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Positron-Matter Collisions

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This work supported by the Robert A. Welch Foundation

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Low-Energy Positron Scattering

- Isolated collision between one target (atom or molecule) and one positron of known kinetic energy
- Only elastic scattering—stay below the energy threshold for electronic excitation of the target or for real positronium formation
- Local, energy-independent interaction potential based on physically-motivated approximations

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Scattering Formulation

Consider the time-independent Schrödinger equation (T.I.S.E.) for an N-electron target and a colliding positron

$$\hat{\mathcal{H}}\,|\Psi> \;=\; E\,|\Psi>$$

where,

$$\hat{\mathcal{H}} \;=\; \hat{\mathcal{H}}_t + \hat{T}_p + \hat{V}_{int},$$

with,

- $\hat{\mathcal{H}}_t \;\equiv\;$ N-particle Target Hamiltonian,
- $\hat{T}_p \;\equiv\;$ K.E. operator for the positron, and
- $\hat{V}_{int} \;\equiv\;$ positron–Target interaction operator.

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Reduction of Scattering Formulation

We "reduce" the problem by expanding the (N+1)-particle ket in a complete set of target and scattering states, viz.

$$|\Psi> = \sum\!\!\!\!\!\!\!\int_{\gamma} F_{\gamma}\Phi_{\gamma}.$$

Using this expansion in the T.I.S.E. and operating on the left with $<\Phi_0|$ eventually leaves the one-particle T.I.S.E. for elastic scattering of the positron

$$\hat{T}_p|F_0> - \frac{k^2}{2}|F_0> = -\hat{V}_{sp}|F_0> .$$

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Interaction Potential

A local approximation to the interaction potential between a colliding positron and the molecular target can be represented as

$$V_{sp}(\vec{r}_p) \;=\; V_{st}(\vec{r}_p) \;+\; V_{pol}(\vec{r}_p),$$

where the static potential is given by,

$$V_{st}(\vec{r}_p) \;=\; \left\langle \Phi_0(\vec{r_i}) \left| \hat{V}_{int} \right| \Phi_0(\vec{r_i}) \right\rangle,$$

with $\hat{V}_{int}$ representing the Coulomb interactions between the positron and the target and where $V_{pol}(\vec{r}_p)$ is the polarization potential.

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Polarization Potential

The polarization potential is defined as the energy difference

$$V_{pol}(\vec{r}_p) \; = \; E^R(\vec{r}_p) - E^U(\vec{r}_p),$$

where the energy from the relaxed (distorted) target orbitals is

$$E^R(\vec{r}_p) \; = \; \left\langle \Phi^R(\vec{r}_i;\vec{r}_p) \left| \hat{\mathcal{H}}_t + \hat{V}_{int} \right| \Phi^R(\vec{r}_i;\vec{r}_p) \right\rangle_{d\vec{r}_i},$$

and the energy from the unrelaxed (ground state) orbitals is

$$E^U(\vec{r}_p) \; = \; \left\langle \Phi^U_0(\vec{r}_i) \left| \hat{\mathcal{H}}_t + \hat{V}_{int} \right| \Phi^U_0(\vec{r}_i) \right\rangle_{d\vec{r}_i}.$$

In the adiabatic approximation, both $E^U(\vec{r}_p)$ and $E^R(\vec{r}_p)$ are calculated by treating the projectile as an additional "proton" (located at $\vec{r}_p$) and using an LCAO:MO—SCF Quantum Chemistry code to provide variational estimates of these energies.

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Nuclear Attraction Integrals

The distortion of the molecular orbitals is driven by the nuclear attraction integrals that involve the positron as an additional "nucleus" at $\vec{r}_p$.

$$I_{i,j}^{NAI} = \langle \alpha_i(\vec{r}_e) \left| V(\vec{r}_e; \rho_{pos}) \right| \beta_j(\vec{r}_e) \rangle ,$$

where the interaction V from a distribution of positive charge ρ_{pos} is given as

$$V(\vec{r}_e; \rho_{pos}) = \int d\vec{r}\, \rho_{pos}(\vec{r})\, \frac{-1}{|\vec{r}_e - \vec{r}|}.$$

For the adiabatic approximation, $\rho_{pos}(\vec{r}) = \delta(\vec{r} - \vec{r}_p)$, which is appropriate for the positive charge distribution in a virtual H atom.

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Virtual Positronium

The adiabatic approximation leads to a polarization potential that is much too attractive in the near-target region. The problem is that since the positron and electron have equal masses, the distribution of positive charge in a virtual Ps atom is not the same as the distribution of positive charge in a virtual H atom (see the figure on the following page). We can approximate the effect of this difference on the polarization potential by replacing the delta function distribution of positive charge in the nuclear attraction integrals involving the positron with one that is more nearly correct for virtual Ps. Thus, we refer to this scheme as the Distributed Positron Model (DPM).

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Ps C.O.M. Figure

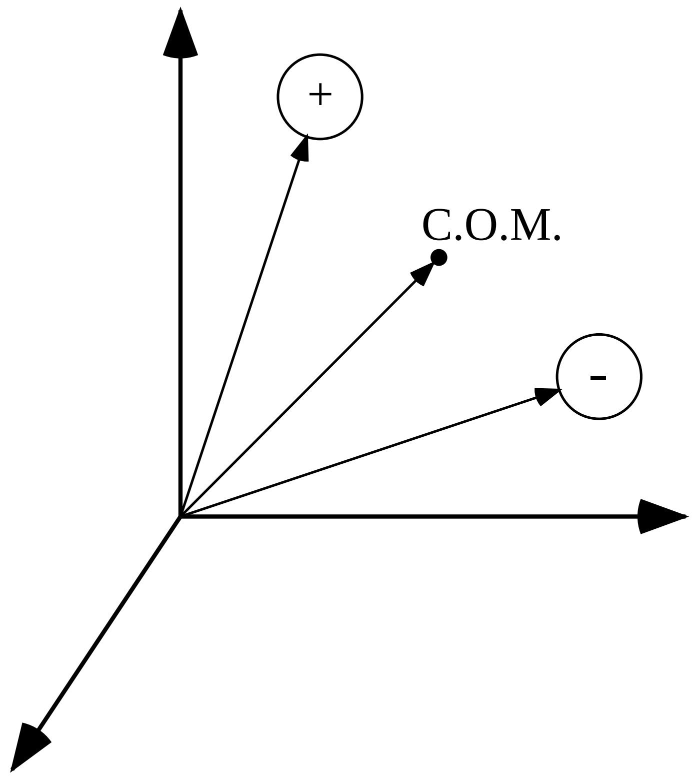

Figure 1: Unlike the H atom, the positive charge in the Ps atom is not localized at the C.O.M. of the atom.

The Distributed Positron Model

We have investigated several simple choices of ρ_{pos} that reflect the distribution of positive charge in a Ps atom and lead to a polarization potential that reduces to the correct long-range behavior of the polarization potential, including:

- Uniform Spherical
  - $R_p = 1.5$ Bohr (Average radius of Ps atom)
  - $R_p = 1.0$ Bohr (Maximum radial probability of Ps atom)
- H1S distribution
- STO-3G distribution

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DPM Figure

For specificity, consider the following case:

- Diatomic target with nuclei at $\vec{A}$ and $\vec{B}$
- Additional "nucleus" (positron) with charge distribution ρ_{pos} located at $\vec{C} \equiv \vec{r}_p$

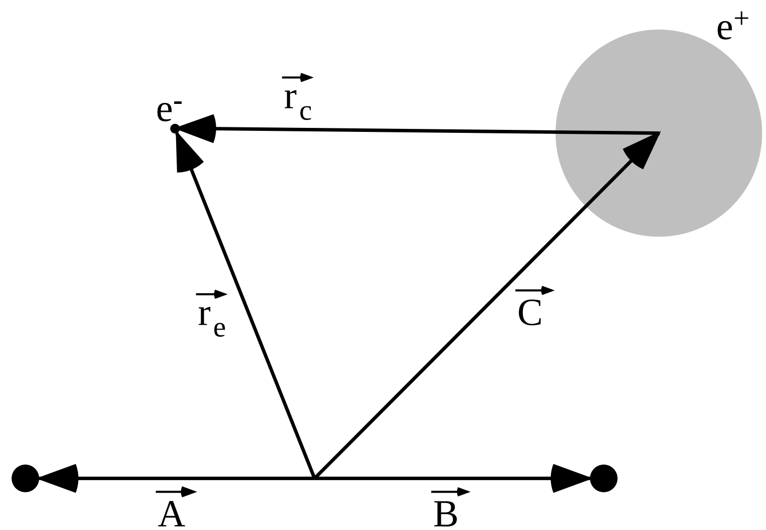

Figure 2: A distribution of positive charge simulates the effect of virtual Ps formation in the DPM.

DPM Distortion Interaction Figure

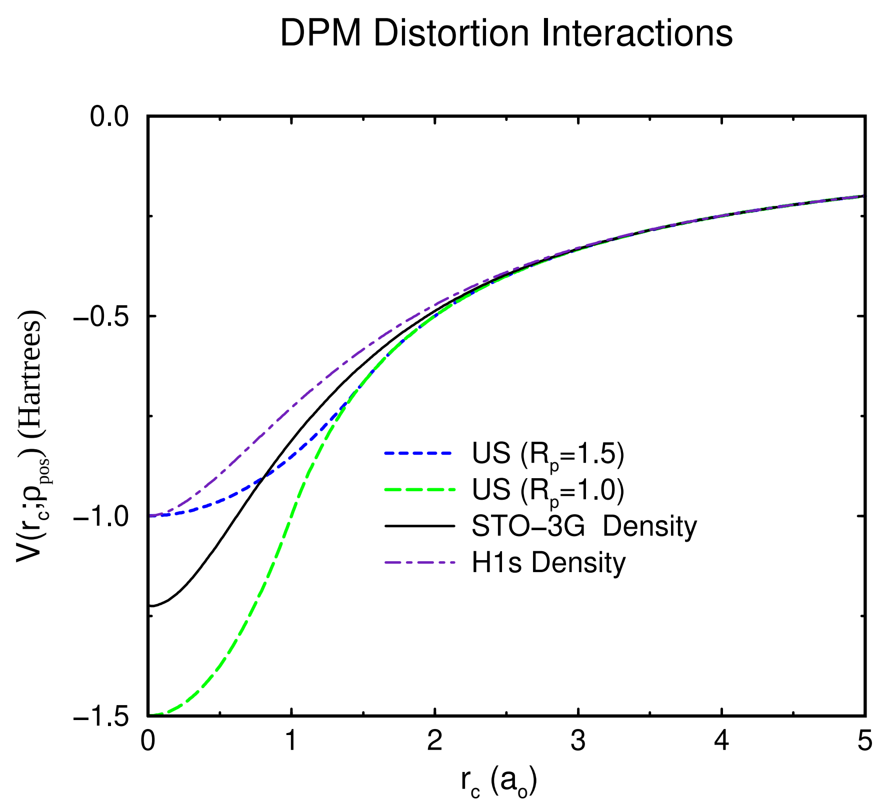

Figure 3: The distortion interaction $V(\vec{r}_c;\rho_{pos})$ for various choices of ρ_{pos} in the DPM.

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Computing the Interaction Potential

Our method of calculating the polarization component of the positron-matter interaction potential involves fixing the positron at a large number of points near the target and then running a variational estimate of the system energy for each of these points. Since most of the required integrals change with the location of the positron and since the number of points required to provide a smooth interpolation of the polarization potential runs from 100's for atoms or linear molecules to 1000's for non-linear molecules, a substantial amount of computer resources is required. Even though we had written our own highly-optimized suite of codes (PATMOL) to perform these operations, larger systems, such as SF_6, remained out of reach.

- **Larger Systems $\Longrightarrow$ More CPU Time**
  - Time to compute V_{pol} for Ar: 12 minutes (serial code)
  - Time to compute V_{pol} for SF_6: 125 days (estimated)
- **Larger Systems $\Longrightarrow$ More Memory**
- **Larger Systems $\Longrightarrow$ More I/O**

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Solution—Concurrent Computing

- **Beowulf Cluster**
  - Performance: 100's to 1000's of Megaflops
  - Memory: Gigabytes
  - I/O: Distributed Across Multiple Nodes
  - **Very** Affordable Hardware
  - Standard Software Available for Free
  - Local Control
    * Configuration Optimized for Problem
    * No Sharing Required

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Beowulf Quote

What is a Beowulf Cluster?

> Beowulf is a project to produce the software for off-the-shelf clustered workstations based on commodity PC-class hardware, a high-bandwidth internal network, and the Linux operating system.
> —*Donald Becker*

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The PATMOL Codes

A Quantum Chemistry Program Suite
written by
Patrick J. Nichols
Texas Tech University

PATMOL is a suite of programs written in C and C++ that we now use to compute polarization potentials for positron-molecule scattering calculations. These codes have the following features:

- A user-friendly interface
- Use of point group symmetry
- An integrals package based on the methods of McMurchie-Davidson [JCP **26**, 218-31 (1978)]
- A properties package
- Serial and Concurrent (MPI) versions

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