Bloch equations for carriers, phonons and excitons from first-principles many-body theory

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Starting from the first-principles Hamiltonian for electrons and phonons, we go through a series of well defined simplifications to derive a set of coupled equations of motion for the electronic occupations and polarizations, nuclear displacements as well as phononic occupations and coherences. These are the semiconductor electron-phonon equations (SEPE), sharing the same scaling with system size and propagation time as the Boltzmann equations. The SEPE treat coherent and incoherent degrees of freedom on equal footing, widen the scope of the semiconductor Bloch equations and Boltzmann equations, and reduce to them under additional simplifications. The new features of the SEPE pave the way for first-principles studies of phonon squeezed states and coherence effects in time-resolved absorption and diffraction experiments. The SEPE are suited to describe the coupled dynamics of carriers and phonons, but ignore excitonic effects. Current approaches to the exciton dynamics rely on model Hamiltonians depending on already screened electron-electron and electron-phonon couplings. We show that these approaches are affected by an overscreening of the electron-phonon interaction. We therefore extend the first-principles many-body theory underlying the SEPE, and show how to formulate excitonic Bloch equations (XBE) free from overscreening. The XBE describe the time-evolution of coherent, irreducible, and incoherent excitons during and after the optical excitation, and are applicable even beyond the linear regime.