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Beyond the Born-Oppenheimer approximation with quantum Monte Carlo NORM TUBMAN, University of Illinois - Urbana Champaign, ILKKA KYLANPAA, Tampere University of Technology, SHARON HAMMES-SCHIFFER, DAVID CEPERLEY, University of Illinois - Urbana Champaign — We develop tools that enable the study of non-adiabatic effects with variational and diffusion Monte Carlo methods. We introduce a highly accurate wave function ansatz for electron-ion systems that can involve a combination of both clamped ions and quantum nuclei. We explicitly calculate the ground state energies of H_2, LiH, H_2O and FHF^- using fixed-node quantum Monte Carlo with wave function nodes that explicitly depend on the ion positions. The obtained energies implicitly include the effects arising from quantum nuclei and electron-nucleus coupling. We compare our results to the best theoretical and experimental results available and find excellent agreement.

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