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PIMC Simulation of Thermal Dissociation of Dipositronium

ILKKA KYLÄNPÄÄ, TAPIO RANTALA¹, Department of Physics, Tampere University of Technology, P.O.Box 692, FI-33101 Tampere, Finland — Positronium is a hydrogen atom like pair of a positron and an electron, and correspondingly, dipositronium is a four-particle molecule formed by two positronium atoms. Stability of the dipositronium molecule was established by Hylleraas in 1947 [1], already, but not experimentally observed until recently [2]. This system of four light particles sets challenges for both theoretical and experimental consideration and in finite temperature, in particular. The experimental observations are based on the observation of positronium decay rate and the changes related to dipositronium formation or dissociation. The finite-temperature modeling of such light quantum particles has to be done fully nonadiabatically, that we have accomplished with the Path-Integral Monte Carlo (PIMC) method for the thermal equilibrium. As the dissociation energy of dipositronium is about 0.4 eV, the recent observation of the thermal activation energy of about 0.07 eV was interpreted to follow from the experiment related desorption process [2]. With our quantum statistical simulation we show, however, that the observed low energy obviously relates to the dissociation of the molecule, directly. [1] Hylleraas, E.A. and Ore A., Phys. Rev.71, 493 (1947). [2] Cassidy D.B. and Mills A.P. Jr., Nature 449, 195 (2007).

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