## 0.1 A module for QSE-based calculations of IPs and Green's function

Given a Hamiltonian, $\hat{H}$, and a quantum circuit describing a preliminary VQE calculation for a system of $N$ particles, we can compute excited states in the $N-1$ particle sector formulating the following Ansatz

$$|\Psi_\mu\rangle = \sum_I c_{I\mu} \hat{E}_I |\Psi_{\rm vqe}\rangle \quad . \tag{1}$$

Here, the operators $\hat{E}_I$ have the form

$$\hat{E}_I \in \{\hat{a}_{p\sigma}\}_{p\sigma} \quad , \quad \hat{E}_I \in \{\hat{a}_{p\sigma} \Big[ \sum_\tau \hat{a}^\dagger_{r\tau} \hat{a}_{s\tau} \Big] \}_{prs,\sigma} \quad \text{undressed/dressed} \tag{2}$$

and the coefficients $c$ are determined solving the eigenvalue equation

$$H\, c = \varepsilon\, S\, c \quad , \tag{3}$$

with

$$S_{IJ} = \langle \Psi_{\rm vqe} | \hat{E}^\dagger_J \hat{E}_I | \Psi_{\rm vqe} \rangle \quad , \quad H_{IJ} = \langle \Psi_{\rm vqe} | \hat{E}^\dagger_J \hat{H} \hat{E}_I | \Psi_{\rm vqe} \rangle \quad . \tag{4}$$

### 0.1.1 Green's functions

Green's functions in real-time are defined as

$$C_{AB}(t) = \langle \Psi_{\rm vqe} | A(t) B | \Psi_{\rm vqe} \rangle \simeq \langle \Psi_{\rm vqe} | A e^{-it(H-E_{\rm vqe})} B | \Psi_{\rm vqe} \rangle \tag{5}$$

The Lehmann representation is

$$C_{AB}(t) \simeq \sum_\mu \langle \Psi_{\rm vqe} | A | \Psi_\mu \rangle e^{-it(\varepsilon_\mu - E_{\rm vqe})} \langle \Psi_\mu | B | \Psi_{\rm vqe} \rangle \rangle \tag{6}$$

or equivalently

$$C_{AB}(t) \simeq \sum_\mu \langle \Psi_\mu | A^\dagger | \Psi_{\rm vqe} \rangle^* e^{-it(\varepsilon_\mu - E_{\rm vqe})} \langle \Psi_\mu | B | \Psi_{\rm vqe} \rangle \tag{7}$$

and depends on matrix elements of the form

$$X_\mu = \langle \Psi_\mu | B | \Psi_{\rm vqe} \rangle = \sum_I c^*_{I\mu} \langle \Psi_{\rm vqe} | \hat{E}^\dagger_I B | \Psi_{\rm vqe} \rangle \tag{8}$$