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Annihilating States in Close-Coupling Method for Collisions between Hadronic and Ordinary Atoms

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Usual close-coupling method for 2-body collisions

$$A(i) + B \Rightarrow A(j) + B :$$

expansion of the total wave function $\Psi(\mathbf{R}, \xi)$ in terms of inner stationary states $\phi_k(\xi)$ of colliding subsystems,

$$\Psi(\mathbf{R}, \xi) = \sum_k \phi_k(\xi)\psi_k(\mathbf{R}),$$

$+$ standard boundary conditions for $\psi_k(\mathbf{R})$ at $R \to \infty$ (incoming and outgoing waves in open channels, and damping in closed channels).
But: In real quantum systems (atoms, nuclei, etc.) any excited state has a finite life time $\tau_k = \hbar/\Gamma_k < \infty$.
When the state can be considered as a stationary during collision?
Evident condition:
life time is large as compare with a collision time,

$$\tau_k \gg \tau_{\text{coll}} \sim R_i/v,$$

(R_i is an interaction radius).

The parameter $\nu_k = \tau_{\rm coll}/\tau_k = \Gamma_k R_i/\hbar v$ gives a criterion of the state stationarity during collisions: at $\nu_k \ll 1$ the state non-stationarity during collision can be neglected.

The condition $\nu_k \ll 1$ is fulfilled for the most of atomic and nuclear states.

However the states of hadronic atoms with low angular momenta $(ns,\, np)$ have large annihilation (nuclear absorbtion) widths Γ_{nl} and small life times $\tau_{nl} = \hbar/\Gamma_{nl}$, $\therefore$ the condition $\nu_k \ll 1$ can be violated.

The state with $\nu_k \gtrsim 1$

- $\diamond$ can not be a state of incoming channels,
- $\diamond$ can disappear during collision, being admixed to other states.

★ PROBLEM:

How to take into account effects of very short-lived (annihilating) states on collisions of hadronic atoms with environment atoms?

Existing approaches:

$\diamond$ Semiclassical approximations with regard to annihilation (nuclear absorbtion) during collisions
(M. Leon and H.A. Bethe, Phys. Rev. **127** (1961) 636;
T.P. Terada and R.S. Hayano, Phys. Rev. **C 55** (1997) 73; ...).
holds for "hot" hadronic atoms: $ka \gg 1\,(E \gtrsim 1$ eV for $(p\bar{p})_{nl} + H)$

$\diamond$ Quantum close-coupling method
The single attempt within the quantum close-coupling method:
T.S. Jensen and V.E. Markushin (Eur. Phys. J. **D 19** (2002) 165) taken into account nuclear absorbtion in ns-states for the collisions $(\pi^- p)_{nl} + H$.
However the authors use an artificial assumption that the Γ_{nl} is turned off at distances between two atoms $R > R_0 = 5a_0$ that contradicts to the physical reality.

OUR AIM:

Extended close-coupling method to include short-lived (annihilating) states into the basis set with correct asymptotic conditions

General consideration

For definiteness we consider collisions of hadronic atom (or ion) $(\bar{p}Z)_{nl}$ with a neutral atom B

$$(\bar{p}Z)_{nl} + B \to (\bar{p}Z)_{n'l'} + B,$$

where Z is a bar nucleus (e.g., p or He^{++}). Heavy particles (nuclei and antiproton) are slow ($v_{hp} \ll v_e$),

$\therefore$ electronic variables can be separated out within adiabatic approximation reducing the problem to the 3-body $(\bar{p} - Z - B)$.

Total effective 3-body hamiltonian:

$$H = T_R + V(\mathbf{R}, \mathbf{r}) + h(\mathbf{r}),$$

h and $\mathbf{r}$ are inner hamiltonian and coordinates of $(\bar{p}Z)$,

$$T = (-1/2m)\nabla^2_{\mathbf{R}},$$

$\mathbf{R}$ and m are the kinetic energy operator, relative coordinates and reduced mass of colliding subsystems,
$V(\mathbf{R}, \mathbf{r})$ is an operator of the interaction potential between antiprotonic and ordinary atoms.

Model of Hadronic Atom:

$$h = h_0 + U_{opt}(r),$$

h_0 is a hamiltonian of hydrogen-like atom with the nucleus charge Z and the reduced mass μ,
$U_{opt}(r)$ is a short-range complex optical potential of the $\bar{p}$-nucleus interaction, and $\mathrm{Im}U_{opt}(r) \leq 0$
that has to be taken into account for s and p-states.
For $l \geqslant 2$: $U_{opt}(r)$ is negligible, $h \Rightarrow h_0$, eigenfunctions $\phi_{nlm}(\mathbf{r})$ and eigenvalues $e_n = -\mu Z^2/2n^2$ of h are hydrogen-like.
For s and p-states: eigenvalues are complex, $E_{nl} = e_n + \Delta E_{nl}$, where $\Delta E_{nl} = -\epsilon_{nl} - \mathrm{i}\Gamma_{nl}/2$. Eigenfunctions $\phi_{nlm}(\mathbf{r})$ are in general differ from hydrogen-like.

Coupled channels approach:

Basis for close-coupling expansion:

$$\Phi_j(\mathbf{r},\Omega_R) = (\phi_{nl}(\mathbf{r}) \otimes Y_L(\Omega_R))_{JM}\,,$$

where L and J are relative and total angular momenta.

Total wave function: $\Psi_i(\mathbf{R},\mathbf{r}) = \sum_j \Phi_j(\mathbf{r},\Omega_R)\psi_{ji}(R)/R$,
where i is a number of an incoming channel

System of coupled-channel equations:

$$\psi''_{ji}(R) + \left[k_j^2 - L_j(L_j+1)/R^2\right]\psi_{ji}(R) = 2m\sum_k V_{jk}(R)\psi_{ki}(R)$$

$$k_j^2 = \begin{cases} 2m(E-e_n) & \text{if } l_j \geqslant 2\,(\text{real } k_j), \\ 2m(E-e_n+\epsilon_{nl}+\frac{\mathrm{i}}{2}\Gamma_{nl}) & \text{if } l_j \leqslant 1\,(\mathrm{Im}\,k_j > 0). \end{cases}$$

BOUNDARY CONDITIONS:

$$\psi_{ji}(R) \xrightarrow[R\to 0]{} 0,$$

$$\psi_{ji}(R) = 0 \text{ at } l_i \leqslant 1, \text{ all } j, \text{ any } R$$

$$\psi_{ji}(R) \xrightarrow[R\to\infty]{} \begin{cases} \frac{\delta ij}{\sqrt{k_i}} \exp[-i(k_i R - L_i \pi/2)] - \frac{1}{\sqrt{k_j}} \exp[i(k_j R - L_j \pi/2)] S_{ji} \\ \text{at } l_j, l_i \geqslant 2 \\ \\ -\frac{1}{\sqrt{k_j}} \exp[i(k_j R - L_j \pi/2)] \sim \exp[-\mathrm{Im}(k_j R)] \\ \text{at } l_j \leqslant 1, l_i \geqslant 2 \end{cases}$$

(standard conditions in the channels with $l_j, l_i \geqslant 2$, but in the channels with $l_j \leqslant 1, l_i \geqslant 2$ $\psi_{ji}(R) \to\sim \exp(-\mathrm{Im}(k_j)R)$, and $\psi_{ji}(R) = 0$ at $l_i \leqslant 1$)

In order to solve close-coupling equations with the above-mentioned boundary conditions, we divide the total space of N channels into the subspace α of the stationary states ($l \geq 2$) and the subspace β of the annihilating states ($l = 0, 1$) and construct two types of the ($N \times N$) matrix solutions $X(r)$ and $Y(r)$, which are defined by the asymptotic forms at $r \to \infty$: $X_{ji}, Y_{ji} \to 0$ at $i \neq j$, X_{ii} and Y_{ii} at $i \in \alpha$ tend to ordinary incoming and outgoing waves, whereas at $i \in \beta$ $X_{ii}(R) \equiv 0$, and $Y_{ii}(R)$ tends to *damping* outgoing wave. Total matrix of solutions with the correct asymptotic behaviour is

$$F(r) = [X(r) - Y(r)C].$$

At a small $r = r_s$ it has to be sewed with the ($N \times N$) matrix of regular solutions $U(r)A$, where $U(r)$ is obtained by a standard way with account for the complex energy shifts in the annihilating channels, and A is an arbitrary matrix.

This procedure yields the $(N \times N)$ matrix

$$C = \begin{pmatrix} C_{\alpha\alpha} & 0 \\ C_{\beta\alpha} & 0 \end{pmatrix}$$

The submatrix $C_{\alpha\alpha} = S$ is the S-matrix of the transitions between the states in the subspace α, whereas other elements $(C_{\beta\alpha})$ don't have a real physical meaning.

The S-matrix is not unitary, because the hamiltonian of the problem is non-hermitian. The 'unitary defect'

$$(1 - \sum_{j \in \alpha} |S_{ji}|^2)$$

might be used to obtain the cross section of induced annihilation for the initial state $i \in \alpha$.

EXAMPLE OF APPLICATION:

Stark transitions and annihilation in collisions $(\bar{p}\mathrm{He}^{++})_{nl} + \mathrm{He}$ at $E \sim 10$ K

Potential $V(\mathbf{R}, \mathbf{r})$ can be calculated by quantum-chemistry methods. But in our problem: $\langle r \rangle \sim n^2/\mu \sim 0.3$, $R_{eff} \gtrsim 1$ a.u., $\therefore$

$$V(\mathbf{R}, \mathbf{r}) \simeq V_0(R) + (\mathbf{d} \cdot \nabla_{\mathbf{R}}) V_0(R) + \ldots$$

$V_0(R)$ is an adiabatic potential of interaction between He atom and single positive charge of the ion, $\mathbf{d}$ is a dipole operator of $(\bar{p}\mathrm{He}^{++})$ that can mix nl states.

Analytical approximation of the numerical potential (J.Russel, J.Cohen):

$$V_0(R) = V_M(R) + V_p(R),$$

$$V_M(R) = D_0\left(\exp[-2\beta(R - R_e)] - 2\exp[-\beta(R - R_e)]\right) \text{ (Morse)},$$

$$V_p(R) = -\frac{\alpha}{2R^4}[1 - \exp(-\gamma(R - R_e)^4] \text{ at } R > R_e$$

(polarization long-range interaction)

Parameters:

$D_0 = 0.075$, $R_e = 1.46$, $\beta = 1.65$, $\alpha = 1.383$, $\gamma = 0.005$ a.u.

For ns- and np-states:

$$\Delta E_{ns} = \Delta E_{1s}/n^3, \quad \Delta E_{np} = \Delta E_{2p} \cdot \frac{32(n^2-1)}{3n^5}$$

For $\bar{p} -^4$ He:

$$\Gamma_{1s} \simeq 11\,\mathrm{keV}, \quad \Gamma_{2p} \simeq 36\,\mathrm{eV}, \quad \epsilon_{nl} \simeq 0.3\Gamma_{nl}$$

Some technical details of the numerical solution of the system of differential equation:

♦ The solutions $X(R)$ and $Y(R)$ are taken in the asymptotic form (i.e., are reduced to Hankel-Riccatti function) for 'normal' channels at $R > 150$ a.u.

Matrix elements of channel coupling

$$V_{jk}(R) = \langle \Phi_j(\mathbf{r}, \Omega_R) | V(\mathbf{R}, \mathbf{r}) | \Phi_k(\mathbf{r}, \Omega_R) \rangle$$

are taken into account

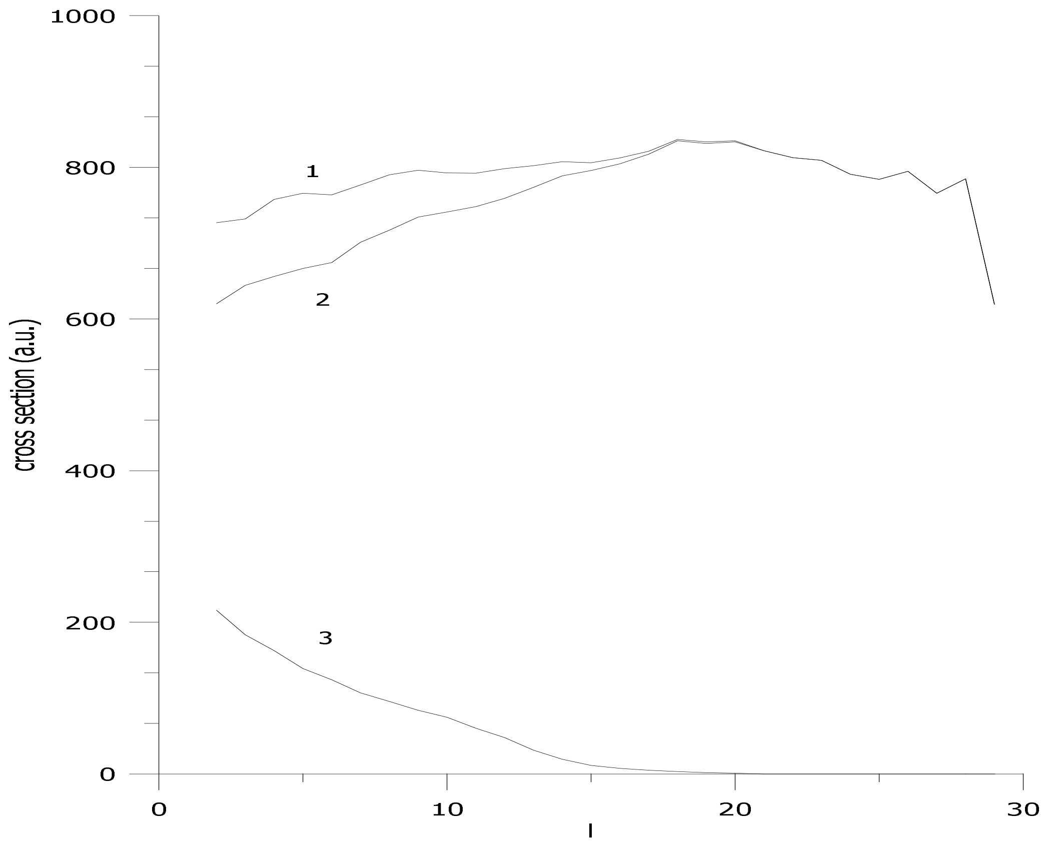
♦ up to $R = 150$ a.u. for $l_j, l_k \geqslant 2$,

♦ up to $R = 10$ a.u. for (l_j, l_k) =(1, 2) or (2, 1), and up to $R = 5$ a.u. for (l_j, l_k) =(0, 1) or (1, 0), because of large complex energy shifts as compare with $V_{jk}(R)$ at these distances.

♦ In addition, the matrix elements $V_{jk}(R)$ are calculated with H-like wave functions for all the states, because the wave functions of the annihilating states are disturbed by a strong interaction only at very small distances ($\sim 10^{-13}$ cm).

Note: Jensen& Markushin supposed $\Gamma_{nl} = 0$ at $R > R_0$. Instead, we have $V_{\alpha\beta}(R) \to 0$ at some R.

Dependence of total Stark and induced annihilation cross section on initial state ($n = 30$, $E = 10K$)



1 - σ_{St} without annihilation, 2 - σ_{St} with account for annihilation, 3 - σ_{annih}

CONCLUSION

♦ We have formulated extended quantum close-coupling method with account for short-lived (annihilating) states in the basis set with correct asymptotic conditions in the annihilating channels.

♦ The method is applied to calculations of Stark transition and induced annihilation in the collisions $(\bar{p}\mathrm{He}^{++})_{nl} + \mathrm{He}$ at $E \sim 10$ K

♦ This approach can be applied to collisions of many other hadronic atoms with ordinary atoms in media