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Exciton band structure of monolayer MoS_2 FENGCHENG WU, Department of Physics, University of Texas at Austin, FANYAO QU, Department of Physics, University of Texas at Austin; Instituto de Física, Universidade de Brasília, ALLAN MACDONALD, Department of Physics, University of Texas at Austin — We describe a theory of the momentum-dependent exciton spectrum of monolayer molybdenum disulfide. Low-energy excitons occur both at the Brillouin zone center and at the Brillouin-zone corners. We find that binding energies at the Brillouin-zone center deviate qualitatively from the $(n-1/2)^{-2}$ pattern of the two-dimensional hydrogenic model. Moreover, the four $2p$ states of A series are lower in energy than the corresponding $2s$ states and not degenerate. The two-fold ground-state valley degeneracy is lifted linearly at small momenta by electron-hole exchange processes that establish inter valley coherence. We conclude that atlhough monolayer MoS_2 is a direct-gap semiconductor when classified by its quasiparticle band structure it may well be an indirect gap material when classified by its excitation spectra, and speculate on the role of this property in luminescence characteristics.

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