

Abstract Submitted
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Dipole moment of ultra-cold polar molecules: A quantum Monte Carlo study SHI GUO, LUBOS MITAS, North Carolina State University — There has been recently a great interest in the ultra-cold heteronuclear molecules that have a large electric dipole moment interaction both theoretically and experimentally. In this work, we calculate the dipole moment of a two-atom alkaline molecule, LiSr. We use two approaches: the configuration interaction and the quantum Monte Carlo method. We take the wavefunction calculated by configuration interaction and add the correlated terms, optimize the wavefunction to get a good candidate for Quantum Monte Carlo calculation. In order to reach a better accuracy for dipole moment, not only a diffusion Monte Carlo but a repetition Monte Carlo method is also implemented to better treat the quantity which does not commute with the Hamiltonian. We are also trying to evaluate the modifications coming from the spin orbit coupling term using quantum Monte Carlo method

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