Splitting methods with complex coefficients for the Schrödinger equation in imaginary time

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An efficient method to compute the ground states of the Schrödinger equation is the propagation in imaginary time. In this work, we propose new splitting methods with complex coefficients in order to obtain higher order methods that cannot be achieved with classical splittings because of a problem that is analogous to integrating the heat equation backward in time - numerical instabilities occur for the computation of exp(hA), where A is the Laplacian and h > 0 for methods of order greater than two. Complex coefficients allow us to overcome this limitation. The study is complemented with numerical results.