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Maximizing the hyperpolarizability poorly determines the potential ROLFE PETSCHEK, TIMOTHY ATHERTON, JOSEPH LESNEFSKY, GREG WIGGERS, Case Western Reserve University — Increasing the non-linear response of materials to an electric field, characterized by quantities such as the first hyperpolarizibility β, is a mattter of importance for applications. We optimized the zero frequency β of a one-dimensional potential well containing a single electron by freely adjusting the shape of that potential. It is shown that with careful optimization the maximum hyperpolarizability converges quickly with increasing numbers of parameters in the potential to approximately 0.708951 of the proven upper bound. The Hessian of β at the maximum makes it clear that there is a very wide range of nearby, nearly optimal potentials: with several measures of differences between potentials, this Hessian has only two large eigenvalues with the others diminishing quickly. The optimum potentials are substantially different and more affected by small eigenvectors than the wavefunctions. Thus, wavefunctions are superior for describing the conditions that optimize the hyperpolarizability. Prospects for a concise description of the two important constraints on near-optimum potentials and wavefunctions are discussed.

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