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Two-electron R-matrix approach to calculations of potential-energy curves of long-range Rydberg molecules[1] MICHAL TARANA, ROMAN ČURíK, Academy Sci of the Czech Rep — We introduce a computational method developed for study of long-range molecular Rydberg states of such systems that can be approximated by two electrons in a model potential of the atomic cores [1]. The method is based on a two-electron R-matrix approach inside a sphere centered on one of the atoms. The wave function is then connected to a Coulomb region outside the sphere via a multichannel version of the Coulomb Green's function. This approach is applied to a study of Rydberg states of Rb_2 for internuclear separations R from 40 to 320 bohrs and energies corresponding to n from 7 to 30. We report bound states associated with the low-lying $^3P^o$ resonance and with the virtual state of the rubidium atom that turn into ion-pair-like bound states in the Coulomb potential of the atomic Rydberg core. The results are compared with previous calculations based on single-electron models employing a zero-range contact-potential [2] and short-range modele potential [3]. [1] M. Tarana and R. Čurík, Phys. Rev. A 93, 012515 (2016). [2] C. H. Greene, A. S. Dickinson, and H. R. Sadeghpour, Phys. Rev. Lett. 85, 2458 (2000). [3] A. A. Khuskivadze, M. I. Chibisov, and I. I. Fabrikant, Phys. Rev. A 66, 042709 (2002).

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