Notes on approximating a unitary matrix by a parameterized quantum circuit

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Reference unitary we want to approximate: U, for example a time step of a given quantum Hamiltonian H, i.e.,

$$U = \mathrm{e}^{-iH\Delta t}\,. \tag{1}$$

Goal:

$$\max_V \mathrm{Re}(\mathrm{Tr}[VU^\dagger]) \tag{2}$$

with V some Ansatz unitary, here: sequence of single and two-qubit gates (can be regarded as quantum circuit).

One can re-write Eq. (2) as follows: Let $\{|\psi_j\rangle\,, \mathrm{e}^{-\lambda_j}\}$ be a spectral decomposition of U, such that

$$U = \sum_j \mathrm{e}^{-\lambda_j}\,|\psi_j\rangle\,\langle\psi_j|\,. \tag{3}$$

Then the target function reads

$$\mathrm{Re}(\mathrm{Tr}[VU^\dagger]) = \sum_j \mathrm{Re}\left(\mathrm{e}^{\lambda_j}\,\langle\psi_j|\,V\,|\psi_j\rangle\right). \tag{4}$$

The states $|\psi_j\rangle$ can thus be interpreted as inputs to the quantum circuit V.