Canonical Quantization of Crystal Dislocation and Electron-Dislocation Scattering in an Isotropic Media MINGDA LI, MIT, WENPING CUI, Boston College, M. S. DRESSELHAUS, GANG CHEN, MIT, MIT TEAM, BOSTON COLLEGE TEAM — Crystal dislocations govern the plastic mechanical properties of materials but also affect the electrical and optical properties. However, a fundamental and decent quantum-mechanical theory of dislocation remains undiscovered for decades. Here we present an exact and manageable Hamiltonian theory for both edge and screw dislocation line in an isotropic media, where the effective Hamiltonian of a single dislocation line can be written in a harmonic-oscillator-like form, with closed-form quantized 1D phonon-like excitation. Moreover a closed-form, position dependent electron-dislocation coupling strength is obtained, from which we obtained good agreement of relaxation time when comparing with classical results. This Hamiltonian provides a platform to study the effect of dislocation to materials' non-mechanical properties from a fundamental Hamiltonian level.

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