I will discuss numerical analysis issues that arise in approximations of observables in quantum systems described by many-body Schroedinger equation. I will present quantitative error estimates for molecular dynamics observables compared with observables determined by the time-independent Schrödinger equation, including the case with crossing or nearly crossing electron potential surfaces that can yield large errors. The derivation combines mathematical stability analysis of eigenvalue problems with quantitative numerical Ehrenfest molecular dynamics computations of perturbations. This is a joint work with Håkon Hoel (KAUST), Ashraful Kadir (KTH), Mattias Sandberg (KTH) and Anders Szepessy (KTH). (Received January 28, 2014)