In this section we work out explicitly the reduction of the exact N interacting Fermion Hamiltonian to a reduced "complete active space" of orbitals. That is, beginning from the second-quantized interacting Hamiltonian

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l, \tag{1}$$

we will assume that some index set $\mathcal{I}_C$ is now fully occupied, or is the frozen "core" and some index set $\mathcal{I}_V$ is totally unoccupied, or virtual. The active set of orbitals belongs to the index set $\mathcal{I}_A$. All Hamiltonians here will assume the integrals have been worked out in the spin-orbital basis so as to include the spin properly. We will denote the total number of spin-orbitals/sites to be M and total number of fermions to be N_e. Without loss of generality we will order the orbitals such that the first N_c orbitals are frozen. Under this convention, all wavefunctions in the active space may be written as

$$|\Psi\rangle = \prod_{j=N_c+1}^{N} \left(\sum_{k=N_c+1}^{M} c_k^j a_j^\dagger \right) \prod_{\lambda=1}^{N_c} a_\lambda^\dagger \, |\rangle \tag{2}$$

where the product operator is assumed to fill from the right, e.g. $\prod_{\lambda=1}^{2} a_\lambda^\dagger = a_2^\dagger a_1^\dagger$. Thus to find a Hamiltonian with equivalent action on the active space under the assumption of filled core orbitals, we examine the action of the dressed Hamiltonian on the resulting subsystem of $N - N_c$ electrons in $M - N_c$ orbitals which is given by

$$\tilde{H} = \left(\prod_{\lambda=N_c}^{1} a_\lambda \right) H \left(\prod_{\lambda=1}^{N_c} a_\lambda^\dagger \right). \tag{3}$$

To proceed, it will be useful to work out the dressing for a single term for both the 1- and 2-fermion operators, which after copious use of Wick's theorem and an assumption that the index λ will not appear in the remaining wavefunction, turn out to be

$$ca_\lambda a_\lambda^\dagger = c \tag{4}$$

$$a_\lambda h_{ij} a_i^\dagger a_j a_\lambda^\dagger = h_{ij}\left[a_i^\dagger a_j + \delta_{\lambda i}\delta_{j\lambda}\right] \tag{5}$$

$$\begin{aligned} a_\lambda h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l a_\lambda^\dagger = h_{ijkl} \Big[& a_i^\dagger a_j^\dagger a_k a_l \\ & - \delta_{\lambda i}\delta_{k\lambda} a_j^\dagger a_l + \delta_{\lambda i}\delta_{l\lambda} a_j^\dagger a_k \\ & + \delta_{\lambda j}\delta_{k\lambda} a_i^\dagger a_l - \delta_{\lambda j}\delta_{l\lambda} a_i^\dagger a_k \Big] \end{aligned} \tag{6}$$

where c is any generic constant. The form of these terms allows one to extend by induction to a dressing of all N_c terms with the same assumptions, which yields

$$c \prod_\lambda a_\lambda \prod_\lambda a_\lambda^\dagger = c \tag{7}$$

$$\prod_\lambda a_\lambda h_{ij} a_i^\dagger a_j \prod_\lambda a_\lambda^\dagger = h_{ij}\left[a_i^\dagger a_j + \sum_\lambda \delta_{\lambda i}\delta_{j\lambda}\right] \tag{8}$$

$$\begin{aligned} \prod_\lambda a_\lambda h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \prod_\lambda a_\lambda^\dagger = h_{ijkl} \Big[& a_i^\dagger a_j^\dagger a_k a_l \\ & + \sum_\lambda \Big(-\delta_{\lambda i}\delta_{k\lambda} a_j^\dagger a_l + \delta_{\lambda i}\delta_{l\lambda} a_j^\dagger a_k \\ & + \delta_{\lambda j}\delta_{k\lambda} a_i^\dagger a_l - \delta_{\lambda j}\delta_{l\lambda} a_i^\dagger a_k \Big) \\ & + \sum_{\lambda\sigma} (-\delta_{\lambda i}\delta_{k\lambda}\delta_{\sigma j}\delta_{l\sigma} + \delta_{\lambda i}\delta_{l\lambda}\delta_{\sigma j}\delta_{k\sigma} \\ & + \delta_{\lambda j}\delta_{k\lambda}\delta_{\sigma i}\delta_{l\sigma} - \delta_{\lambda j}\delta_{l\lambda}\delta_{\sigma i}\delta_{k\sigma}) \Big] . \end{aligned}$$

Regrouping these terms by the number of fermions they act on and using the symmetry of the two-fermion integrals in physicist notation, we arrive at the Hamiltonian which takes the form

$$H_{\text{core}} = \sum_{\lambda} h_{\lambda\lambda} + \frac{1}{2}\sum_{\lambda\sigma} -h_{\lambda\sigma\lambda\sigma} + h_{\lambda\sigma\sigma\lambda} + h_{\sigma\lambda\lambda\sigma} - h_{\sigma\lambda\sigma\lambda} \tag{9}$$

$$= \sum_{\lambda} h_{\lambda\lambda} + \sum_{\lambda\sigma} \left(h_{\lambda\sigma\sigma\lambda} - h_{\lambda\sigma\lambda\sigma}\right) \tag{10}$$

$$H_{\text{one}} = \sum_{ij}\left[h_{ij} + \sum_{\lambda}\left(h_{\lambda ij\lambda} - h_{\lambda i\lambda j}\right)\right] a_i^\dagger a_j \tag{11}$$

$$H_{\text{two}} = \frac{1}{2}\sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \tag{12}$$

$$H = H_{\text{core}} + H_{\text{one}} + H_{\text{two}}. \tag{13}$$

The assumption of unoccupied virtual states enters as a trivial restriction of the range of the sums in the operators. As a result, the new Hamiltonian operator acts only on sites from $N_c + 1$ to $N - N_v - 1$, and has at most N_e electrons in it. The simplest way to summarize this result is by defining the transformed active space Hamiltonian with its new effective coefficients

$$\tilde{H} = \sum_{ij\in\mathcal{I}_A} \tilde{h}_{ij} a_i^\dagger a_j + \sum_{ijkl\in\mathcal{I}_A} \tilde{h}_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \tilde{C} \tag{14}$$

$$\tilde{C} = \sum_{\lambda\in\mathcal{I}_C} h_{\lambda\lambda} + \sum_{\lambda\sigma\in\mathcal{I}_C} \left(h_{\lambda\sigma\sigma\lambda} - h_{\lambda\sigma\lambda\sigma}\right) \tag{15}$$

$$\tilde{h}_{ij} = h_{ij} + \sum_{\lambda\in\mathcal{I}_C} \left(h_{\lambda ij\lambda} - h_{\lambda i\lambda j}\right) \tag{16}$$

$$\tilde{h}_{ijkl} = h_{ijkl} \tag{17}$$