $V(r)$. However, it is well known that different cut–off to the Coulomb problem can lead to different limits which do not necessarily agree with the exact Coulomb transition matrix. The limit $R_0 \to \infty$ requires a careful study.

QUESTION:

What are the consequences of cutting the potential ONLY on RHS?

What is the meaning of the solution in the outer region?

ANSWER:

Unphysical solution in the outer region ($r>R_0$).

Discontinuous derivative of the wave function at R_0.

Incompatible with standard amplitude extraction (at least in Coulomb case)

A balanced cut-off treatment is more appropriate/consistent

(i.e. using a cut potential from the outset)

but the limit $R_0 \rightarrow \infty$ needs to be investigated

SUMMARY

COULOMB CASE

- **Coulomb distorted wave reformulation (TWO PROPOSALS).**

  A similar reformulation for the three-body case? (need asymptotic solution!)

- **ANALYTICAL STUDY**

  - Cut-off procedure (ECS): unbalanced treatment of the potential.
  - Alternative cut-off procedure: balanced treatment **more appropriate.**

  Inner solution is proportional to the exact solution (cornerstone of ECS).

  A similar demonstration for the three-body case?

SUMMARY

- ECS method: numerically very sucessful
  - … but raised some questions
  - … and provided some answers + reinforce method!
  - … but some questions remain open (3 body!)

> Ultimately, however, the fundamental correctness of our procedure relies on the empirical observation that the computed results are in perfect agreement with absolute experimental measurements that probe the most intimate details of the collision dynamics at energies where long-range correlation effects are very important.

FIRST *take home message*:

ECS works numerically but not on solid formal footing

Another question

Can the cut-off procedure be avoided altogether ?

-YES by using $\Psi_{0,dis}(r)$ with known exact asymptotic solution

If not known: better to use a balanced treatment.

- YES by using complex basis with appropriate asymptotic behavior

Use of real L^2 basis functions with a complex Hamiltonian (through ECS rotation)

$\Leftrightarrow$

Use of complex basis functions with a real Hamiltonian

Basis is rotated NOT the driven equation !!

BUT incoming part (e^{-ikr}) leads to divergencies on RHS → CUT-OFF !

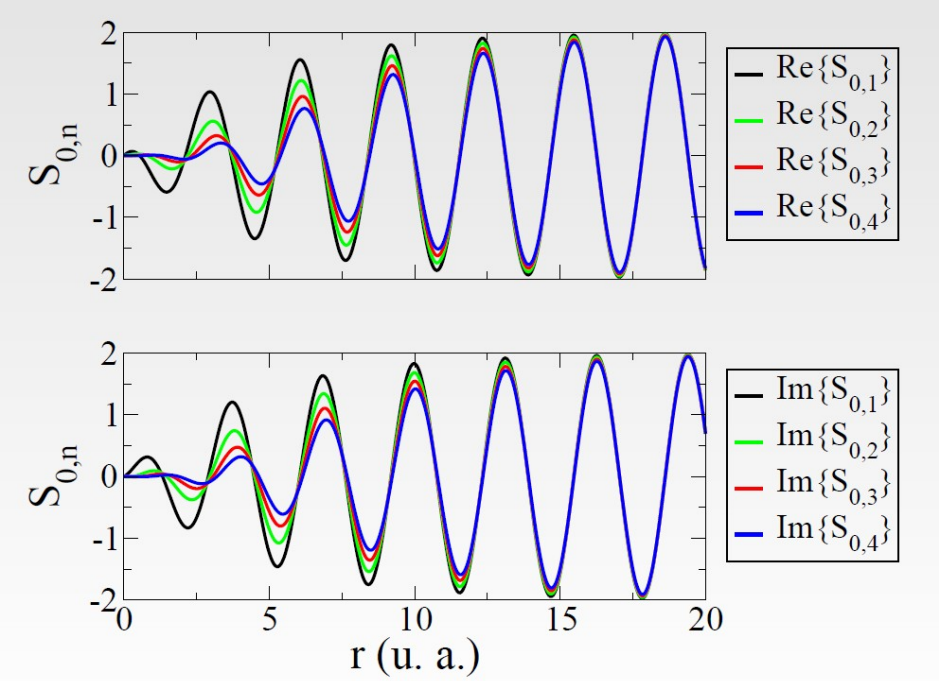
PROPOSAL: use STURMIAN basis functions

$$S_{n,l}(r=0) = 0$$

$$S^{+}_{n,l}(r \to \infty) = e^{i\left(kr - \alpha \ln(2kr) - \frac{\pi}{2}l\right)}$$

EXAMPLE

$S_{n,l}(r) \sim e^{ikr} = \cos(kr) + i\sin(kr)$



STURMIAN BASIS FUNCTIONS

AIM: solve Schrödinger equation $(H-E)\Psi = 0$

TWO-BODY CASE: standard approach

U(r) : central potential

$$\Psi(\mathbf{r}) = \frac{1}{r} R_l(r) Y_l^m(\hat{r})$$

Radial equation:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + U(r) - E \right] R_l(r) = 0$$

Eigenvalue E

$R_l(r)$: eigenfunctions of the ENERGY

Complete and orthogonal set

TWO-BODY CASE: Sturmian approach

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}+U(r)-E\right]S_{n,l}(r)=-\beta_n V_g(r)S_{n,l}(r)$$

U(r) : auxiliary potential (short or long range, usually related to the potential to be solved)

$$\lim_{r\to\infty} rU(r)=Z$$

$V_g(r)$: generating potential (short range)

$$\lim_{r\to\infty} rV(r)=0$$

E: externally fixed parameter

β_n: eigenvalues

$S_{n,l}(r)$: **Eigenfunctions of the potential**

Complete and orthogonal (potential $V_g(r)$ weighted) set

→ **BASIS SET**

Asymptotically:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+U(r)-E\right]S_{n,l}(r)=0$$

→ All $S_{n,l}(r)$: asymptotic behavior dictated by U(r)

TWO-BODY CASE: Sturmian approach

Boundary conditions (for all n)

BOUND STATES ($E=-k^2/2\mu<0$)

$$S_{n,l}(r=0)=0$$

$$S_{n,l}(r\to\infty)=e^{-\kappa r}$$

CONTINUUM STATES ($E=k^2/2\mu>0$)

$$S_{n,l}(r=0)=0$$

$$S_{n,l}(r\to\infty)=H_l^{\pm}(\alpha,r)\longrightarrow e^{\pm i\left(kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right)}$$

Incoming (-) or outgoing (+) wave
(just a plane wave if U(r) not coulombic)

ADVANTAGES OF STURMIAN BASIS

- All basis elements have correct asymptotic behavior
  (with correct energy for continuum states)
- They concentrate the effort in the inner part
- « Diagonalize » the kinetic energy and the potential if U(r) appropriately chosen
- Their orthogonality property transforms the Schrödinger equation
  into a matricial problem (by projection on the basis functions)

→ **VERY EFFICIENT BASIS**
(require smaller computational resources)

STURMIAN basis functions $S^{+}_{n,l}(r \to \infty) = e^{i\left(kr - \alpha \ln(2kr) - \frac{\pi}{2}l\right)}$

AIM: solve driven equation: $\left[\mathcal{T}_l + V(r) - E\right] \Psi_{\mathrm{SC}}(r) = -V(r)\Psi_0(r)$

Expand in Sturmian functions:

$$\Psi_{sc}(r) = \sum_n a_n S_{n,l}(r)$$
$$-V(r)\Psi_0(r) = \sum_n b_n S_{n,l}(r)$$

$\Longrightarrow$

$$\sum_n \beta_n \delta_{n',n} a_n = b_{n'}$$

Matrix equation

Asymptotic limit:

$$\Psi_{sc}(r) \to \sum_n a_n e^{i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2}l\right]} = T_l e^{i\left[kr - \alpha \ln(2kr) - \frac{\pi}{2}l\right]}$$

Transition amplitude:

$$T_l = \sum_n a_n$$

STURMIAN basis functions

Exterior Complex Scaling

$$S_{n,l}(q(r,\eta)) \rightarrow H_l^+(\alpha, re^{i\eta})$$

Asymptotic limit:

$$H_l^+(\alpha, re^{i\eta}) \rightarrow e^{i\left[kre^{i\eta} - \alpha \ln\left(2kre^{i\eta}\right) - \frac{\pi}{2}l\right]} \rightarrow 0$$

AS DESIRED !

No need of CUT-OFF (as no incoming part) !!!

The proposal is promising … applications on the way

SECOND *take home message*:
CUT-OFF can be avoided by using appropriate complex basis functions

Thank you for your attention!

THREE-BODY CASE

Several successful applications:

- bound atomic states (ground and excited), resonances
  (e.g. BEST ground state energy with uncorrelated product)
- H_2^+ molecule (see POSTER)
- electron-atom ionization in Temkin-Poet model
  (reproduce SDCS benchmark results)

REFERENCES:

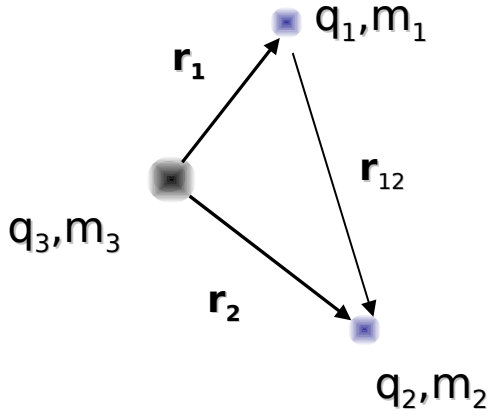
Frapiccini et al, JPB, 2010
Randazzo et al, PRA, 2010
Frapiccini et al, Int. J. Q. Chem, 2009
Frapiccini et al, PRA, 2010
Mitnik et al, Comp. Phys. Comm., 2011

… to come

- Electron-hydrogen ionization for L>0
- Double photo-ionization of He

- With smaller computational resources
- Possibly opening on more complex systems

THREE-BODY CASE



ECS ingredients (1)

THREE-BODY CASE

A three-body scattering problem can be described using the time-independent Schrödinger equation

$$[H - E]\,\Psi^+ = 0.$$

Let H_0 be an Hamiltonian where some part W has been neglected: $H = H_0 + W$

Set $\Psi^+ = \Psi_0 + \Psi_{sc}^+$

- Ψ_0 is a given **initial state** solving an approximate (asymptotic, unperturbed) Hamiltonian H_0
- Ψ_{sc}^+ is the **scattering wave function** . It is defined with outgoing wave asymptotic behavior and possesses all the information about the collisional problem.

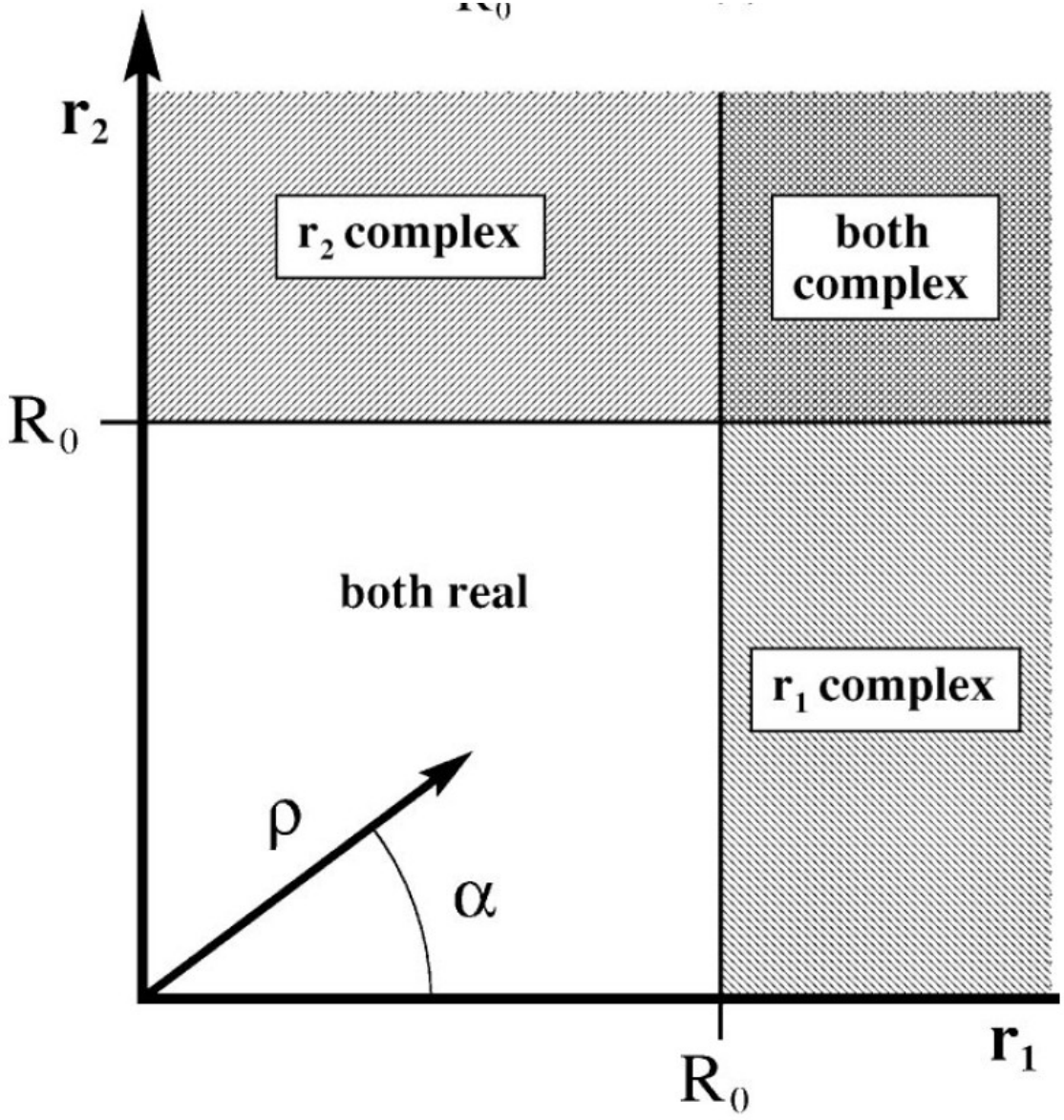
$\longrightarrow$ Ψ_{sc}^+ solves **the driven Schrödinger equation:**

$$[H - E]\,\Psi_{sc}^+ = -W\Psi_0.$$

BOUNDARY CONDITIONS: - regularity at the origin
- pure outgoing behavior

EXAMPLE OF INITIAL STATE (3-body): $\Psi_0 = \frac{\sin r_1}{r_1}\, e^{-r_2}$ [BOUND-FREE]

HERE: TWO-BODY CASE


r2
r2 complex
both complex
R0
both real
r1 complex
ρ
α
R0
r1