Localization of electrons in liquid parahydrogen from Density Functional calculations.

F. Ancilotto^a, M. Barranco^b, J Navarro^c, and M. Pi^b

 $^a\mathrm{Dipartimento}$ di Fisica 'G. Galilei', Universita' di Padova, via Marzolo 8, I-35131 Padova, Italy and CNR-IOM-Democritos, I-34014 Trieste, Italy

^bDepartament ECM, Facultat de Fisica, and IN2UB, Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain

 $^c \rm IFIC$ (CSIC University of Valencia) Apartado 22085, 46071 Valencia, Spain

We have developed a finite-temperature density functional approach to describe the properties of parahydrogen (pH_2) in the liquid-vapor coexistence region. Our scheme is based on a finite-range free density functional which, while it is fitted to reproduce bulk pH_2 properties only, it is shown to yield liquid-vapor interface properties in good agreement with experiments in the whole temperature range from the triple point to near the critical point. We have studied the localized states of electrons in liquid pH_2 using a suitable representation for the electron-hydrogen interaction potential. The effect of electrons as seeds of heterogeneous cavitation is also investigated.