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Iterative computation of band edge states for semi-conductor nano structures

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The so-called band edge states determine optical and electronical properties of semi-conductor nano structures. They can be computed from an eigenproblem where the eigenvalues are typically clustered and well at the interior of the spectrum. For computational purposes, the eigenproblem can also be reformulated via a spectral transformation such as folding of the operator. We study the robustness and performance of state-of-the-art iterative eigensolvers on large quantum dots and wires, focusing on variants of preconditioned CG, Lanczos, and Davidson methods. Preconditioning aspects are also addressed.