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Multiscale analytic calculation of valley splitting in silicon quantum wells.[1] SUCISMITA CHUTIA, SUSAN COPPERSMITH, MARK FRIESEN, University of Wisconsin-Madison — Valley splitting in Si/SiGe quantum wells is a central issue for Si based quantum dot quantum computers. The valley coupling arises due to the mixing of states at a sharp quantum well interface. The effective mass theory provides an essential tool for studying the valley splitting in various geometries. However, the magnitude of the splitting must still be determined microscopically, e.g., from atomistic theories. Here, we develop a multiscale theory that bridges the effective mass and atomistic approaches. Since the valley coupling occurs within just a few atomic layers of the interface, we splice a tight binding treatment of the interface into an effective mass treatment of the extended wavefunction. This multiscale theory yields analytical solutions for the valley splitting with no adjustable parameters.

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