Consider a quadratic Hamiltonian

$$\hat{H} = \sum_{i,j} c_i^\dagger H_{ij} c_j \tag{1}$$

The matrix H is Hermitian. Therefore, there exists a unitary matrix, U, that diagonalizes H. The columns of U are the eigenvectors of H. We define the quasiparticles

$$c_i = \sum_n U_{in} f_n \tag{2}$$

$$\begin{aligned}
\hat{H} =& \sum_{i,j,m,n} f_m^\dagger U_{im}^* H_{ij} U_{jn} f_n & (3)\\
=& \sum_{m,n} f_m^\dagger (U^\dagger H U)_{mn} f_n & (4)\\
=& \sum_n E_n f_n^\dagger f_n & (5)
\end{aligned}$$

The anti-commutation relations are

$$\begin{aligned}
\{f_m, f_n\} =& \sum_{i,j} U_{im}^* U_{jn}^* \{c_i, c_j\} = 0 & (6)\\
\{f_m, f_n^\dagger\} =& \sum_{i,j} U_{im}^* U_{jn} \{c_i, c_j^\dagger\} = \sum_i U_{im}^* U_{in} = \delta_{mn} & (7)
\end{aligned}$$

where we used $U^\dagger U = I$. Therefore, f_n obey fermionic commutation relations.
We get the time-dependence using the Baker-Campbell-Hausdorff formula

$$f_n(t) = e^{iHt} f_n e^{-iHt} = f_n + [iHt, f_n] + \frac{1}{2!}[iHt, [iHt, f_n]] + \dots \tag{8}$$

The commutator is given by

$$[H, f_n] = \sum_k E_k [f_k^\dagger f_k, f_n] = -E_n f_n \tag{9}$$

Therefore, the time-dependent quasiparticles are given by

$$f_n(t) = \sum_k \frac{(-iE_n t)^k}{k!} f_n = f_n e^{-iE_n t} \tag{10}$$

and the time-dependent electron operators are given by

$$c_i(t) = e^{iHt} c_i e^{-iHt} = \sum_n U_{in} e^{iHt} f_n e^{-iHt} = \sum_n U_{in} f_n(t) \tag{11}$$

Green's functions

The six Green's functions are given by

$$\begin{aligned}
G_{ij}^{>}(t,t') =& -i \langle c_i(t) c_j^\dagger(t') \rangle & (12)\\
G_{ij}^{<}(t,t') =& i \langle c_j^\dagger(t') c_i(t) \rangle & (13)\\
G_{ij}^{T}(t,t') =& \Theta(t-t') G_{ij}^{>}(t,t') + \Theta(t'-t) G_{ij}^{<}(t,t') & (14)\\
G_{ij}^{\tilde{T}}(t,t') =& \Theta(t'-t) G_{ij}^{>}(t,t') + \Theta(t-t') G_{ij}^{<}(t,t') & (15)\\
G_{ij}^{R}(t,t') =& -i\Theta(t-t') \langle \{c_i(t), c_j^\dagger(t')\} \rangle & (16)\\
G_{ij}^{A}(t,t') =& i\Theta(t'-t) \langle \{c_i(t), c_j^\dagger(t')\} \rangle & (17)
\end{aligned}$$

The six functions are the greater, lesser, time-ordered, anti-time-ordered, retarded, and advanced Green's function, respectively. The Green's functions have the relations

$$G^R = G^T - G^< = G^> - G^{\bar{T}} \tag{18}$$

$$G^A = G^T - G^> = G^< - G^{\bar{T}} \tag{19}$$

$$G^R - G^A = G^> - G^< \tag{20}$$

Retarded Green's function

The retarded Green's function is

$$G^R_{ij}(t,t') = -i\Theta(t-t')\left\langle\{c_i(t), c_j^\dagger(t')\}\right\rangle \tag{21}$$

$$= -i\Theta(t-t')\sum_{m,n}\left\langle\{U_{im}f_m e^{-iE_m t}, U^*_{jn}f_n^\dagger e^{iE_n t'}\}\right\rangle \tag{22}$$

$$= -i\Theta(t-t')\sum_n U_{in}e^{-iE_n(t-t')}U^*_{jn} \tag{23}$$

The Green's function only depends on the difference $t-t'$, so we can set $t'=0$. In frequency space, we have

$$G^R_{ij}(\omega) = \int_{-\infty}^{\infty} dt G^R_{ij}(t,0)e^{i(\omega+i\delta)t} \tag{24}$$

$$= -i\sum_n \int_0^\infty dt U_{in}e^{i(\omega+i\delta-E_n)t}U^*_{jn} \tag{25}$$

$$= -i\sum_n U_{in}\frac{-1}{i(\omega+i\delta-E_n)}U^*_{jn} \tag{26}$$

$$= \sum_n U_{in}\frac{1}{\omega+i\delta-E_n}U^*_{jn} \tag{27}$$

where the infinitesimal $i\delta$ was introduced for convergence. Since the columns of U are the eigenvectors of H, we can write the elements as $U_{in} = \langle i|\psi_n\rangle$.

$$G^R_{ij}(\omega) = \sum_n \langle i|\psi_n\rangle \frac{1}{\omega+i\delta-E_n}\langle\psi_n|j\rangle \tag{28}$$

We can also write the Green's function matrix as

$$G^R(\omega) = U((\omega+i\delta)I-E)^{-1}U^\dagger = \left((\omega+i\delta)I - UEU^\dagger\right)^{-1} = ((\omega+i\delta)I-H)^{-1} \tag{29}$$

Advanced Green's function

The advanced Green's function is

$$G^A_{ij}(t,t') = i\Theta(t'-t)\left\langle\{c_i(t), c_j^\dagger(t')\}\right\rangle \tag{30}$$

$$= i\Theta(t'-t)\sum_n U_{in}e^{-iE_n(t-t')}U^*_{jn} \tag{31}$$

In frequency space,

$$G^A_{ij}(\omega) = \int_{-\infty}^{\infty} dt G^A_{ij}(t,0)e^{i(\omega-i\delta)t} \tag{32}$$

$$= \sum_n U_{in}\frac{1}{\omega-i\delta-E_n}U^*_{jn} \tag{33}$$

$$= \sum_n \langle i|\psi_n\rangle \frac{1}{\omega-i\delta-E_n}\langle\psi_n|j\rangle \tag{34}$$

In matrix form,

$$G^A(\omega) = ((\omega - i\delta)I - H)^{-1} \tag{35}$$

Since H is Hermitian, we get the relation

$$G^A(\omega) = \left(G^R(\omega)\right)^\dagger \tag{36}$$

Lesser Green's function

The lesser Green's function is given by

$$\begin{aligned}
G^<_{ij}(t,t') =& i \langle c_j^\dagger(t') c_i(t) \rangle & (37)\\
=& i \sum_{m,n} U^*_{jm} U_{in} \langle f_m^\dagger f_n \rangle e^{iE_m t' - iE_n t} & (38)\\
=& i \sum_n U_{in} n_F(E_n) U^*_{jn} e^{-iE_n(t-t')} & (39)
\end{aligned}$$

where n_F is the Fermi distribution function and we used $\langle f_m^\dagger f_n \rangle = \delta_{mn} n_F(E_n)$ in thermal equilibrium. In frequency space,

$$\begin{aligned}
G^<_{ij}(\omega) =& \int_{-\infty}^{\infty} dt G^<_{ij}(t,0) e^{i\omega t} & (40)\\
=& i \sum_n U_{in} n_F(E_n) U^*_{jn} \int_{-\infty}^{\infty} dt e^{i(\omega - E_n)t} & (41)\\
=& i \sum_n U_{in} n_F(E_n) U^*_{jn} 2\pi \delta(\omega - E_n) & (42)\\
=& 2\pi i n_F(\omega) \sum_n \langle i|\psi_n\rangle \delta(\omega - E_n) \langle \psi_n | j \rangle & (43)
\end{aligned}$$

Greater Green's function

The greater Green's function is given by

$$\begin{aligned}
G^>_{ij}(t,t') =& -i \langle c_i(t) c_j^\dagger(t') \rangle & (44)\\
=& -i \sum_{m,n} U^*_{jm} U_{in} \langle f_n f_m^\dagger \rangle e^{iE_m t' - iE_n t} & (45)\\
=& -i \sum_n U_{in} (1 - n_F(E_n)) U^*_{jn} e^{-iE_n(t-t')} & (46)
\end{aligned}$$

In frequency space,

$$G^>_{ij}(\omega) = -2\pi i (1 - n_F(\omega)) \sum_n \langle i|\psi_n\rangle \delta(\omega - E_n) \langle \psi_n | j \rangle \tag{47}$$

Spectral function

We define the spectral function as

$$\begin{aligned}
A_{ij}(\omega) =& -\frac{1}{2\pi i} \left(G^R_{ij}(\omega) - G^A_{ij}(\omega)\right) & (48)\\
=& -\frac{1}{2\pi i} \sum_n \langle i|\psi_n\rangle \left(\frac{1}{\omega + i\delta - E_n} - \frac{1}{\omega - i\delta - E_n} \right) \langle \psi_n | j \rangle & (49)\\
=& \sum_n \langle i|\psi_n\rangle \frac{1}{\pi} \frac{\delta}{(\omega - E_n)^2 + \delta^2} \langle \psi_n | j \rangle & (50)\\
\xrightarrow{\delta \to 0}& \sum_n \langle i|\psi_n\rangle \delta(\omega - E_n) \langle \psi_n | j \rangle & (51)
\end{aligned}$$

For $i = j$, we get $G_{ii}^A = \left(G_{ii}^R\right)^*$. Therefore,

$$A_{ii}(\omega) = -\frac{1}{2\pi i}\left(G_{ii}^R(\omega) - \left(G_{ii}^R(\omega)\right)^*\right) \tag{52}$$

$$= -\frac{1}{\pi}\mathrm{Im}\left[G_{ii}^R(\omega)\right] \tag{53}$$

In thermal equilibrium, we get the relations

$$G_{ij}^<(\omega) = 2\pi i n_F(\omega) A_{ij}(\omega) \tag{54}$$

$$= -n_F(\omega)\left(G_{ij}^R(\omega) - G_{ij}^A(\omega)\right) \tag{55}$$

$$G_{ij}^>(\omega) = -2\pi i(1 - n_F(\omega))A_{ij}(\omega) \tag{56}$$

$$= (1 - n_F(\omega))\left(G_{ij}^R(\omega) - G_{ij}^A(\omega)\right) \tag{57}$$

Numerical evaluation of LDOS

We want to calculate

$$A_{ii}(\omega) = -\frac{1}{\pi}\mathrm{Im}\left[G_{ii}^R(\omega)\right] \tag{58}$$

$$= \frac{1}{\pi}\sum_n |U_{in}|^2 \frac{\delta}{(\omega - E_n)^2 + \delta^2} \tag{59}$$

Let

$$K_n(\omega) = \frac{1}{\pi}\frac{\delta}{(\omega - E_n)^2 + \delta^2} \tag{60}$$

The LDOS becomes

$$A_{ii}(\omega) = \sum_n |U_{in}|^2 K_n(\omega) \tag{61}$$

which can be calculated using a dot product.