Quadrature scheme for higher-order energy derivative of density functional theory

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Abstract:
A knowledge of higher energy derivative facilitate determination of reaction path Hamiltonian, cubic force constant, quartic force constant, vibration-rotation interaction constant, vibrational anharmonic constants. Anharmonic effects are also relevant to thermochemistry and chemical kinetics. Even Density functional theory, which provides route to include electron-correlation in computationally inexpensive manner, becomes expensive for higher energy derivative calculation, as one need to take larger grid and derivative of the grid-weight. To decrease the computational error, we discuss the inherent problems with the available quadrature schemes and propose Hermite-polynomial interpolation based Gauss-Turan quadrature which uses self-associated orthogonal polynomial to generate grid weights and points. The proposed quadrature scheme will provide better polynomial degree of exactness than the current available ones.