What we need for the sparse solver is

$$V\psi_0\,,\quad V^\dagger\psi_0\lambda = V^\dagger\psi_1\,. \tag{1}$$

Using the singular value decomposition of V,

$$V = ASB^\dagger \tag{2}$$

with A, B $N\times M$-matrices, and S a diagonal $M\times M$-matrix, it is enough for us to actually compute

$$\tilde\psi_0 = B^\dagger\psi_0\,,\quad \tilde\psi_1 = A^\dagger\psi_1 \tag{3}$$

as we can get from this information easily the desired terms.

The Schrödinger equation in the lead reads

$$\begin{gathered}\lambda H\psi_0 + V\psi_0 + \lambda V^\dagger\psi_1 = \\ \lambda H\psi_0 + AS\tilde\psi_0 + \lambda BS\tilde\psi_1 = 0\end{gathered} \tag{4}$$

or equivalently

$$H\psi_1 + V\psi_0 + \lambda V^\dagger\psi_1 = 0 \tag{5}$$

We can now insert in these equations

$$\begin{aligned}0 &= \lambda(A'A^\dagger\psi_0 + B'B^\dagger\psi_0 - A'A^\dagger\psi_0 + B'B^\dagger\psi_0)\\ &= \lambda(A'A^\dagger + B'B^\dagger)\psi_0 - A'\tilde\psi_1 - \lambda B'\tilde\psi_0\,,\end{aligned} \tag{6}$$

where A' and B' can be in principle arbitrary $N\times M$-matrices (useful choices are discussed below).

Eqs. (4) and (5) still contain the full ψ_0 and ψ_1, that we would like to replace with $\tilde\psi_0$ and $\tilde\psi_1$. Defining

$$\tilde H = H + A'A^\dagger + B'B^\dagger\,, \tag{7}$$

we can rewrite Eq. (4) as

$$\psi_0 = \frac{1}{\lambda}\tilde H^{-1}\left[\lambda B'\tilde\psi_0 + A'\tilde\psi_1 - AS\tilde\psi_0 - \lambda BS\tilde\psi_1\right]\,, \tag{8}$$

i.e. express ψ_0 in terms of $\tilde\psi_0$ and $\tilde\psi_1$. This equation is well-defined as long as $\tilde H$ is invertible. Inserting the 0 of Eq. (6) such has the function to regularize the inversion. H is Hermitian and as such has only real eigenvalues. In general, choosing $A' = iA$ and $B' = iB$ is therefore a good choice: $AA^\dagger$ and $BB^\dagger$ are nonzero on the lattice sites reached by V and $V^\dagger$ respectively. Adding something imaginary there is like adding a self-energy due to some sort of leads (I guess it's actually identical to the leads we discussed about last week). The inversion can thus only fail if there is an exact eigenstate in the lead, that is not touched by the hopping - this is a state that would correspond to a dispersionless band in the *whole* Brillouin zone (which is possible, see the various $S=1$-Dirac lattices recently). However, in this case scattering matrices are also supposed to fail. Hence, this insertion of 0 seems to be equivalent to scattering matrices.

There is some reason speaking against making this choice always: If one deals with real matrices only, staying in real arithmetics is typically 3-4 times faster than switching to complex arithmetics.

By multiplying Eq. (4) with $B^\dagger\tilde H^{-1}$ from the right, and Eq. (5) with $A^\dagger\tilde H^{-1}$ from the right, we finally obtain a generalized eigenproblem for $\tilde\psi_0$ and $\tilde\psi_1$ only:

$$\begin{pmatrix}B^\dagger\tilde H^{-1}A\,S & -B^\dagger\tilde H^{-1}A'\\ A^\dagger\tilde H^{-1}A\,S & 1 - A^\dagger\tilde H^{-1}A'\end{pmatrix}\begin{pmatrix}\tilde\psi_0\\ \tilde\psi_1\end{pmatrix} = \lambda\begin{pmatrix}B^\dagger\tilde H^{-1}B' - 1 & -B^\dagger\tilde H^{-1}B\,S\\ A^\dagger\tilde H^{-1}B' & -A^\dagger\tilde H^{-1}B\,S\end{pmatrix}\begin{pmatrix}\tilde\psi_0\\ \tilde\psi_1\end{pmatrix} \tag{9}$$

This equation is a $2M\times 2M$ generalized eigenvalue problem. The reduction in size is thus not only necessary for our sparse solver, but can also result in a very considerable speedup.