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Nonanalyticity, Valley Quantum Phases, and Massless Excitons in Monolayer Transition Metal Dichalcogenides¹ DIANA Y. QIU, TING CAO, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — Exciton dispersion as a function of center-of-mass momentum \mathbf{Q} is essential to the understanding of exciton dynamics, relaxation, and condensation. We use the ab initio GW-Bethe-Salpeter equation (GW-BSE) method to calculate the dispersion of excitons in monolayer MoS₂ and find a nonanalytic lightlike dispersion. This behavior arises from the interplay of an unusual $|Q|$ -term in both the intra- and intervalley exchange of the electron-hole interaction, which concurrently gives rise to a valley quantum phase of winding number two. We have derived a simple, effective Hamiltonian and analytic solutions, which quantitatively describe this physics, and we predict that signatures of this unusual dispersion can be measured with a linearly polarized optical beam tilted away from normal incidence. The existence of a nonanalytic exciton dispersion can be generalized to other 2D semiconductors with excitons whose amplitudes are localized in a small region of the Brillouin zone.

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