Stochastic Evaluation of Multidimensional Integrals for Time-Dependent Perturbations to the Hamiltonian Operator for Electrons in Wurtzite III-Nitride Crystals

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Abstract

Two-body problems, such as electron-electron interactions, pose fundamental numerical challenges to first-principles modeling of charge transport in semiconductor crystals. One such example is the process of impact ionization, whereby high-energy electrons ionize bound valence charge. Applications include highly sensitive telecommunications systems, quantum cryptography, and the detection of biological pathogens. Calculations of the rate at which high-energy electrons initiate impact ionization events involve integration over 9 dimensions in momentum-space:

$$S_{II}(E) = \frac{1}{4\pi^2\hbar} \sum_{n_c n_v' n_c' n_c''} \sum_{G,G'} \iiint d^3k\, d^3k'\, d^3p' \left| M_{G,G'}(nk, n_v p; n_c' k', n_c'' p') \right|^2$$
$$\times \delta\left(E_{n_c}(k) + E_{n_v}(p) - E_{n_c'}(k') - E_{n_c''}(k'') \right)$$

The integrands, however, are sharply peaked, with non-zero contributions only along certain non-analytic manifolds. Even on such manifolds, the integrands exhibit significant variation, especially in the case of contributions from electronic states of comparable momentum. To date, successful calculations have been performed only by stochastic means, where the variance of the estimator for the integral is quite large, and only for crystals of cubic symmetry. In the present work, we discuss our stochastic evaluation of impact ionization rate in bulk wurtzite III-nitride semiconductor material, including statistical error analysis and stopping criteria.