1 Krylov subspace

The order-n Krylov subspace is defined as

$$\mathcal{K}_n(H, |v_0\rangle) = \text{span}\left\{|v_0\rangle, H|v_0\rangle, H^2|v_0\rangle, \ldots, H^{n-1}|v_0\rangle\right\} \tag{1}$$

By approximating H in this subspace, we can calculate eigenvalues and eigenvectors using Lanczos iteration. We can also calculate spectral functions and Green's functions using the kernel polymial method.

2 Power method

Let $|v_0\rangle$ be an arbitrary vector. We define the recurrence relation

$$|\tilde{v}_{n+1}\rangle = H|v_n\rangle \tag{2}$$

$$|v_{n+1}\rangle = \frac{|\tilde{v}_{n+1}\rangle}{\sqrt{\langle\tilde{v}_{n+1}|\tilde{v}_{n+1}\rangle}} \tag{3}$$

i.e., we multiply by H and normalize. If $|v_n\rangle$ converges to a vector $|v_\infty\rangle$, then we get

$$|v_\infty\rangle \propto H|v_\infty\rangle \tag{4}$$

Therefore, $|v_\infty\rangle$ is an eigenvector of H. This method usually converges on an eigenvector associated with the dominant (largest magnitude) eigenvalue since any non-zero component of the dominant eigenvector will get larger after each iteration.

3 Lanczos algorithm

Combining the power method with Gram-Schmidt orthonormalization, we can approximate H on the Krylov subspace $\mathcal{K}_{N+1}$ after N iterations. These notes are based on The Lanczos Method - Erik Koch.
Assume H is Hermitian. Let $|v_0\rangle$ be an arbitrary normalized vector, $\langle v_0|v_0\rangle = 1$. We multiply $|v_0\rangle$ by H and orthogonalize the new vector $H|v_0\rangle$ to $|v_0\rangle$.

$$|\tilde{v}_1\rangle = H|v_0\rangle - |v_0\rangle\langle v_0|H|v_0\rangle \tag{5}$$

Define

$$a_n = \langle v_n|H|v_n\rangle \tag{6}$$

$$b_n^2 = \langle\tilde{v}_n|\tilde{v}_n\rangle \tag{7}$$

Eq. (5) becomes

$$b_1|v_1\rangle = H|v_0\rangle - a_0|v_0\rangle \tag{8}$$

Rearranging gives

$$H|v_0\rangle = a_0|v_0\rangle + b_1|v_1\rangle \tag{9}$$

For the next iteration step, we multiply $|v_1\rangle$ by H and orthogonalize $H|v_1\rangle$ w.r.t. all previous vectors.

$$b_2|v_2\rangle = |\tilde{v}_2\rangle = H|v_1\rangle - \sum_{i=0}^{1}|v_i\rangle\langle v_i|H|v_1\rangle = H|v_1\rangle - a_1|v_1\rangle - b_1|v_0\rangle \tag{10}$$

Rearranging gives

$$H|v_1\rangle = b_1|v_0\rangle + a_1|v_1\rangle + b_2|v_2\rangle \tag{11}$$

Continuing the iteration, we get

$$b_3 |v_3\rangle = |\tilde{v}_3\rangle = H |v_2\rangle - \sum_{i=0}^{2} |v_i\rangle \langle v_i|H|v_2\rangle = H |v_2\rangle - a_2 |v_2\rangle - b_2 |v_1\rangle \tag{12}$$

Here, the term $|v_0\rangle \langle v_0|H|v_2\rangle$ vanishes. This can be seen from Eq. (9)

$$\langle v_2|H|v_0\rangle = a_0 \langle v_2|v_0\rangle + b_1 \langle v_2|v_1\rangle \tag{13}$$

The vectors are orthogonal by construction. Therefore, $\langle v_0|H|v_2\rangle = 0$. Rearranging gives

$$H |v_2\rangle = b_2 |v_1\rangle + a_2 |v_2\rangle + b_3 |v_3\rangle \tag{14}$$

We can repeat the process to get

$$H |v_n\rangle = b_n |v_{n-1}\rangle + a_n |v_n\rangle + b_{n+1} |v_{n+1}\rangle \tag{15}$$

This process is called tridiagonalization. After N iterations, the Hamiltonian on the $N+1$-dimensional Krylov subspace is

$$H_{\mathcal{K}_N(|v_0\rangle)} = \begin{pmatrix} \langle v_0|H|v_0\rangle & \dots & \langle v_0|H|v_N\rangle \\ \vdots & \ddots & \vdots \\ \langle v_N|H|v_0\rangle & \dots & \langle v_N|H|v_N\rangle \end{pmatrix} = \begin{pmatrix} a_0 & b_1 & & & & \\ b_1 & a_1 & b_2 & & & \\ & b_2 & a_2 & b_3 & & \\ & & & \ddots & & \\ & & & b_{N-1} & a_{N-1} & b_N \\ & & & & b_N & a_N \end{pmatrix} \tag{16}$$

3.1 Eigensolution

Let V be the matrix with columns $|v_0\rangle, \dots, |v_N\rangle$ and T be the tridiagonal matrix. Then $H \approx VTV^\dagger$. If $T |x\rangle = \lambda |x\rangle$ ($|x\rangle$ is an eigenvector of T), then $V |x\rangle$ is the corresponding eigenvector to H with eigenvalue λ.

$$HV |x\rangle \approx VTV^\dagger V |x\rangle = VT |x\rangle = \lambda V |x\rangle \tag{17}$$

This is beneficial since T is of lower dimension than H and also, there are specialized algorithms for diagonalizing tridiagonal matrices. However, like the power method, this converges on dominant eigenvalues. To find eigenvalues near σ, we can use the shift-invert method. This method uses Lanczos iteration on the matrix $(H - \sigma I)^{-1}$. The dominant eigenvalues of this matrix are near σ and the eigenvectors for $(H - \sigma I)^{-1}$ are the same as H. Also, this method is numerically unstable since after many iterations, orthogonality is lost. To circumvent this, implementations will "restart" after a certain number of iterations. These methods are implemented in scipy as scipy.sparse.linalg.eigsh.

3.2 Green's function

Consider

$$G(z) = \langle \psi_0|(z - H)^{-1}|\psi_0\rangle \tag{18}$$

By initializing the Lanczos algorithm with the vector $|\psi_0\rangle$, we get the tridiagonalization

$$z - H \approx V(z - T)V^\dagger = V \begin{pmatrix} z - a_0 & -b_1 & & & & \\ -b_1 & z - a_1 & -b_2 & & & \\ & -b_2 & z - a_2 & -b_3 & & \\ & & & \ddots & & \\ & & & -b_{N-1} & z - a_{N-1} & -b_N \\ & & & & -b_N & z - a_N \end{pmatrix} V^\dagger \tag{19}$$

To get $G(z)$, we need to calculate $[(z-T)^{-1}]_{00}$. We can use block inversion to get the inverse

$$z - T = \begin{pmatrix} z - a_0 & -B^{(1)T} \\ -B^{(1)} & z - T^{(1)} \end{pmatrix} \tag{20}$$

$$B^{(1)} = \begin{pmatrix} b_1 \\ 0 \\ \vdots \end{pmatrix} \qquad z - T^{(1)} = \begin{pmatrix} z - a_1 & -b_2 & & & \\ -b_2 & z - a_2 & -b_3 & & \\ & & \ddots & & \\ & & -b_{N-1} & z - a_{N-1} & -b_N \\ & & & -b_N & z - a_N \end{pmatrix} \tag{21}$$

$$[(z-T)^{-1}]_{00} = \left(z - a_0 - B^{(1)T}(z - T^{(1)})^{-1}B^{(1)}\right)^{-1} = \left(z - a_0 - b_1^2[(z - T^{(1)})^{-1}]_{00}\right)^{-1} \tag{22}$$

The inverse $(z - T^{(1)})^{-1}$ can similarly be inverted using block matrices. Repeating the inversion, we get the continued fraction

$$G(z) = \cfrac{1}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \dots}}} \tag{23}$$

which terminates with $-\frac{b_N^2}{z - a_N}$.

4 Kernel Polynomial Method

This section is based on Kernel Polynomial Method.

4.1 Chebyshev polynomials

The Chebyshev polynomials of the first kind are given by

$$\{T_n(x) = \cos(n \arccos(x)) : n = 0, 1, 2, 3, \dots\} \tag{24}$$

which are orthogonal under the inner product

$$\langle f, g \rangle = \int_{-1}^{1} \frac{f(x)g(x)}{\pi\sqrt{1 - x^2}} dx \tag{25}$$

with the orthogonality relation

$$\langle T_m, T_n \rangle = \begin{cases} 0 & m \neq n \\ 1 & m = n = 0 \\ 1/2 & m = n \neq 0 \end{cases} \tag{26}$$

A useful property of the Chebyshev polynomials is that they can be generated using the recurrence relation

$$T_0(x) = 1 \tag{27}$$
$$T_1(x) = x \tag{28}$$
$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \tag{29}$$

The Chebyshev expansion for a function f defined on the domain $[-1, 1]$ is

$$f(x) = \sum_{n=0}^{\infty} \frac{\langle f, T_n \rangle}{\langle T_n, T_n \rangle} T_n(x) = \alpha_0 + 2\sum_{n=1}^{\infty} \alpha_n T_n(x) \tag{30}$$

with coefficients

$$\alpha_n = \int_{-1}^{1} \frac{f(x)T_n(x)}{\pi\sqrt{1-x^2}}dx \tag{31}$$

The denominator in the integral is troublesome so we rearrange the expansion

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}}\left(\mu_0 + 2\sum_{n=1}^{\infty}\mu_n T_n(x)\right) \tag{32}$$

$$\mu_n = \int_{-1}^{1} f(x)T_n(x)dx \tag{33}$$

4.1.1 Proof of rearrangement

Define a new inner product

$$\langle f, g\rangle_1 = \int_{-1}^{1} \pi\sqrt{1-x^2}f(x)g(x)dx \tag{34}$$

and polynomials

$$\phi_n(x) = \frac{T_n(x)}{\pi\sqrt{1-x^2}} \tag{35}$$

These polynomials have the same orthogonality relations

$$\langle \phi_m, \phi_n\rangle_1 = \langle T_m, T_n\rangle = \begin{cases} 0 & m \neq n \\ 1 & m = n = 0 \\ 1/2 & m = n \neq 0 \end{cases} \tag{36}$$

The expansion becomes

$$f(x) = \sum_{n=0}^{\infty} \frac{\langle f, \phi_n\rangle_1}{\langle \phi_n, \phi_n\rangle_1}\phi_n(x) = \frac{1}{\pi\sqrt{1-x^2}}\left(\mu_0 + 2\sum_{n=1}^{\infty}\mu_n T_n(x)\right) \tag{37}$$

$$\mu_n = \langle f, \phi_n\rangle_1 = \int_{-1}^{1} f(x)T_n(x)dx \tag{38}$$

4.1.2 Rescaling

Expanding $f(x)$ with Chebyshev polynomials requires $x \in [-1, 1]$. We will expand functions of energy so the eigenvalues of the Hamiltonian should be in the interval $E_k \in [-1, 1]$. To fit the spectrum in the interval, we apply a linear transformation to the Hamiltonian and energies.

$$H' = (H - b)/a \tag{39}$$
$$\omega' = (\omega - b)/a \tag{40}$$
$$a = (E_{max} - E_{min})/(2 - \epsilon) \tag{41}$$
$$b = (E_{max} + E_{min})/2 \tag{42}$$

ϵ is a small cut-off for numerical stablity. All H and ω used afterwards refer to the scaled Hamiltonian and energies.

4.2 Density of states

The first basic application of Chebyshev expansion is the calculation of the density of states

$$\rho(\omega) = \sum_k \delta(\omega - E_k) \tag{43}$$

where E_k are the eigenvalues of the Hamiltonian matrix. The moments are calculated by

$$\begin{aligned}
\mu_n =& \int_{-1}^{1} \rho(\omega) T_n(\omega) d\omega && (44)\\
=& \sum_k T_n(E_k) && (45)\\
=& \sum_k \langle k|T_n(H)|k\rangle && (46)\\
=& \mathrm{Tr}(T_n(H)) && (47)
\end{aligned}$$

4.3 Local density of states

The retarded Green's function in terms of eigenvectors is

$$G^R(\omega) = \lim_{\delta\to 0^+} \sum_k \frac{|k\rangle \langle k|}{\omega + i\delta - E_k} \tag{48}$$

The local density of states is

$$\begin{aligned}
\rho_i(\omega) =& -\frac{1}{\pi} \mathrm{Im} G^R_{ii}(\omega) && (49)\\
=& \lim_{\delta\to 0^+} -\frac{1}{\pi} \sum_k \mathrm{Im} \frac{\langle i|k\rangle \langle k|i\rangle}{\omega + i\delta - E_k} && (50)\\
=& \lim_{\delta\to 0^+} \frac{1}{\pi} \sum_k |\langle i|k\rangle|^2 \frac{\delta}{(\omega - E_k)^2 + \delta^2} && (51)\\
=& \sum_k |\langle i|k\rangle|^2 \delta(\omega - E_k) && (52)
\end{aligned}$$

The moments are

$$\begin{aligned}
\mu_n =& \int_{-1}^{1} \rho_i(\omega) T_n(\omega) d\omega && (53)\\
=& \sum_k |\langle i|k\rangle|^2 T_n(E_k) && (54)\\
=& \sum_k \langle i|T_n(H)|k\rangle \langle k|i\rangle && (55)\\
=& \langle i|T_n(H)|i\rangle && (56)
\end{aligned}$$

4.4 Spectral function

The spectral function is

$$A(\omega) = -\frac{G^R(\omega) - G^A(\omega)}{2\pi i} \tag{57}$$

$$= -\frac{1}{2\pi i}\lim_{\delta\to 0^+}\sum_k |k\rangle\langle k|\left(\frac{1}{\omega + i\delta - E_k} - \frac{1}{\omega - i\delta - E_k}\right) \tag{58}$$

$$= \lim_{\delta\to 0^+}\sum_k |k\rangle\langle k|\frac{1}{\pi}\frac{\delta}{(\omega - E_k)^2 + \delta^2} \tag{59}$$

$$= \sum_k |k\rangle\langle k|\,\delta(\omega - E_k) \tag{60}$$

For a matrix element $A_{ij}(\omega)$, the moments are

$$\mu_n = \int_{-1}^{1} A_{ij}(\omega)T_n(\omega)d\omega \tag{61}$$

$$= \sum_k \langle i|k\rangle\langle k|j\rangle\, T_n(E_k) \tag{62}$$

$$= \sum_k \langle i|T_n(H)|k\rangle\langle k|j\rangle \tag{63}$$

$$= \langle i|T_n(H)|j\rangle \tag{64}$$

4.5 Lesser Green's function

The lesser Green's function in equilibrium is

$$G^<_{ij}(\omega) = 2\pi i n_F(\omega)A_{ij}(\omega) \tag{65}$$

4.5.1 Mean-field equation

The expectation value is an integral over energy of the lesser Green's function given by

$$\langle c_j^\dagger c_i\rangle = \int_{-1}^{1}\frac{d\omega}{2\pi i}G^<_{ij}(\omega) \tag{66}$$

$$= \int_{-1}^{1} d\omega n_F(\omega)A_{ij}(\omega) \tag{67}$$

4.5.2 Current

The current is given by

$$I_{ij} = \frac{-2e}{\hbar}\int\frac{d\omega}{2\pi}\mathrm{Re}[t_{ji}G^<_{ij}(\omega)] \tag{68}$$

$$= \frac{2e}{\hbar}\int d\omega n_F(\omega)\mathrm{Im}[t_{ji}A_{ij}(\omega)] \tag{69}$$

4.5.3 Superconducting order parameter

An example of solving the mean-field equation is for the the superconducting order parameter Δ_{ij}

$$\Delta_{ij} = -V\langle c_i^\dagger c_j^\dagger\rangle = -V\int_{-1}^{1}\frac{d\omega}{2\pi i}F^<_{ij}(\omega) \tag{70}$$

$$= -V\int_{-1}^{1} d\omega n_F(\omega)A^{12}_{ij}(\omega) \tag{71}$$

where A^{12} is the spectral function of the Bogoliubov-de-Gennes Hamiltonian in the anamolous block.

4.6 Calculating moments

Usually, H is a sparse matrix. In general, $T_n(H)$ is not a sparse matrix. However, $T_n(H)$ usually acts on a vector. Instead of storing the matrix $T_n(H)$, we can store the vector $|\alpha_n\rangle = T_n(H)\,|\alpha\rangle$.

4.6.1 $\mu_n = \langle\beta|T_n(H)|\alpha\rangle$

Starting from the state $|\alpha\rangle$, we can iteratively construct states $|\alpha_n\rangle = T_n(H)\,|\alpha\rangle$ using the recurrence relations

$$|\alpha_0\rangle = |\alpha\rangle \tag{72}$$
$$|\alpha_1\rangle = H\,|\alpha\rangle \tag{73}$$
$$|\alpha_{n+1}\rangle = 2H\,|\alpha_n\rangle - |\alpha_{n-1}\rangle \tag{74}$$
$$\mu_n = \langle\beta|\alpha_n\rangle \tag{75}$$

Note that for a single starting vector α, the expansion coefficients can be calculated for many different β.

4.6.2 $\mu_n = \mathbf{Tr}(AT_n(H))$

We can use a stochastic method to estimate the trace.

$$\mathrm{Tr}(AT_n(H)) \approx \frac{1}{R}\sum_{r=0}^{R-1} \langle r|AT_n(H)|r\rangle$$

where $|r\rangle$ is a random vector, R is the number of random vectors, and the relative error is of the order $O(1/\sqrt{RD})$. The i-th component $\langle i|r\rangle = \xi_i$ can be Gaussian distributed or have a uniform random phase.

$$\xi_i = x \quad \text{or} \quad \xi_i = e^{i\phi}$$

where $x \in \mathbb{R}$ is a gausian distributed random number and $\phi \in [0, 2\pi)$ is a uniformly distributed random number. Then, we use the procedure for $\mu_n = \langle\beta|T_n(H)|\alpha\rangle$ for each random vector $|r\rangle$

$$\langle\beta_r| = \langle r|\,A \tag{76}$$
$$|\alpha_{rn}\rangle = T_n(H)\,|r\rangle \tag{77}$$
$$\mu_n = \frac{1}{R}\sum_{r=0}^{R-1} \langle\beta_r|\alpha_{rn}\rangle \tag{78}$$

4.6.3 $|\beta\rangle = |\alpha\rangle$

Using the product relation

$$2T_m(x)T_n(x) = T_{m+n}(x) + T_{m-n}(x) \tag{79}$$

the recurrence relation can be simplified even further to

$$\mu_{2n} = 2\,\langle\alpha_n|\alpha_n\rangle - \mu_0 \tag{80}$$
$$\mu_{2n+1} = 2\,\langle\alpha_{n+1}|\alpha_n\rangle - \mu_1 \tag{81}$$

4.7 Kernel

The Chebyshev expansion is exact for an infinite number of moments. However, we must approximate the expansion given a finite number of N moments μ_n. Truncating the series leads to Gibbs oscillations near points where the function $f(x)$ is not continuously differentiable. To damp these oscillations, we modify the expansion coefficients $\bar{\mu}_n = g_n\mu_n$.

4.7.1 Jackson kernel

$$g_n = \frac{(N-n+1)\cos\frac{\pi n}{N+1} + \sin\frac{\pi n}{N+1}\cot\frac{\pi}{N+1}}{N+1} \tag{82}$$

which is related to a Gaussian

$$\delta(x-a) \approx \frac{1}{\sqrt{2\pi\sigma^2}}\exp(-\frac{(x-a)^2}{2\sigma^2}) \tag{83}$$

$$\sigma^2 = \frac{N-a^2(N-1)}{2(N+1)}\left(1-\cos\frac{2\pi}{N+1}\right) \tag{84}$$

$$\approx \left(\frac{\pi}{N}\right)^2\left(1-a^2+\frac{4a^2-3}{N}\right) \tag{85}$$

4.7.2 Lorentz kernel

$$g_n = \frac{\sinh(\lambda(1-n/N))}{\sinh(\lambda)} \tag{86}$$

which is related to a Lorentzian

$$\delta(x-a) \approx \frac{1}{\pi}\frac{\epsilon}{(x-a)^2+\epsilon^2} \tag{87}$$

$$\epsilon = \lambda/N \tag{88}$$

λ is a free parameter related to the width of the Lorentzian. A small λ gives good resolution but increases the Gibbs oscillations. A good value for λ is between 3 and 5.
For both of these kernels, a strictly positive function remains positive and delta functions are approximated using a Gaussian or Lorentzian. For most applications, the Jackson kernel converges best, but for approximating Green's functions the Lorentz kernel is best.

4.8 Discrete cosine transform

For a set $\{x_m\}$ of M points, the Chebyshev expansion is

$$f(x_m) = \frac{1}{\pi\sqrt{1-x_m^2}}\left(\bar{\mu}_0 + 2\sum_{n=1}^{N-1}\bar{\mu}_n T_n(x_m)\right) \tag{89}$$

By making a special choice for our data points x_m,

$$x_m = \cos\frac{\pi(m+1/2)}{M} \quad \text{with} \quad m = 0,\ldots,M-1 \tag{90}$$

we have $T_n(x_m) = \cos(n\arccos(x_m)) = \cos\frac{\pi n(m+1/2)}{M}$. We then obtain

$$\gamma_m = \pi\sqrt{1-x_m^2}f(x_m) = \bar{\mu}_0 + 2\sum_{n=1}^{N-1}\bar{\mu}_n\cos\frac{\pi n(m+1/2)}{M} \tag{91}$$

which can be efficiently calculated using a fast discrete cosine transform found in many FFT packages. After discrete cosine transform of the moments, the approximated function at the data points $\{x_m\}$ are

$$f(x_m) = \frac{\gamma_m}{\pi\sqrt{1-x_m^2}} \tag{92}$$

4.9 Chebyshev-Gauss quadrature

In numerical analysis, Chebyshev-Gauss quadrature is a method of approximating integrals as

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx \approx \frac{\pi}{M} \sum_{m=0}^{M-1} f(x_m) \quad \text{with} \quad x_m = \cos \frac{\pi(m+1/2)}{M} \tag{93}$$

The special choice of data points $\{x_m\}$ from the discrete cosine transform corresponds to the abscissas of Chebyshev-Gauss quadrature. Hence, integrals of the form $\int_{-1}^{1} f(x)g(x)dx$ become simple averages.

$$\int_{-1}^{1} f(x)g(x)dx = \int_{-1}^{1} \frac{\sqrt{1-x^2} f(x)g(x)}{\sqrt{1-x^2}} dx \tag{94}$$

$$\approx \frac{\pi}{M} \sum_{m=0}^{M-1} \sqrt{1-x_m^2} f(x_m)g(x_m) \tag{95}$$

$$= \frac{1}{M} \sum_{m=0}^{M-1} \gamma_m g(x_m) \tag{96}$$

4.10 Retarded Green's function

We can calculate the Retarded Green's function in terms of the spectral function using the relation

$$\frac{1}{\omega + i\delta} = \mathcal{P}\frac{1}{\omega} - i\pi\delta(\omega) \tag{97}$$

where $\mathcal{P}$ denotes the principal value.

$$G^R(\omega) = \lim_{\delta \to 0^+} \sum_k \frac{|k\rangle \langle k|}{\omega + i\delta - E_k} \tag{98}$$

$$= \sum_k |k\rangle \langle k| \left(\mathcal{P}\frac{1}{\omega - E_k} - i\pi\delta(\omega - E_k) \right) \tag{99}$$

$$= \mathcal{P} \int d\nu \frac{A(\nu)}{\omega - \nu} - i\pi A(\omega) \tag{100}$$

Using the Chebyshev expansion of the spectral function,

$$A(\nu) = \frac{1}{\pi\sqrt{1-\nu^2}} \left(\mu_0 + 2\sum_{n=1}^{\infty} \mu_n T_n(\nu) \right) \tag{101}$$

the integral becomes

$$\mathcal{P} \int d\nu \frac{A(\nu)}{\omega - \nu} = 2\sum_{n=1}^{\infty} \mu_n \int \frac{d\nu}{\pi\sqrt{1-\nu^2}} \frac{T_n(\nu)}{\omega - \nu} \tag{102}$$

The Chebyshev polynomials of the first and second kind have the integral relation

$$\mathcal{P} \int_{-1}^{1} \frac{dy}{\pi\sqrt{1-y^2}} \frac{T_n(y)}{y - x} = U_{n-1}(x) \tag{103}$$

where the Chebyshev polynomials of the second kind are

$$U_n(\cos(\theta)) \sin(\theta) = \sin\left((n+1)\theta\right) \tag{104}$$

Plugging this into the retarded Green's function, we get

$$G^R(\omega) = -2\sum_{n=1}^{\infty}\mu_n U_{n-1}(\omega) - i\pi\frac{1}{\pi\sqrt{1-\omega^2}}\left(\mu_0 + 2\sum_{n=1}^{\infty}\mu_n T_n(\omega)\right) \tag{105}$$

$$= -\frac{i}{\sqrt{1-\omega^2}}\left[\mu_0 + 2\sum_{n=1}^{\infty}\mu_n\left(T_n(\omega) - i\sqrt{1-\omega^2}U_{n-1}(\omega)\right)\right] \tag{106}$$

$$= -\frac{i}{\sqrt{1-\omega^2}}\left(\mu_0 + 2\sum_{n=1}^{\infty}\mu_n e^{-in\arccos(\omega)}\right) \tag{107}$$

Therefore, we can calculate the retarded Green's function using the same expansion coefficients as the spectral function. The advanced Green's function can similarly be calculated.

$$G^A(\omega) = \frac{i}{\sqrt{1-\omega^2}}\left(\mu_0 + 2\sum_{n=1}^{\infty}\mu_n e^{in\arccos(\omega)}\right) \tag{108}$$

4.10.1 Fourier transform

We use the same set of points as the discrete cosine transform.

$$\omega_m = \cos\frac{\pi(m+1/2)}{M} \quad \text{with} \quad m = 0, \ldots, M-1 \tag{109}$$

First, we define

$$\gamma_m = i\sqrt{1-\omega_m^2}G^R(\omega_m) = \bar{\mu}_0 + 2\sum_{n=1}^{N-1}\bar{\mu}_n e^{-in\arccos(\omega_m)} \tag{110}$$

where $\bar{\mu}_n$ are the modified expansion coefficients. Next, we define

$$\lambda_n = \begin{cases} \bar{\mu}_0 & n = 0 \\ 2\bar{\mu}_n e^{-i\pi n/2M} & 0 < n < N \\ 0 & N \leq n \end{cases} \tag{111}$$

Eq. (110) becomes

$$\gamma_m = \sum_{n=0}^{M-1}\lambda_n e^{-\pi inm/M} \tag{112}$$

Using the standard FFT,

$$\hat{\lambda}_m = \sum_{n=0}^{M-1}\lambda_n e^{-2\pi inm/M} \tag{113}$$

we get the even and odd indices

$$\gamma_{2m} = \hat{\lambda}_m \tag{114}$$

$$\gamma_{2m+1} = \hat{\lambda}^*_{M-1-m} \tag{115}$$

4.11 Improving accuracy using projections

We have seen that most of the functions that we want to calculate can be calculated from the spectral function. Often, we want to increase the accuracy in some energy range. To do this, we first calculate a subset of eigenfunctions in this energy range (using the Lanczos method). We then calculate the spectral

function exactly in this subspace. Finally, we approximate the contributions from the rest of the spectrum using the kernel polynomial method.
Let

$$P = \sum_k{}' |k\rangle \langle k| \tag{116}$$

$$Q = 1 - P \tag{117}$$

where the primed sum goes over some subset of eigenfunctions. The spectral function in the P subspace is

$$A^P(\omega) = \sum_k{}' |k\rangle \langle k| \, \delta(\omega - E_k) \tag{118}$$

The Chebyshev expansion coefficients are

$$\mu_n^P = \int_{-1}^{1} A_P(\omega) T_n(\omega) d\omega \tag{119}$$

$$= \sum_k{}' |k\rangle \langle k| \, T_n(E_k) \tag{120}$$

$$= P T_n(H) \tag{121}$$

Similarly, the spectral function in the Q subspace has the expansion coefficients

$$\mu_n^Q = Q T_n(H) \tag{122}$$

The spectral function over the full space is

$$A(\omega) = A^P(\omega) + A^Q(\omega) \tag{123}$$

and has the coefficients

$$\mu_n = \mu_n^P + \mu_n^Q = T_n(H) \tag{124}$$

Originally, the approximation to the spectral function was

$$A(\omega) \approx \frac{1}{\pi\sqrt{1-\omega^2}} \left(\mu_0 + 2 \sum_{n=1}^{N-1} \mu_n T_n(\omega) \right) \tag{125}$$

We split the spectral function into the P and Q subspace and calculate the P subspace contribution exactly.

$$A(\omega) \approx \sum_k{}' |k\rangle \langle k| \, \delta(\omega - E_k) + \frac{1}{\pi\sqrt{1-\omega^2}} \left(\mu_0^Q + 2 \sum_{n=1}^{N-1} \mu_n^Q T_n(\omega) \right) \tag{126}$$

Usually, the coefficients μ_n have already been calculated. The energies in the P subspace have also been calculated. We can use Eq. (120, 124) to get

$$\mu_n^Q = \mu_n - \mu_n^P \tag{127}$$

$$\mu_n^P = \sum_k{}' |k\rangle \, T_n(E_k) \langle k| \tag{128}$$

Following the same procedure for the retarded Green's function, we get

$$G^R(\omega) = \sum_k{}' \frac{|k\rangle \langle k|}{\omega + i\delta - E_k} - \frac{i}{\sqrt{1-\omega^2}} \left(\mu_0^Q + 2 \sum_{n=1}^{N-1} \mu_n^Q e^{-in \arccos(\omega)} \right) \tag{129}$$