1. Prove the Thouless theorem.

2. Assuming the spectral theorem for normal matrices, prove that every unitary matrix can be written as $\mathbf{U} = \exp(\mathbf{X} - \mathbf{X}^\dagger)$ for some square matrix $\mathbf{X}$. If the dimension of these matrices is m, explain why $m(m-1)/2$ of the elements in $\mathbf{X}$ are redundant for this parametrization. Note that, when $\mathbf{X}$ is real, the diagonal elements are redundant as well.

3. Prove the following.

$$\exp(G)\, a_p^\dagger \exp(-G) = \sum_q a_q^\dagger \left(\exp(\mathbf{G})\right)_{qp} \qquad\qquad G = \sum_{pq} (\mathbf{G})_{pq}\, a_p^\dagger a_q \tag{1}$$

4. Show that the creation and annihilation operators associated with a set of spin-orbitals $\{\psi'_p\}$ transformed from the original basis by $\mathbf{U} = \exp(\mathbf{X} - \mathbf{X}^\dagger)$ can be written as follows.

$$\begin{aligned} a_p'^\dagger &= \exp(X - X^\dagger) a_p^\dagger \exp(X^\dagger - X) \\ a'_p &= \exp(X - X^\dagger) a_p \exp(X^\dagger - X) \end{aligned} \qquad\qquad X \equiv \sum_{pq} (\mathbf{X})_{pq}\, a_p^\dagger a_q \tag{2}$$

5. Prove the following.

$$|\Phi'_{(p_1 \cdots p_n)}\rangle = \exp(X - X^\dagger) |\Phi_{(p_1 \cdots p_n)}\rangle \qquad\qquad \begin{aligned} |\Phi'_{(p_1 \cdots p_n)}\rangle &= a'^\dagger_{p_1} \cdots a'^\dagger_{p_n} |\mathrm{vac}\rangle \\ |\Phi_{(p_1 \cdots p_n)}\rangle &= a^\dagger_{p_1} \cdots a^\dagger_{p_n} |\mathrm{vac}\rangle \end{aligned} \tag{3}$$

6. Derive the following conditions for Brueckner/optimized orbitals

$$\{\psi_p\}_\mathrm{B} \,:\, \langle \Phi_i^a | \Psi \rangle \stackrel{!}{=} 0 \qquad\qquad \{\psi_p\}_\mathrm{O} \,:\, \langle \Psi | [a_a^i, H] | \Psi \rangle \stackrel{!}{=} 0 \tag{4}$$

   from the best-overlap/best-energy criteria. Explain why the Brueckner condition is equivalent to requiring that singles coefficients vanish, for both the coupled-cluster and configuration interaction Ansätze.

7. Write down an algorithm for computing BCC orbitals. In particular, explain how to rotate the orbitals each iteration in order to satisfy the Brueckner condition.

8. Write down an algorithm for computing OCC orbitals. In particular, explain how to rotate the orbitals each iteration in order to satisfy the optimization condition.

9. Derive an explicit formula for the orbital Newton-Raphson step, using a zeroth-order approximation for the orbital Hessian.

10. Derive density matrices for the CEPA_0 approximation. Give both the diagrams and algebraic expressions.