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Extrapolation of elliptic eigenvalue calculations on the whole space by the virial theorem.

The calculations of eigenvalues of partial differential operators posed on the whole space are important in many applications. A typical model is the Schrodinger equation with various types of potentials in chemical physics where the eigenvalues are energy levels of an atom or molecule. The partial differential operator normally consists of sums of Laplacians signifying the quantized kinetic energy, and the potential energy operators can take various forms. The eigenvalues are then sums of the respective kinetic and potential energies. A common feature of these systems is that the kinetic and potential energy operators often have power law scaling properties such that the virial theorem is applicable. In this paper, we propose and prove extrapolation schemes that can be used to improve the accuracy of eigenvalue calculations by utilizing the virial theorem. Concrete data and examples from the finite element computation of the hydrogen atom and a quartic harmonic oscillator in three dimensions are illustrated.

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