Linear Method as Used in VQE's

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1 Real Eigenvalues

This derivation shows that if you have a generalized eigenvalue equation of the form $Av = Bv\lambda$, where both A and B are Hermitian and B is postive definite. Then the eigenvalues will be real. First all the steps will be shown mathematically and then some comments will be given on certain steps.

This is the generalized eigenvalue equation which we aim to solve:

$$\underline{\boldsymbol{A}}\boldsymbol{v} = \underline{\boldsymbol{B}}\boldsymbol{v}\Lambda \tag{1}$$

First we do a spectral decomposition of B into the eigenvalues of matrix B and the eigenvectors.

$$B = \Phi_B \Lambda_B \Phi_B^T \tag{2}$$

Then we define the following three expressions:

$$\Phi_B^{'} = \Phi_B \Lambda^{-1/2} \tag{3}$$

$$\Phi_B^{'T} = \Lambda^{-1/2} \Phi_B^{-1} \tag{4}$$

$$A^{'} = \Phi_B^{'T} A \Phi_B^{'} \tag{5}$$

Similarly to what we did in formula 2 for B we also decompose this new A' matrix into its eigenvalues and eigenvectors.

$$A^{'} = \Phi_{A'} \Lambda_{A'} \Phi_{A'}^T \tag{6}$$

Rewriting this gives that the the eigenvalues are:

$$\Lambda_{A'} = \Phi_{A'}^T A' \Phi_{A'} \tag{7}$$

Filling in the definition of A'

$$\Lambda_{A'} = \Phi_{A'}^T \Phi_B^{'T} A \Phi_B^{'} \Phi_{A'} \tag{8}$$

Now we define:

$$\Phi = \Phi_B^{'} \Phi_{A'} \tag{9}$$

which results in:

$$\Lambda_{A'} = \Phi^T A \Phi \tag{10}$$

It can be shown that the following expression is equal to the identity. This will be shown in formula 12 until 16. It makes use of substitions of previous expressions.

$$\Phi^T B \Phi = I \tag{11}$$

$$\Phi^T B\Phi = \Phi_{A'}^T \Phi_B'^T B \Phi_B' \Phi_A' \tag{12}$$

$$= \Phi_{A'}^T \Lambda_B^{-1/2} \Phi_B^T B \Phi_B \Lambda_B^{-1/2} \Phi_{A'} \tag{13}$$

$$= \Phi_{A'}^T \Lambda_B^{-1/2} \Phi_B^T \Phi_{B B} \Phi_B^T \Phi_B \Lambda_B^{-1/2} \Phi_{A'} \tag{14}$$

$$= \Phi_{A'}^T \Lambda_B^{-1/2}{}_B \Lambda_B^{-1/2} \Phi_{A'} \tag{15}$$

$$= \Phi_{A'}^T \Phi_{A'} = I \tag{16}$$

Because it is equal to the identity we can write it in front of the eigenvalues of A' and then rewrite it to get an expression which is the same as our original eigenvalue equation.

$$\Phi^T B \Phi \Lambda_{A'} = \Lambda_{A'} \tag{17}$$

$$\Phi^T B \Phi \Lambda_{A'} = \Phi^T A \Phi \tag{18}$$

$$B \Phi \Lambda_{A'} = A \Phi \tag{19}$$

Therefore the eigenvalues of A' are the same as the eigenvalues of our original generalized eigenvalue equation. And because A' was a symmetric matrix we know that its eigenvalues are real.

$$\Lambda_{A'} = \Lambda \tag{20}$$