

## Effect of Quantum Fluctuations on the Binding Nature of Three- and Four-body Coulomb systems

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In treatment of the ground-state properties of atoms and molecules, we usually resort to the adiabatic (AA), assuming electrons to respond instantaneously to the change in positions of nuclei. Because their mass ratio is larger than one thousand, AA approximation succeeds in the prediction of the ground-state property. However, it does not work for the complex systems such as an excitonic molecule or a dipositronium. In such cases, quantum fluctuations of counterparts, holes or positrons, of electrons are so large that electrons no longer lock on them. The purpose of this study is to investigate when and how the breakdown of AA caused by quantum fluctuations.

The three- and four-body Coulomb systems composed of one or two “electrons  $m^-$ ” and two “protons  $M^+$ ” are appropriate to study this purpose. Varying the mass ratio  $m/M$  from zero to unity, these systems show the change from hydrogen-molecule-like to dipositronium-like systems due to the enhancement of quantum fluctuations of protons. We can calculate accurately the ground-state of these systems with the diffusion Monte Carlo (DMC) which fully incorporates quantum fluctuations of all the constituent particles. The result of DMC shows the existence of the stable bound states for the entire mass ratio. On the other hand, that of AA deviates from DMC’s for  $m/M > 0.1$  and no longer provides a bound state for  $m/M > 0.2$ . Our calculation shows that the kinetic energy of protons in AA increases monotonically but that in DMC stops increasing with  $m/M$  increasing. From the comparison of the pair-distribution of protons,  $g_{pp}(r)$ , it is found that the poor description of the effective potential between protons  $V_{pp}(r)$  causes the breakdown of AA.  $V_{pp}(r)$  derived from  $g_{pp}(r)$  in DMC is shallower than in AA, and then it suppresses the increase in the kinetic energy of protons with increase of  $m/M$ . The difference of  $V_{pp}(r)$  between DMC and AA indicates the manifestation of the non-adiabaticity.

The binding properties of the three- and four-body systems are almost the same. We will discuss how to overcome AA and incorporate the non-adiabaticity to the three-body systems.