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Algorithm for extraction of quantum oscillation orbits from band structure data PATRICK ROURKE, STEPHEN JULIAN, University of Toronto — In determining the Fermi surface of a material, quantum oscillation measurements are often compared to band structure calculations. Each oscillation frequency corresponds to an electron (or hole) orbit on the Fermi surface, perpendicular to the applied magnetic field; only orbits enclosing areas that are locally extremal are detected. To facilitate comparisons between theory and experiment, we have developed an algorithm, "SKEAF," which finds extremal orbits in band structure calculations and determines quantum oscillation frequencies, effective masses and band specific heat contributions. Our code uses a k-space supercell approach, and can successfully locate geometrically-complicated orbits. Example results will be presented for the heavy fermion material UPt_3.

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