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Theoretical interpretation of donor wavefunctions STM images in silicon[1] BELITA KOILLER, A. L. SARAIVA, RODRIGO B. CAPAZ, Instituto de Física, Universidade Federal do Rio de Janeiro, Brazil, M.J, CALDERÓN, ICMM-CSIC, Madrid, Spain, J. SALFI, B. VOISIN, J. BOCQUEL, S. ROGGE, Centre for Quantum Computation and Communication Technology, Sydney, Australia — Single dopant wavefunctions in Si have recently been probed by scanning tunneling spectroscopy, revealing localized patterns of resonantly enhanced tunneling currents. We show that the shapes of the conducting splotches resemble cuts through Kohn-Luttinger (KL) hydrogenic envelopes, which modulate the interfering Bloch states of conduction electrons. All the non-monotonic features of the current profile are consistent with the charge density fluctuations observed between successive {001} atomic planes, including a counter-intuitive reduction of the symmetry – a heritage of the lowered point group symmetry at these planes. A model-independent analysis of the diffraction figure constrains the value of the electron wavevector to $k_0 = (0.82 \pm 0.03)(2\pi/a_{\mathrm{Si}})$. Unlike prior measurements, averaged over a sizeable density of electrons, this estimate is obtained directly from isolated electrons. We further investigate the model-specific anisotropy of the wave function envelope, related to the effective mass anisotropy. This anisotropy appears in the KL variational wave function envelope as the ratio between Bohr radii b/a.

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