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Calculation of the Vibrational Continuum in Helical Polymers from First Principles: Application to Single-walled Carbon Nanotubes HADLEY LAWLER, CARTER WHITE, Naval Research Laboratory, JOHN MINTMIRE, Oklahoma State University — A first-principles method for calculation of the full vibrational continuum in helical polymers is presented, with application to chiral single-walled carbon nanotubes. The dynamical matrix is calculated within a helical symmetry, utilizing a cylindrical basis for nuclear displacements. Sum rules within a helical symmetry, helical speeds of sound and helical flexure modes are addressed.

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