FEAST Eigensolver for non-Hermitian Problems in Quantum Mechanics

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One can identify several instances of non-Hermitian problems in quantum mechanics. The perfectly matched layer (PML) technique or complex absorbing potentials can be used to approximate open boundary conditions for electron transport and nanoelectronics modeling. Complex band structure calculations give rise to non-Hermitian system matrices. A complex scaled Hamiltonian has also recently been proposed to compute quantum resonant states [1]. Currently these problems have few robust options for computing the eigen-decomposition.

Here, we propose to extend the capabilities of the FEAST eigenvalue algorithm and solver [2,3] for addressing the non-symmetric problem. The main computation behind the eigenvalue problem is transformed into solving a set of linear systems along a complex contour. Non-symmetric FEAST is capable of obtaining the imaginary eigenvalues in any given region of the complex plane as well as the right and left eigenvectors forming a bi-orthonormal basis [4,5]. This algorithm retains all computational benefits of the original Hermitian algorithm including parallelism and scalability.

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