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Novel Exciton States in Monolayer MoS_2: Unconventional Effective Hamiltonian FELIPE DA JORNADA, DIANA QIU, STEVEN LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Recent well-converged ab inito GW-BSE calculations show that monolayer MoS_2 has a large number of strongly bound excitons with varying characters. We show that these excitonic states cannot be even qualitatively described by an effective mass hydrogenic model without a detailed understanding of the 2D screening. Additionally, we identify and analyze one exciton series having an unusually high binding energy, which originates around the Γ point of the Brillouin zone. We show that this excitonic series arises from a fundamentally different effective Hamiltonian with a kinetic energy term resembling a Mexican hat in momentum space, which is responsible for the unusual ordering of the energy levels and distribution of oscillator strength. This work was supported by NSF grant No. DMR10-1006184 and the U.S. DOE under Contract No. DE-AC02-05CH11231.

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