Iterative diagonalization

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The Hilbert space dimension of a many-body system increases exponentially with the number of single-particle bases (e.g., number of lattice/chain sites). To keep the tensor size manageable, tensor-networks-based methods use various ways to truncate the Hilbert space.

Iterative diagonalization is such an approach. Let's consider a one-dimensional system having N sites. At the n-th iteration of iterative diagonalization, we diagonalize the Hamiltonian of the subsystem ranging from site 1 to site n. The N_{keep} (and a few more) lowest-lying energy eigenvalues and the corresponding eigenstates are kept to span the Hilbert space for the enlarged subsystem, ranging from site 1 to site $n+1$, to be treated at the next iteration.

Here we need to **keep all degenerate states whose energies are close to the truncation threshold.** So the actual number of kept states at an iteration can be larger than N_{keep}, hence "a few more". The closeness to the threshold is determined by the tolerance parameter `tol`, chosen in terms of numerical precision; the states separated within this tolerance are regarded as degenerate. The degeneracy often comes from physical symmetries, such as spin and particle-hole symmetries. If we keep only the part of the degenerate states, then the Hilbert space will not respect the symmetries anymore. This artificial symmetry breaking would lead to qualitatively wrong result. (Of course, we can discard the degenerate states altogether, rather than keeping them, which also preserves the symmetries.)

Exercise (a): Non-interacting tight-binding chain

In this Exercise, we implement iterative diagonalization codes for computing the ground-state energy of non-interacting spinless fermions on a tight-binding chain. Since it's non-interacting, we can compare the iterative diagonalization results with numerically exact single-particle calculations (namely, via `nonIntTB`). The Hamiltonian is given by

$$\hat{H} = \sum_{\ell=1}^{N-1} (-t_\ell \hat{c}_{\ell+1}^\dagger \hat{c}_\ell - t_\ell^* \hat{c}_\ell^\dagger \hat{c}_{\ell+1}),$$

where the chain has N sites and $\hat{c}_\ell^\dagger$ creates a particle at a site $\ell \in [1, N]$. Here we consider two different chain types (i) with uniform hopping amplitudes, $t_\ell = 1$, and (ii) with logarithmic hopping amplitudes, $t_\ell = 2^{-(\ell-1)/2}$. Compute the ground-state energies of both types for various chain lengths, $N = 2, 3, \cdots, 50$, and compare them the single-particle calculations. Use $N_{\mathrm{keep}} = 300$.