Calculation of Z_{eff} using the SMC method with an optical potential

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The annihilation of positrons with molecules has been a source of major studies in the past years. The high annihilation rates encountered in the experimental data are still puzzling. Many models have been proposed to explain the phenomenon, but up to date none have given a completely satisfactory explanation [1].

The Schwinger Multichannel Method was originally created to calculate the low energy electron scattering by molecules [2], being later adapted for positron scattering and for the calculation of the annihilation parameter (Z_{eff}) [3]. The success obtained for the differential (DCS) and integral cross section (ICS) was not followed on the calculation of Z_{eff} [4]. This can be explained by two major reasons: the SMC method is a variational method for the scattering amplitude (and therefore for the calculation of the ICS and DCS), but not for the Z_{eff} parameter. The other reason is that it uses Cartesians Gaussians as basis set on the expansions of the bound and continuum molecular orbitals. These are smooth functions and do not reproduce the "cusp" always present in virtual positronium states.

In an attempt to better understand the high values found for the Z_{eff}, an optical potential initially proposed by Ivanov and Mitroy and later applied by Igarashi *et al.* [5] was included in the SMC method in order to make the calculation of the annihilation parameter variationally stable. In this work, the potential will be described and the first results obtained for the Helium atom and the Hydrogen molecule will be shown [6]. A basis set study for the He atom will be presented as a way to obtain the functions that could better reproduce the behavior encountered in the calculation of the Z_{eff}.

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