

Block-diagonalization of Toeplitz matrices

Consider Hermitian block Toeplitz matrix

$$T = \begin{pmatrix} A & B & B^\dagger \\ B^\dagger & A & B \\ B & B^\dagger & A \end{pmatrix}$$

is block-diagonalized by the Vandermonde matrix

$$P = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ v_0 & v_1 & v_2 \\ v_0^2 & v_1^2 & v_2^2 \end{pmatrix}, \quad \text{with} \quad v_n = e^{2\pi i n/3}.$$

Upon the substitution of v_n we get

$$P = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & e^{2\pi i/3} & e^{-2\pi i/3} \\ 1 & e^{-2\pi i/3} & e^{2\pi i/3} \end{pmatrix}.$$

Check:

$$(P^\dagger \otimes I) T (P \otimes I) = \begin{pmatrix} A + B + B^\dagger & 0 & 0 \\ 0 & A + e^{2\pi i/3} B + e^{-2\pi i/3} B^\dagger & 0 \\ 0 & 0 & A + e^{-2\pi i/3} B + e^{2\pi i/3} B^\dagger \end{pmatrix}$$

Now, the blocks can be diagonalized separately. For the hexagonal mesh used in the code there arises a 6-fold symmetry and, therefore, 6 blocks. If one is concerned with s - excitons states, only the first block is needed, which reduces the size of the matrix to be diagonalized by 36 times.