7. Exact diagonalization

7.1 Hamiltonian operators for strongly correlated electron systems

7.1.1 The Hubbard model

The **Hubbard model** represents interacting electrons in narrow bands. It was originally proposed to study metal-insulator transitions and ferromagnetism of itinerant electrons in narrow bands but it has also acquired importance in the study of high temperature superconductors. Assuming localized orbitals and a strong screening of the Coulomb interaction, only the local density-density repulsion is included. The model is defined by

$$H = \underbrace{-t \sum_{<i,j>,\sigma} a^{\dagger}_{i\sigma} a_{j\sigma}}_{H_0} + \underbrace{U \sum_{i} n_{i\downarrow} n_{i\uparrow}}_{H_1} - \mu \hat{N} \tag{7.1}$$

where $a^{\dagger}_{i\sigma}(a_{i\sigma})$ create (annihilate) fermions of spin $\sigma = \downarrow, \uparrow$ in a Wannier orbital centered at site i. $n_{i\sigma} = a^{\dagger}_{i\sigma} a_{i\sigma}$ represents the occupation number operator. The electrons move in tight binding bands, with a transfer integral t between nearest neighbor sites, as indicated by $< i, j >$. The Coulomb interaction strength is U. The chemical potential μ couples to the particle number operator $\hat{N} = \sum_i (n_{i\downarrow} + n_{i\uparrow})$.

7.1.2 The t-J model

The **t-J model** consists of a constrained hopping term for the charge degrees of freedom, allowing no double occupancies. It can be derived as strong U limit of the Hubbard model. In the restricted space the eliminated double occupancies result in an effective spin-spin interaction:

$$H = t \sum_{<i,j>,\sigma} (1 - n_{i\,-\sigma}) a^{\dagger}_{i\sigma} a_{j\sigma} (1 - n_{j\,-\sigma}) + J \sum_{<i,j>} \left(\mathbf{S}_i \mathbf{S}_j - \frac{n_i n_j}{4} \right) \tag{7.2}$$

The projection operators $(1 - n_{i\,-\sigma})$ in the kinetic term ensure that no site is occupied by more than two electrons. The spin operators at site i

are $\mathbf{S}_i = \sum_{\sigma\sigma'} a^\dagger_{i\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} a^\dagger_{i\sigma'}$ with Pauli matrices $\boldsymbol{\sigma}_{\sigma\sigma'}$. S_i describes magnetic moments with $S = 1/2$ for occupied sites and $S = 0$ for empty sites. The t-J model can be viewed as a generic model for the interplay of spin and charge degrees of freedom.

7.1.3 The Heisenberg model

While the Hubbard type models treat itinerant electrons, the **Heisenberg Hamiltonian** describes the situation that the charge degrees of freedom are bound to the atomic positions and only the spin degrees of freedom remain active. This fundamental model in the theory of magnetism of local magnetic moments is defined by

$$H = \sum_{ij} J^z_{ij} S^z_i S^z_j + J^\perp_{ij} (S^x_i S^x_j + S^y_i S^y_j) + B \sum_i S^z_i \tag{7.3}$$

where $S^\alpha_i, \alpha = x, y, z$ is the α component of the spin operator and J stands for the exchange integrals. The last term describes the coupling to an external magnetic field B in z direction. Special cases are the isotropic Heisenberg model $J^z = J^\perp$, the Ising model $J^\perp = 0$ and the XY model $J^z = 0$. The spin operators obey

$$[S^\alpha_i, S^\beta_j] = i\delta_{ij} \epsilon_{\alpha\beta\gamma} S^\gamma_i \tag{7.4}$$

For numerical purposes it is convenient to use ladder operators

$$S^\pm_i = S^x_i \pm i\, S^y_i \tag{7.5}$$

so that the operators S^x and S^y can be written as

$$S^x_i = \frac{1}{2}(S^+_i + S^-_i) \qquad S^y_i = \frac{1}{2i}(S^+_i - S^-_i) \tag{7.6}$$

Replacing S^x and S^y in the Hamiltonian leads to

$$H = \sum_{i \neq j} \left(J^z_{ij} S^z_i S^z_j + \frac{1}{2}(S^+_i S^-_j + S^-_i S^+_j) \right) + B \sum_i S^z_i \tag{7.7}$$

7.2 Principle of the exact diagonalization method

To see why we have to employ special methods to make the diagonalization of Hamilton matrices possible, we have to consider the dimension of the

Hamilton matrix produced by a given lattice and model.
If we study the Heisenberg Hamiltonian on a lattice of N sites, we have two possible states for each site: Spin up and spin down. Thus the lattice has 2^N states, and this is the dimension of the Hamilton matrix. Similarly we find for the t-J model 3^N states and for the Hubbard model 4^N states. This exponential growth of the matrix with lattice size makes even small lattices of typically 10 sites difficult to handle with standard diagonalization techniques.
In order to make the matrix size for a given lattice size accessible to the available computing power, it is important to exploit the **model symmetries**.
Many models, including those given above, show conservation of total spin number, total spin in the z direction and total charge, *i.e.*

$$\left[H, \mathbf{S}^2\right] = \left[H, S^z\right] = [H, \hat{N}] = 0 \tag{7.8}$$

where H is the model Hamiltonian and

$$\mathbf{S} = \sum_i \mathbf{s}_i \qquad \hat{N} = \sum_i n_i \tag{7.9}$$

In addition, these operators also commute with each other

$$\left[\mathbf{S}^2, S^z\right] = \left[S^z, \hat{N}\right] = [\hat{N}, \mathbf{S}^2] = 0 \tag{7.10}$$

so that the eigenvalues of H, $\mathbf{S}^2$, S^z and $\hat{N}$ are simultaneous good quantum numbers which we can denote by E, $S(S+1)$, S^z and N.
In order to build the Hamilton matrix, we have to choose a basis set that is easily generated, allows fast computation of matrix elements, is economical with memory and allows us to access states quickly. We also have to find a numerical representation of the basis set.
For representing **spin-1/2 systems**, we can use integers $n_i = (\sigma_i + 1)/2 \in \{0, 1\}$. If we identify the sequence of n_i values with the bit pattern of the integer $I = \sum_{l=1}^{N} n_l 2^{l-1}$, the basis state $|\psi\rangle = |-1, +1, -1, +1\rangle$ is represented by $n = \{0101\}$ and mapped onto $I = 4$. This representation saves memory and speeds up some numerical operations.
As $S^z = \sum_{i=1}^{N} S_i^z$ commutes with the Hamiltonian, the Hamilton matrix is block diagonal in the sectors with fixed S^z values, *i.e.* fixed numbers N^σ of σ spins.

For a given S^z sector, the number of ones in the bit pattern is fixed which reduces the number of basis states to

$$L = \binom{N}{N^\uparrow} \tag{7.11}$$

where N is the number of lattice sites and

$$S^z = \frac{1}{2}\left(2N^\uparrow - N\right) \tag{7.12}$$

For example, if the number of sites is $N = 16$ there are $2^{16} = 65536$ possible basis states in total, but only $\binom{16}{8} = 12870$ for $S^z = 0$, *i.e.* $N^\uparrow = N^\downarrow = 8$. In principle, translation and rotation could be exploited to reduce the number of basis states even further.

Now we are ready to list all permissible configurations. Not every integer is included since the number of ones and zeros in the bit pattern is fixed. We generate the basis states in such a way that the corresponding integer values are in increasing order. The basis states and their integer representations are therefore

$$\begin{aligned}
|\phi_1\rangle &= \{\overbrace{0,0,\ldots,0,0}^{N-N^\uparrow},\overbrace{1,1,1,\ldots,1}^{N^\uparrow}\}; \quad I_1 = 2^{N^\uparrow} - 1 \\
|\phi_2\rangle &= \{0,0,\ldots,0,1,0,1,1,\ldots,1\}; \quad I_2 = 2^{N^\uparrow+1} - 1 - 2^{N^\uparrow-1} \\
|\phi_3\rangle &= \{0,0,\ldots,0,1,1,0,1,\ldots,1\}; \quad I_3 = 2^{N^\uparrow+1} - 1 - 2^{N^\uparrow-2} \\
&\vdots \quad \vdots \\
|\phi_L\rangle &= \{\underbrace{1,1,\ldots,1,1}_{N^\uparrow},\underbrace{0,0,0,\ldots,0}_{N-N^\uparrow}\}; \quad I_L = 2^N - 2^{N-N^\uparrow}
\end{aligned} \tag{7.13}$$

Consider a four site cluster with $S^z = 0$ as an example:

number	1	2	3	4	5	6
bit	0011	0101	0100	1001	1010	1100
integer	3	5	6	9	10	12

As the basis states are ordered, their spin representations can be found rapidly by bisection search.

Representation of **electronic systems**: The basis for Hubbard, Anderson or t-J Hamiltonians can be conveniently constructed in real space. Restricting the discussion to a single orbital per lattice site, the state vector can

be writen as

$$|\psi\rangle = \prod_{i=1}^{N^\uparrow} a^\dagger_{\Gamma_i^\uparrow} \prod_{j=1}^{N^\downarrow} a^\dagger_{\Gamma_j^\downarrow} |0\rangle \tag{7.14}$$

where $|0\rangle$ denotes the vacuum state and $\Gamma_i^\uparrow$ is the lattice site of the i-th spin up electron and $\Gamma_j^\downarrow$ is the lattice site of the j-th spin down electron. For example

$$|\psi\rangle = \left| \begin{matrix} 1 & 2 & 3 & 4 \\ \uparrow & \sqcup & \downarrow & \Updownarrow \end{matrix} \right\rangle \tag{7.15}$$

is represented by $\Gamma^\uparrow = \{1, 4\}$ and $\Gamma^\downarrow = \{3, 4\}$

Another way of representing this basis is by

$$|\psi\rangle = \prod_{i=1}^{N} \left(a^\dagger_{i\uparrow}\right)^{n_i^\uparrow} \prod_{j=1}^{N} \left(a^\dagger_{j\downarrow}\right)^{n_j^\downarrow} |0\rangle \tag{7.16}$$

where $n_i^\uparrow, n_j^\downarrow \in \{0, 1\}$ indicate whether or not site i is occupied by a spin up or spin down electron. The state Eq. (7.15) is represented by $n^\uparrow = \{1, 0, 0, 1\}$ and $n^\downarrow = \{0, 0, 1, 1\}$.
Yet another way to encode the same basis is

$$|\psi\rangle = \prod_{i=1}^{N} O_i |0\rangle \quad O_i \in \{\hat{1}, a^\dagger_{i\uparrow}, a^\dagger_{i\downarrow}, a^\dagger_{i\uparrow} a^\dagger_{i\downarrow}\} \tag{7.17}$$

where the operator O_i creates either an empty site, a site occupied by an up or down electron, or a doubly occupied site.
The number of basis states is 4^N. In the case of the t-J model, doubly occupied site are forbidden and therefore the number of basis states reduces to 3^N.
Since the electronic spin is conserved, $N^\uparrow$ and $N^\downarrow$ are good quantum numbers. For spin σ there are

$$L^\sigma = \binom{N}{N^\sigma} \tag{7.18}$$

basis states. The total number of basis states in the sector of fixed N^σ values $N^\uparrow, N^\downarrow$ is therefore

$$L = L^\uparrow L^\downarrow = \binom{N}{N^\uparrow} \binom{N}{N^\downarrow} \tag{7.19}$$

For example, $N = 16$ and $N^{\uparrow} = N^{\downarrow} = 8$. The number of basis states is then $4^{16} = 4\,294\,967\,296$, while $\binom{16}{8}\binom{16}{8} = 165\,636\,900$.
In the t-J model there the additional constraint of no double occupancy reduces the number of basis states to (below half-filling)

$$L = \frac{N!}{N^{\downarrow}!\, N^{\uparrow}!\, N^{h}!} \tag{7.20}$$

where $N^{h} = N - N^{\downarrow} - N^{\uparrow}$ is the number of empty sites (holes). In the previous example, the number of states would only be $L = 12870$.

As before, it is recommended to use a memory saving representation, and for that Eq. (7.16) is well suited because the two spin species are separately treated and we can interpret the sequence of values of n_i^{σ} as a bit pattern. Then in the example above $n^{\uparrow} = \{1, 0, 0, 1\}$ corresponds to the integer $I^{\uparrow} = 9$, $n^{\downarrow} = \{0, 0, 1, 1\}$ corresponds to $I^{\downarrow} = 3$. Each basis state is therefore represented as a pair of integers $(I^{\uparrow}, I^{\downarrow})$.
The generation of basis states is now similar to that of spin-1/2 systems. The only difference is that we have to generate two integers for the two spin species.

7.2.1 Computation of the Hamilton matrix

Now we have to calculate the matrix elements

$$h_{\nu'\nu} = \langle \Phi_{\nu'} | H | \Phi_{\nu} \rangle \tag{7.21}$$

of the Hamiltonian H in suitable basis states $|\Phi_{\nu}\rangle$. For this purpose we split the Hamiltonian into individual contributions $H^{(l)}$

$$H = \sum_{l} H^{(l)} \tag{7.22}$$

such that the application of one term $H^{(l)}$ to a basis state $|\Phi_{\nu}\rangle$ yields again a basis state or the null vector:

$$H^{(l)} |\Phi_{\nu}\rangle = h^{(l)}_{\nu'\nu} |\Phi_{\nu'}\rangle \tag{7.23}$$

The full matrix element $\langle \Phi_{\nu'} | H | \Phi_{\nu} \rangle$ is obtained by summing up all contributions $h^{(l)}_{\nu'\nu}$. If there is only one term $H^{(l)}$ in the Hamiltonian that mediates between the two basis states $|\Phi_{\nu}\rangle$ and $|\Phi_{\nu'}\rangle$ then $h_{\nu'\nu} = h^{(l)}_{\nu'\nu}$.

Let's consider building the Hubbard Hamilton matrix in the real space basis of Eq. (7.16) characterized by the set of occupation numbers $|\Phi_\nu\rangle = |\{n^\nu_{i\sigma}\}\rangle$ for all lattice sites i and the two spin directions, with $n^\nu_{i\sigma} \in \{0, 1\}$. The Hubbard interaction H_1 of Eq. (7.1) is diagonal in this basis, so we have

$$h_{\nu\nu} = U \sum_i n^\nu_{i\uparrow} n^\nu_{i\downarrow} \tag{7.24}$$

There are no other contributions to the diagonal elements. Each summand in the kinetic energy of Eq. (7.1) represents an individual contribution to Eq.(7.22). But it is better to combine the back-and-forth hopping processes for a particular nearest-neighbour pair (i_0, j_0)

$$H^{(l)}_0 = -t\big(a^\dagger_{i_0\sigma_0} a_{j_0\sigma_0} + a^\dagger_{j_0\sigma_0} a_{i_0\sigma_0}\big) \tag{7.25}$$

Application of this term $H^{(l)}_0$ to a basis state $|\Phi_\nu\rangle = |\{n^\nu_{i\sigma}\}\rangle$ results either in the null vector if $n^\nu_{i_0\sigma_0}$ and $n^\nu_{j_0\sigma_0}$ are both occupied or empty

$$H^{(l)}_0 |\{n^\nu_{i\sigma}\}\rangle = 0 \qquad \text{if } n^\nu_{i_0\sigma_0} = n^\nu_{j_0\sigma_0} \tag{7.26}$$

Otherwise the hopping process is possible and results in another basis state $|\Phi_{\nu'}\rangle = |\{n^{\nu'}_{i\sigma}\}\rangle$ which differs from $|\Phi_\nu\rangle$ only in the exchange of the occupation number $n^\nu_{i_0\sigma_0}$ and $n^\nu_{j_0\sigma_0}$, *i.e.*

$$\begin{aligned} n^{\nu'}_{i\,-\sigma_0} &= n^\nu_{i\,-\sigma_0} \quad \forall i \\ n^{\nu'}_{i\sigma_0} &= n^\nu_{i\sigma_0} \qquad \forall i \neq i_0, j_0 \\ n^{\nu'}_{i_0\sigma_0} &= n^\nu_{j_0\sigma_0} \qquad n^{\nu'}_{j_0\sigma_0} = n^\nu_{i_0\sigma_0} \end{aligned} \tag{7.27}$$

There is only one hopping process $H^{(l)}$ mediating between the two basis states under consideration.
The respective matrix element is therefore

$$h_{\nu'\nu} = \begin{cases} -t\,S & \text{if } n^\nu_{i_0\sigma_0} \neq n^\nu_{j_0\sigma_0} \text{ for one set } (i_0\sigma_0, j_0\sigma_0) \\ 0 & \text{otherwise} \end{cases} \tag{7.28}$$

The hopping process can result in a sign S due to the Fermi statistics of the electrons. Consider for example a two-dimensional (4x4) lattice with sites enumerated as

$$\begin{array}{cccc} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{array}$$

(The numbering of sites is arbitrary but must be kept fixed.)
Now we consider hopping between sites 2 and 6 of one spin species The state $|\Phi_\nu\rangle$ be given by $\{n_{i\sigma}\} = \{0,0,1,1,\ 1,1,0,0,\ 0,0,0,0,\ 0,0,0,0\}$ (we suppress the spin indices from now on). The state reads according to Eq. (7.16)

$$|\Phi_\nu\rangle = a_3^\dagger a_4^\dagger a_5^\dagger a_6^\dagger |0\rangle \tag{7.29}$$

Application of the hopping operator

$$H_0^{(l)} = -t\big(a_2^\dagger a_6 + a_6^\dagger a_2\big) \tag{7.30}$$

results in the state

$$|\Phi_{\nu'}\rangle = a_3^\dagger a_4^\dagger a_5^\dagger a_2^\dagger |0\rangle = -a_2^\dagger a_3^\dagger a_4^\dagger a_5^\dagger |0\rangle \tag{7.31}$$

Thus, the new state is given by

$$|\Phi_{\nu'}\rangle = -\{0,1,1,1,\ 1,0,0,0,\ 0,0,0,0,\ 0,0,0,0\} \tag{7.32}$$

The hopping operator has shifted a bit and created a fermionic phase factor. For periodic boundary conditions, care must be taken of possible minus signs whenever an electron is wrapped around the boundary and the number of electrons it commutes through is odd. The sign is given by

$$S = (-1)^{\Delta n} \tag{7.33}$$

where Δn is the number of electrons at the lattice sites between the site i_0 and j_0, in the example $\Delta n = 3$.

Now that we know how the individual terms of the Hamiltonian $H^{(l)}$ couple a basis state $\{n_{i\sigma}^\nu\}$ represented by a bit pattern to another basis state $\{n_{i\sigma}^{\nu'}\}$ or to its integer representation $(I_\uparrow^{\nu'} I_\downarrow^{\nu'})$.

It is still necessary to find the index ν' of the basis state. As they have been generated in increasing order of their integer representation, we can apply a bisection search to find the index. This is important if we compare the computational cost $O(L)$ steps of a brute force search to $O(\log_2 L)$ operations of the bisection search. For example, for $L = 10^8$ there is a factor of 10^6 between the two methods.

7.3 The Lanczos method

In the previous section, exact diagonalization was introduced as a method to solve manybody Hamiltonians by calculating the Hamiltonian matrix

in a basis and diagonalizing it. But the corresponding matrices are of the order $(10^8 \times 10^8)$ or larger and cannot be treated by Householder tridiagonalization.
The **Lanczos** (pronounced ['la:ntsoʃ]) **method** avoids the problem of calculating and saving huge matrices in the computer memory by constructing a basis that directly leads to a tridiagonal matrix. It is an example of a family of projection techniques known as Krylov subspace methods.
The procedure is as follows. Consider an arbitrary normalized wave function $|\Phi_1\rangle$ which we assume not to be an eigenvector of the Hamiltonian $\hat{\mathsf{H}}$. Then application of $\hat{\mathsf{H}}$ on this wave function produces a function $|\mathbf{U}_1\rangle$ that is different from $|\Phi_1\rangle$:

$$\hat{\mathsf{H}}|\Phi_1\rangle = |\mathbf{U}_1\rangle \tag{7.34}$$

In general, $|\mathbf{U}_1\rangle$ will not be normalized, and we can determine the normalization constant N_1 from

$$\langle \mathbf{U}_1|\mathbf{U}_1\rangle = \mathsf{N}_1^2 \tag{7.35}$$

A normalized vector $|\Psi_1\rangle$ is obtained by

$$|\Psi_1\rangle = \mathsf{N}_1^{-1}|\mathbf{U}_1\rangle \tag{7.36}$$

As $|\Phi_1\rangle$ is not an eigenvector of $\hat{\mathsf{H}}$, $|\Psi_1\rangle$ and $|\Phi_1\rangle$ are different, and we can write $|\Psi_1\rangle$ as a linear combination of $|\Phi_1\rangle$ and another function $|\Phi_2\rangle$ which we conveniently chose to be normalized and orthogonal to $|\Phi_1\rangle$:

$$\langle \Phi_2|\Phi_2\rangle = 1 \qquad \langle \Phi_2|\Phi_1\rangle = 0 \tag{7.37}$$

Now we can write $|\Psi_1\rangle$ as

$$|\Psi_1\rangle = \alpha_1|\Phi_1\rangle + \beta_1|\Phi_2\rangle \qquad \text{with } \alpha_1^2 + \beta_1^2 = 1 \tag{7.38}$$

If we multiply both sides of Eq. (7.34) by $\langle \Phi_1|$ and integrate over all independent variables, we find

$$\langle \Phi_1|\hat{\mathsf{H}}|\Phi_1\rangle = \mathsf{N}_1\langle \Phi_1|\Psi_1\rangle = \alpha_1\mathsf{N}_1 \tag{7.39}$$

As N_1 is known from Eq. (7.35), we find α_1 by calculating the diagonal matrix element of $\hat{\mathsf{H}}$ with $|\Phi_1\rangle$. With Eq. (7.38) we find

$$|\Phi_2\rangle = \frac{1}{\beta_1}\big(|\Psi_1\rangle - \alpha_1|\Phi_1\rangle\big) \tag{7.40}$$

The value of β_1 can be found from Eq. (7.38) or from the normalization requirement of $|\Phi_2\rangle$. This is very similar to the Gram-Schmidt orthogonalization method of constructing a set of orthonormal vectors from an arbitrary set. Now we can define two more quantities:

$$\mathsf{d}_1 \equiv \langle\Phi_1|\hat{\mathsf{H}}|\Phi_1\rangle = \alpha_1 \mathsf{N}_1 \tag{7.41}$$

$$\mathsf{f}_2 \equiv \langle\Phi_2|\hat{\mathsf{H}}|\Phi_1\rangle = \mathsf{N}_1\langle\Phi_2|\Psi_1\rangle = \beta_1 \mathsf{N}_1 \tag{7.42}$$

These will turn out to be the first diagonal and superdiagonal elements we are looking for. Now we apply $\hat{\mathsf{H}}$ on $|\Phi_2\rangle$ which in general also will not be an eigenvector:

$$\hat{\mathsf{H}}|\Phi_2\rangle = \mathsf{N}_2|\Psi_2\rangle \tag{7.43}$$

where again $|\Psi_2\rangle$ is a normalized state, N_2 is a constant. $|\Psi_2\rangle$ cannot be a linear combination of $|\Phi_1\rangle$ and $|\Phi_2\rangle$ alone (the reason is given later), and we express it as a linear combination with yet another function $|\Phi_3\rangle$ thrown in:

$$|\Psi_2\rangle = \alpha_2|\Phi_1\rangle + \beta_2|\Phi_2\rangle + \gamma_2|\Phi_3\rangle \tag{7.44}$$

Choosing $|\Phi_3\rangle$ normalized and orthogonal to $|\Phi_1\rangle$ and $|\Phi_2\rangle$ gives us the condition (obtained by squaring Eq. (7.44) and integrating over all independent variables).

$$\alpha_2^2 + \beta_2^2 + \gamma_2^2 = 1 \tag{7.45}$$

From the fact that the Hamiltonian is Hermitian, we find that

$$\langle\Phi_2|\hat{\mathsf{H}}|\Phi_1\rangle = \langle\Phi_1|\hat{\mathsf{H}}|\Phi_2\rangle = \mathsf{f}_2 \tag{7.46}$$

On the other hand, from Eqs. (7.43) and (7.44) we find

$$\langle\Phi_1|\hat{\mathsf{H}}|\Phi_2\rangle = \mathsf{N}_2\langle\Phi_1|\Psi_2\rangle = \mathsf{N}_2\alpha_2 \tag{7.47}$$

which gives us the value of $\alpha_2 = \mathsf{f}_2/\mathsf{N}_2$. With $|\Phi_2\rangle$ we obtain

$$\mathsf{d}_2 \equiv \langle\Phi_2|\hat{\mathsf{H}}|\Phi_2\rangle = \mathsf{N}_2\langle\Phi_2|\Psi_2\rangle = \mathsf{N}_2\beta_2 \tag{7.48}$$

and thus $\beta_2 = \mathsf{d}_2/\mathsf{N}_2$.
We can write

$$|\Phi_3\rangle = \frac{1}{\gamma_2}\big(|\Psi_2\rangle - \alpha_2|\Phi_1\rangle - \beta_2|\Phi_2\rangle\big) \tag{7.49}$$

and we define again

$$f_3 \equiv \langle \Phi_3 | \hat{H} | \Phi_2 \rangle \tag{7.50}$$

Note that the matrix element

$$\langle \Phi_3 | \hat{H} | \Phi_1 \rangle = 0 \tag{7.51}$$

because the state produced by the action of $\hat{H}$ on $|\Phi_1\rangle$ is only a linear combination of $|\Phi_1\rangle$ and $|\Phi_2\rangle$, both orthogonal to $|\Phi_3\rangle$. Another application of the Hamiltonian gives the next step in this argument:

$$\hat{H} | \Phi_3 \rangle = N_3 | \Psi_3 \rangle \tag{7.52}$$

Eq. (7.51) and the Hermitian Hamiltonian yield

$$\langle \Phi_1 | \hat{H} | \Phi_3 \rangle = 0 \tag{7.53}$$

This is because by construction the only offdiagonal matrix element of $\hat{H}$ acting on $|\Phi_1\rangle$ is $\langle \Phi_2 | \hat{H} | \Phi_1 \rangle$. It also implies that $|\Psi_3\rangle$ is orthogonal to $|\Phi_1\rangle$. Thus, $|\Psi_3\rangle$ can only be a linear combination of $|\Phi_2\rangle$, $|\Phi_3\rangle$ and a new function $|\Phi_4\rangle$:

$$|\Psi_3\rangle = \alpha_3 |\Phi_2\rangle + \beta_3 |\Phi_3\rangle + \gamma_3 |\Phi_4\rangle \tag{7.54}$$

As before, $|\Phi_4\rangle$ is chosen normalized and orthogonal to $|\Phi_2\rangle$ and $|\Phi_3\rangle$. As $|\Psi_3\rangle$ is orthogonal to $|\Phi_1\rangle$, $|\Phi_4\rangle$ must also be orthogonal to $|\Phi_1\rangle$. Eq. (7.54) already provides the general relation. If we continue to construct basis vectors $|\Phi_1\rangle, |\Phi_2\rangle, \ldots$ until we get to $|\Phi_k\rangle$, we have the relation

$$\hat{H} | \Phi_k \rangle = N_k | \Psi_k \rangle \tag{7.55}$$

in analogy to Eq. (7.43).
It is always possible to express the new state $|\Psi_k\rangle$ as a linear combination of three components

$$|\Psi_k\rangle = \alpha_k |\Phi_{k-1}\rangle + \beta_k |\Phi_k\rangle + \gamma_k |\Phi_{k+1}\rangle \tag{7.56}$$

as demonstrated for $|\Psi_3\rangle$ in Eq. (7.54). The new vector $|\Phi_{k+1}\rangle$ can be made orthogonal to all the previous basis vectors $|\Phi_1\rangle, |\Phi_2\rangle, \ldots, |\Phi_k\rangle$. Furthermore, we see that the Hamiltonian matrix is tridiagonal in the basis formed by $|\Phi_1\rangle, |\Phi_2\rangle, \ldots$.

An exception to Eq. (7.56) occurs when the dimension n of the Hilbert space is finite; in this case, the maximum number of linearly independent basis states that can be constructed is n.
When we reach $k = n$, all required states have been found and no new ones can be generated. Thus

$$|\Phi_{n+1}\rangle = 0 \tag{7.57}$$

What if $\gamma_k = 0$ at some stage for $k < n$ of the basis state construction? This implies that the action of $\hat{H}$ on $|\Phi_k\rangle$ does not contain any component that is not already in the basis states already found. Numerical inaccuracy aside this can only happen if the Hilbert space for the problem consists of two or more independent subspaces. This is closely related to the case when for a tridiagonalized matrix a superdiagonal element $f_k = 0$. This also explains why $|\Psi_2\rangle$ in Eq. (7.44) was written as a linear combination of three mutually orthogonal functions.
In practice, for large n values of γ_k that are close to zero can actually occur due to truncation errors, but the strength of the Lanczos method is that often it may be sufficient for a physical problem to generate only a small fraction of the total number of tridiagonal basis states.
For the general recursion, we label the tridiagonal matrix elements as

$$d_k = \langle\Phi_k|\hat{H}|\Phi_k\rangle \qquad f_k = \langle\Phi_{k-1}|\hat{H}|\Phi_k\rangle \tag{7.58}$$

and find that in general

$$\hat{H}|\Phi_k\rangle = f_k|\Phi_{k-1}\rangle + d_k|\Phi_k\rangle + f_{k+1}|\Phi_{k+1}\rangle \tag{7.59}$$

As an illustration to the working of the Lanczos method, consider finding the ground state energy of a system. From physical intuition we can often guess a starting state $|\Phi_1\rangle$ that is not too far away from the ground state. But as $|\Phi_1\rangle$ is not going to be an eigenfunction, the matrix element $d_1 = \langle\Phi_1|\hat{H}|\Phi_1\rangle$ is not the ground state energy. In fact, if the true ground state energy is denoted by $\mathcal{E}_1$, we expect $d_1 \geqslant \mathcal{E}_1$. Constructing a second basis state $|\Phi_2\rangle$, we can find d_2 and f_2. In this enlarged active space of two tridiagonal basis states, we expect to produce an eigenvector that is a better approximation of the ground state. Let λ_1 be the lower of the eigenvalues formed by the (2×2) matrix formed from d_1, d_2 and f_2. Being a better approximation, we expect λ_1 to be lower in value that d_1 but still higher than $\mathcal{E}_1$. If we proceed to add more tridiagonal basis states to the calculation, we will see the lowest eigenvalue of the growing matrix converge to

the ground state. As in many physical problems this convergence is fast, an active space that is only a small fraction of the complete Hilbert space is sufficient to obtain the ground state energy.

Summary of the Lanczos method

1) Arbitrary normalized $|\Phi_1\rangle$ as starting point.

2) $|\Phi_2\rangle = \frac{1}{f_2}\big(H|\Phi_1\rangle - d_1|\Phi_1\rangle\big)$

3) Iteration

$$|\Phi_{k+1}\rangle = \frac{1}{f_{k+1}}\big(H|\Phi_k\rangle - d_k|\Phi_k\rangle - f_k|\Phi_{k-1}\rangle\big) = \frac{|\gamma_k\rangle}{f_{k+1}} \tag{7.60}$$

with

$$d_k = \langle\Phi_k|H|\Phi_k\rangle, \qquad f_k = \langle\gamma_k|\gamma_k\rangle^{-1}$$

First $|\gamma_k\rangle$ is generated, then normalized to obtain f_{k+1}.

4) The Hamiltonian matrix is

$$\begin{aligned} \langle\Phi_{k-1}|H|\Phi_k\rangle &= f_k \\ \langle\Phi_k|H|\Phi_k\rangle &= d_k \\ \langle\Phi_{k+1}|H|\Phi_k\rangle &= f_{k+1} \end{aligned} \tag{7.61}$$

7.3.1 Lanczos for the anharmonic oscillator

After the abstract discussion of the tridiagonal basis states $|\Phi_i\rangle$ we will now discuss the Lanczos method in terms of some known functions. Let us consider a complete set of orthonormal functions $|\phi_j\rangle$ for $j = 1, 2, \ldots, n$ and express each tridiagonal state in terms of a linear combination

$$|\Phi_i\rangle = \sum_{j=1}^{n} c_{ij}|\phi_j\rangle \tag{7.62}$$

For a given set of $|\phi_j\rangle$ the function $|\Phi_i\rangle$ is completely specified by the coefficients c_{ij}. The $|\phi_j\rangle$ should be chosen both on physical grounds and for mathematical convenience. For example, as in the mentioned example of the anharmonic oscillator $\hat{H} = \mathcal{H}_0 + \mathcal{H}'$, the eigenfunctions of the harmonic oscillator $\mathcal{H}_0$ are a good choice.

Once we also chose a starting tridiagonal basis state $|\Phi_1\rangle$ we have

$$|\Phi_1\rangle = \sum_{j=1}^{n} c_{1j}|\phi_j\rangle \tag{7.63}$$

and proceed as in the abstract example starting with Eq. (7.34):

$$\begin{aligned} |U_1\rangle = \hat{H}|\Phi_1\rangle &= \sum_{j=1}^{n} c_{1j}\hat{H}|\phi_j\rangle \\ &= \sum_{j=1}^{n} c_{1j} \sum_{k=1}^{n} |\phi_k\rangle\langle\phi_k|\hat{H}|\phi_j\rangle = \sum_{k=1}^{n} g_{1k}|\phi_k\rangle \end{aligned} \tag{7.64}$$

where we used the closure property of the set of states and

$$g_{1k} = \sum_{j=1}^{n} c_{1j}\langle\phi_k|\hat{H}|\phi_j\rangle = \sum_{j=1}^{n} c_{1j}H_{kj} \tag{7.65}$$

The Hamiltonian matrix elements are abbreviated by $H_{kj} = \langle\phi_k|\hat{H}|\phi_j\rangle$. Thus we find for the first matrix element

$$d_1 = \langle\Phi_1|\hat{H}|\Phi_1\rangle = \sum_{i,j} c_{1i}c_{1j}H_{ij} \tag{7.66}$$

This can be evaluated by calculating H_{ij} and from the known c_{1i}. Next we determine

$$|\Phi_2\rangle = \sum_{j=1}^{n} c_{2j}\hat{H}|\phi_j\rangle \tag{7.67}$$

with the help of Eq. (7.59) and Eq. (7.64):

$$\hat{H}|\Phi_1\rangle = d_1|\Phi_1\rangle + f_2|\Phi_2\rangle = \sum_{j=1}^{n} g_{1j}|\phi_j\rangle \tag{7.68}$$

Since the basis states are linearly independent, we obtain the relation for the c_{2i} by comparing coefficients:

$$f_2 c_{2j} = g_{1j} - d_1 c_{1j} \tag{7.69}$$

Using the normalization of $|\Phi_2\rangle$ we have $\sum_j c_{2j}^2 = 1$ and thus

$$f_2^2 = \sum_{j=1}^{n} \left(g_{1j} - d_1 c_{1j}\right)^2 \tag{7.70}$$

With f_2 we obtain the values of the coefficients

$$c_{2j} = \frac{g_{1j} - d_1 c_{1j}}{|f_2|} \qquad \text{for } j = 1, 2, \ldots, n. \tag{7.71}$$

There is an overall abiguity of the sign in all coefficients c_{2j} which also affects f_2

$$f_2 = \langle \Phi_1 | \hat{H} | \Phi_2 \rangle = \sum_{ij} c_{1i} c_{2j} H_{ij} \tag{7.72}$$

but not d_2

$$d_2 = \langle \Phi_2 | \hat{H} | \Phi_2 \rangle = \sum_{ij} c_{2i} c_{2j} H_{ij} \tag{7.73}$$

and has no physical consequence.
To derive the general equations, let us assume that we have already proceeded until $|\Phi_k\rangle$ with all coefficients $c_{1j}, c_{2j}, \ldots, c_{kj}$ known. The input quantities needed to calculate the state

$$|\Phi_{k+1}\rangle = \sum_{j=1}^{n} c_{k+1\,j} |\phi_j\rangle \tag{7.74}$$

are diagonal and superdiagonal elements d_k and f_k and coefficients $c_{k-1\,j}$ and c_{kj}. Let

$$|U_k\rangle = \hat{H} |\Phi_k\rangle = \sum_{j=1}^{n} g_{kj} |\phi_j\rangle \quad \text{with } g_{kj} = \sum_{l=1}^{n} c_{kl} H_{jl} \tag{7.75}$$

On the other hand, we have Eq. (7.59)

$$\hat{H} |\Phi_k\rangle = f_k |\Phi_{k-1}\rangle + d_k |\Phi_k\rangle + f_{k+1} |\Phi_{k+1}\rangle \tag{7.76}$$

At this point, f_{k+1} and the $c_{k+1\,j}$ are still unknown. Using Eqs. (7.76) and (7.75), we find for the coefficients

$$f_{k+1} c_{k+1\,j} = g_{kj} - f_k c_{k-1\,j} - d_k c_{kj} \tag{7.77}$$

and with the normalization of $|\Phi_k\rangle$ giving $\sum_j c_{k+1\,j}^2 = 1$ we have

$$f_{k+1}^2 = \sum_{j=1}^{n} \left(g_{kj} - f_k c_{k-1\,j} - d_k c_{kj} \right)^2 \tag{7.78}$$

This yields the value of f_{k+1} up to a sign. Using this, we get the coefficents of $|\Phi_k\rangle$:

$$c_{k+1\,j} = \frac{g_{kj} - f_k c_{k-1\,j} - d_k c_{kj}}{|f_{k+1}|} \tag{7.79}$$

This also allows us to calculate

$$d_{k+1} = \sum_{ij} c_{k+1\,i} c_{k+1\,j} H_{ij} \tag{7.80}$$

This completes the calculations that are necessary for a new tridiagonal basis state. We can now proceed until we have a reasonable number of diagonal and superdiagonal elements and then diagonalize by bisection or QL decomposition. By comparing results for different matrix sizes we can decide whether we have enough tridiagonal basis states in the active space. Let us apply the Lanczos method to the anharmonic oscillator with the Hamiltonian

$$\hat{H} = \mathcal{H}_0 + \mathcal{H}' = -\frac{\hbar}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 + \epsilon\hbar\omega\left(\frac{\mu\omega}{\hbar}\right)^2 x^4 \tag{7.81}$$

With the dimensionless quantity $\rho = x\sqrt{\mu\omega/\hbar}$ the anharmonic term becomes

$$\mathcal{H}' = \epsilon\hbar\omega\rho^4 \tag{7.82}$$

Now we choose the harmonic oscillater wave function as basis states (with the notation $|\phi_i\rangle = |\psi_{i-1}(\rho)\rangle$):

$$\psi_m(\rho) = \frac{1}{\sqrt{2^m m!\sqrt{\pi}}}\, e^{-\rho^2/2}\, H_m(\rho) \tag{7.83}$$

They are eigenfunctions of $\mathcal{H}_0$:

$$\mathcal{H}_0\psi_m = \left(m + \frac{1}{2}\right)\hbar\omega\psi_m \tag{7.84}$$

We now have to determine the matrix elements

$$H_{ij} \equiv \langle\phi_i|\hat{H}|\phi_j\rangle = \langle\psi_{i-1}|\mathcal{H}_0 + \epsilon\hbar\omega\rho^4|\psi_{i-1}\rangle \tag{7.85}$$

With Eq. (7.84) we have

$$\langle\psi_{i-1}|\mathcal{H}_0 + \epsilon\hbar\omega\rho^4|\psi_{i-1}\rangle = \left(i - \frac{1}{2}\right)\hbar\omega\delta_{ij} + \epsilon\hbar\omega\langle\psi_{i-1}|\rho^4|\psi_{i-1}\rangle \tag{7.86}$$

For $m = \min(i, j) - 1$ the matrix elements of ρ^4 are

$$\langle \psi_{i-1}|\rho^4|\psi_{i-1}\rangle = \begin{cases} \frac{3}{2}\left(m^2 + m + \frac{1}{2}\right) & \text{for } i = j \\ \left(m + \frac{3}{2}\right)\sqrt{(m+1)(m+2)} & \text{for } i = j \pm 2 \\ \frac{1}{4}\sqrt{(m+1)(m+2)(m+3)(m+4)} & \text{for } i = j \pm 4 \\ 0 & \text{otherwise} \end{cases} \tag{7.87}$$

A reasonable starting point for constructing the tridiagonal basis states is the ground state of the harmonic oscillator:

$$|\Phi_1\rangle = |\phi_1\rangle \equiv |\psi_0(\rho)\rangle \tag{7.88}$$

This corresponds to the coefficients

$$c_{1j} = \begin{cases} 1 & \text{for } j = 1 \\ 0 & \text{otherwise} \end{cases} \tag{7.89}$$

The first diagonal matrix element in the tridiagonal basis is then

$$d_1 = \langle \Phi_1|\hat{H}|\Phi_1\rangle = \langle \psi_0|\mathcal{H}_0 + \epsilon\hbar\omega\rho^4|\psi_0\rangle = \left(\frac{1}{2} + \frac{3\epsilon}{4}\right)\hbar\omega \tag{7.90}$$

To obtain $|\Phi_2\rangle$ we use Eq. (7.64) to obtain

$$g_{1k} = \sum_{j=1}^{n} c_{1j}H_{kj} = H_{k1} = \begin{cases} d_1 & \text{for } k = 1 \\ \frac{3}{\sqrt{2}}\hbar\omega\epsilon & \text{for } k = 3 \\ \sqrt{\frac{3}{2}}\hbar\omega\epsilon & \text{for } k = 5 \\ 0 & \text{otherwise} \end{cases} \tag{7.91}$$

From these we get

$$f_2^2 = \hbar^2\omega^2\epsilon^2\left(\frac{9}{2} + \frac{3}{2}\right) = 6\hbar^2\omega^2\epsilon^2 \tag{7.92}$$

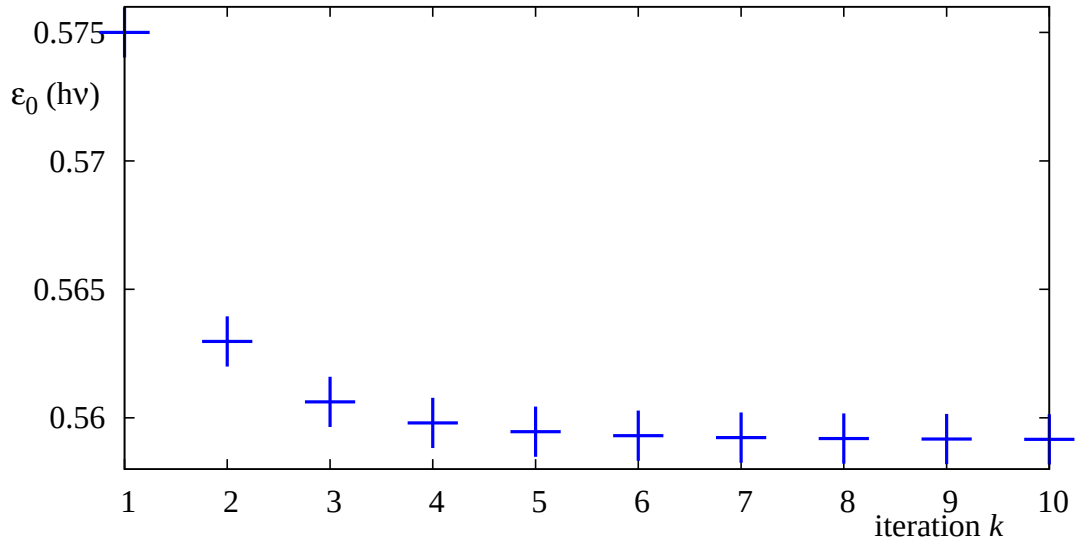
and the values of the coefficients c_{2j}

$$c_{2j} = \left\{0, 0, \frac{\sqrt{3}}{2}, 0, \frac{1}{2}, 0, 0, \ldots, 0\right\} \tag{7.93}$$

The rest of the calculations can be carried out iteratively. For $k \geqslant 2$ we can calculate d_k from

$$d_k = \sum_{ij} = c_{ki}c_{kj}H_{ij} \tag{7.94}$$

and the f_k can be obtained from Eq. (7.78). For each $k \geqslant 2$ the calculations proceeds in the order f_k, c_{kj}, d_k, g_{kj}.
If we repeatedly diagonalize the tridiagonal matrix for each $k = 2, 3, \ldots$, we obtain the following sequence of ground state energies $\mathcal{E}_0$ for $\epsilon = 0.1$.



It is clear that with $k = 10$ steps we already have converged the ground state energy up to an error smaller than $10^{-3}\hbar\omega$.

7.4 Calculation of the Greens function

For an operator $\hat{O}$ the retarded Green's function is defined by

$$\langle\langle \hat{O}(t); \hat{O}^\dagger \rangle\rangle \stackrel{\text{def}}{=} -i\Theta(t)\big(\langle \hat{O}(t)\hat{O}^\dagger\rangle - \varepsilon\langle \hat{O}^\dagger \hat{O}(t)\rangle\big) \tag{7.95}$$

where in the second line the symbol $\langle\rangle$ denotes the thermodynamic average. Commutator ($\varepsilon = +1$) and anticommutator ($\varepsilon = -1$) Green's functions can be chosen. At zero temperature, the average corresponds to the expectation value of the operators in the ground state $|\psi_0\rangle$ of the many-particle system. Here we focus on $T = 0$.

We proceed by inserting the Heisenberg time evolution of the operator $\hat{O}$

$$\hat{O}(t) = e^{i\hat{H}t}\hat{O}(t)e^{-i\hat{H}t} \quad \text{with } \hat{O} = \hat{O}(t=0) \tag{7.96}$$

into Eq. (7.95).
Since $|\psi_0\rangle$ is the exact ground-state with energy E_0 we have

$$e^{-i\hat{H}t}|\psi_0\rangle = e^{-iE_0t}|\psi_0\rangle \qquad e^{i\hat{H}t}|\psi_0\rangle = e^{iE_0t}|\psi_0\rangle \tag{7.97}$$

and with $\omega^+ = \omega + i\delta$, where δ is an infinitesimal positive quantity, we obtain

$$\begin{aligned}
\langle\langle \hat{O}; \hat{O}^\dagger \rangle\rangle_\omega &\stackrel{\text{def}}{=} \int_{-\infty}^{\infty} dt\, e^{i\omega^+ t} \langle\langle \hat{O}(t); \hat{O}^\dagger \rangle\rangle \\
&= -i \int_0^{\infty} dt\, e^{i\omega^+ t} \big(\langle e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t} \hat{O}^\dagger \rangle - \varepsilon \langle \hat{O}^\dagger e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t} \rangle \big) \\
&= -i \int_0^{\infty} dt\, e^{i\omega^+ t} \big(\langle \hat{O} e^{-i(\hat{H}-E_0)t} \hat{O}^\dagger \rangle - \varepsilon \langle \hat{O}^\dagger e^{i(\hat{H}-E_0)t} \hat{O} \rangle \big) \\
&= -i \Big(\Big\langle \hat{O} \int_0^{\infty} dt\, e^{i(\omega^+ - \hat{H} + E_0)t} \hat{O}^\dagger \Big\rangle - \varepsilon \Big\langle \hat{O}^\dagger \int_0^{\infty} dt\, e^{i(\omega^+ + \hat{H} - E_0)t} \hat{O} \Big\rangle \Big)
\end{aligned} \tag{7.98}$$

With the aid of the spectral theorem the integral can be evaluated. Now, taking into account that we perform the average in the ground state $|\psi_0\rangle$, we obtain

$$\begin{aligned}
\langle\langle \hat{O}; \hat{O}^\dagger \rangle\rangle_\omega &= \Big\langle \hat{O} \frac{1}{\omega^+ - (\hat{H} - E_0)} \hat{O}^\dagger \Big\rangle - \varepsilon \Big\langle \hat{O}^\dagger \frac{1}{\omega^+ + (\hat{H} - E_0)} \hat{O} \Big\rangle \\
&= \langle \psi_0 | \hat{O} \hat{O}^\dagger | \psi_0 \rangle \Big\langle \phi_0 \Big| \frac{1}{\omega^+ - (\hat{H} - E_0)} \Big| \phi_0 \Big\rangle \\
&\quad - \varepsilon \langle \psi_0 | \hat{O}^\dagger \hat{O} | \psi_0 \rangle \Big\langle \tilde{\phi}_0 \Big| \frac{1}{\omega^+ + (\hat{H} - E_0)} \Big| \tilde{\phi}_0 \Big\rangle
\end{aligned} \tag{7.99}$$

The normalized state vectors ϕ_0 and $\tilde{\phi}_0$, defined by

$$|\phi_0\rangle = \frac{\hat{O}^\dagger |\psi_0\rangle}{\sqrt{\langle \psi_0 | \hat{O} \hat{O}^\dagger | \psi_0 \rangle}} \qquad |\tilde{\phi}_0\rangle = \frac{\hat{O} |\psi_0\rangle}{\sqrt{\langle \psi_0 | \hat{O}^\dagger \hat{O} | \psi_0 \rangle}} \tag{7.100}$$

are used as initial vectors for two independent Lanczos sequences.
The tridiagonal form of $\hat{H}$, and likewise of the energy denominators $\tilde{H} = \omega \pm (H - E_0)$ in the Lanczos basis can be exploited to determine the expectation value of the inverse of $\tilde{H} = \omega \pm (H - E_0)$ in Eq. (7.99). As for the ground state we calculate the matrix elements for the Lanczos vectors

$$\begin{aligned}
\langle \phi_i | \hat{H} - E_0 | \phi_i \rangle &= \Delta\varepsilon_i \\
\langle \phi_i | \hat{H} - E_0 | \phi_{i+1} \rangle &= k_i \\
\langle \phi_i | \hat{H} - E_0 | \phi_j \rangle &= 0 \quad \forall |i - j| > 1
\end{aligned} \tag{7.101}$$

Together with the orthonormality

$$\langle \phi_i | \phi_j \rangle = \delta_{ij} \tag{7.102}$$

we obtain the tridiagonal form

$$\begin{aligned}
&(\omega^+ \pm (\hat{H} - E_0)) \\
&= \begin{pmatrix}
\omega^+ \pm \Delta\varepsilon_0 & k_1 & & & & \\
k_1 & \omega^+ \pm \Delta\varepsilon_1 & k_2 & & & \\
 & k_2 & \omega^+ \pm \Delta\varepsilon_2 & k_3 & & \\
 & & k_3 & \omega^+ \pm \Delta\varepsilon_3 & k_4 & \\
 & & & k_4 & \ddots &
\end{pmatrix}
\end{aligned} \tag{7.103}$$

We need the $(0,0)$ element of the inverse.
The (i,j) element of an inverse matrix can be expressed by

$$(A^{-1})_{ij} = (-1)^{i+j} \frac{\det \Delta_{ij}}{\det A} \tag{7.104}$$

where Δ_{ij} denotes the submatrix of A obtained by eliminating from A the ith row and the jth column. Especially for the desired $(0,0)$ element of the inverse we have

$$(A^{-1})_{00} = \frac{\det \Delta_{00}}{\det A} \tag{7.105}$$

Because of the tridiagonal structure of the above matrix, the formula simplifies as follows. Consider the matrix

$$A = \begin{pmatrix}
A_{00} & A_{01} & & & \\
A_{10} & A_{11} & A_{12} & & \\
 & A_{21} & A_{22} & A_{23} & \\
 & & A_{32} & A_{33} & A_{34} \\
 & & & A_{43} & A_{44}
\end{pmatrix} \tag{7.106}$$

The determinant can be expanded along the first row and column:

$$\begin{aligned}
\det A = A_{00} \det &\begin{pmatrix}
A_{11} & A_{12} & & \\
A_{21} & A_{22} & A_{23} & \\
 & A_{32} & A_{33} & A_{34} \\
 & & A_{43} & A_{44}
\end{pmatrix} \\
- A_{01} A_{10} \det &\begin{pmatrix}
A_{22} & A_{23} & \\
A_{32} & A_{33} & A_{34} \\
 & A_{43} & A_{44}
\end{pmatrix}
\end{aligned} \tag{7.107}$$

We define the determinant of the submatrix of A beginning with the ith column and row, i.e.

$$D_i \stackrel{\text{def}}{=} \det \begin{pmatrix} A_{ii} & A_{ii+1} & & \\ A_{i+1\,i} & A_{i+1\,i+1} & A_{i+1\,i+2} & \\ & A_{i+2\,i+1} & A_{i+2\,i+2} & A_{i+2\,i+3} \\ & & A_{i+3\,i+2} & A_{i+3\,i+3} \end{pmatrix} \tag{7.108}$$

Then, we can write the desired element of the inverse matrix (7.105) as

$$(A^{-1})_{00} = \frac{1}{\frac{D_0}{D_1}} \tag{7.109}$$

We can now use Eq. (7.107) to express D_0/D_1 by D_1/D_2:

$$\frac{D_0}{D_1} = \frac{A_{00}D_1 - |A_{01}|^2 D_2}{D_1} = A_{00} - \frac{|A_{01}|^2}{\frac{D_1}{D_2}} \tag{7.110}$$

Iterating the above reasoning yields

$$\frac{D_l}{D_{l+1}} = A_{l\,l} - \frac{|A_{l\,l+1}|^2}{\frac{D_{l+1}}{D_{l+2}}} \tag{7.111}$$

This leads to a continued fraction for the desired quantity

$$(A^{-1})_{00} = \frac{1}{\frac{D_0}{D_1}} = \cfrac{1}{A_{00} - \cfrac{|A_{01}|^2}{A_{11} - \cfrac{|A_{12}|^2}{A_{22} - \cfrac{|A_{23}|^2}{A_{33} - \ddots}}}} \tag{7.112}$$

For the original problem $\left((\omega^+ \pm (\hat{H} - E_0))^{-1}\right)_{00}$ the continued fraction reads

$$\begin{aligned} &\left((\omega^+ \pm (\hat{H} - E_0))^{-1}\right)_{00} \\ &= \cfrac{1}{\omega^+ \pm \Delta\varepsilon_0 - \cfrac{|k_1|^2}{\omega^+ \pm \Delta\varepsilon_1 - \cfrac{|k_2|^2}{\omega^+ \pm \Delta\varepsilon_2 - \cfrac{|k_3|^2}{\omega^+ \pm \Delta\varepsilon_3 - \ddots}}}} \end{aligned} \tag{7.113}$$

This expression is well suited for numerical treatment and can be iterated for arbitrary ω. To this end, we introduce the abbreviations

$$\begin{aligned} d_i &= \omega^+ \pm \Delta\varepsilon_i \qquad \text{for } i = 0, 1, \ldots \\ e_i &= |k_i|^2 \qquad\quad \text{for } i = 1, 2, \ldots \end{aligned} \tag{7.114}$$

Beginning with the upper left (2×2) submatrix of A the continued fraction has the form

$$\frac{1}{d_0 - \dfrac{e_1}{d_1 - R_1}} = \frac{d_1 - R_1}{d_0 d_1 - d_1 - d_0 R_1} \equiv \frac{a_1 + a_0 R_1}{b_1 + b_0 R_1} \tag{7.115}$$

In this equation we anticipated the general form. The remainder R_1 has again the form of a continued fraction. In general the remainder reads

$$R_i = \frac{e_{i+1}}{d_{i+1} - R_{i+1}} \tag{7.116}$$

By substituting this for $i = 1$ into Eq. (7.115) we obtain

$$\frac{a_1 + a_0 R_1}{b_1 + b_0 R_1} = \frac{\overbrace{a_1 d_1 + a_0 e_2}^{a_1} + \overbrace{(-a_1)}^{a_0} R_2}{\underbrace{b_1 d_2 + b_0 e_2}_{b_1} + \underbrace{(-b_1)}_{b_0} R_2} \tag{7.117}$$

which is again of the form

$$\frac{a_1 + a_0 R}{b_1 + b_0 R} \tag{7.118}$$

Thus the iteration formula for $i = 1, 2, \ldots$ deduced from the considerations above is given by

$$\begin{aligned} a_1 &\longrightarrow a_1 d_{i+1} + a_0 e_{i+1} \\ a_0 &\longrightarrow -a_1 \\ b_1 &\longrightarrow b_1 d_{i+1} + b_0 e_{i+1} \\ b_0 &\longrightarrow -b_1 \end{aligned} \tag{7.119}$$

with the initial values $a_1 = d_1$, $a_0 = -1$, $b_1 = d_0 d_1 - e_1$, $b_0 = -d_0$. The sequence is iterated for each ω individually and ends if the Krylov space is exhausted or if a desired convergence of

$$g(\omega) = \frac{a_1}{b_1} \tag{7.120}$$

is achieved. In order to avoid numerical instabilities, it is recommended to rescale all quantities a_0, a_1, b_0, b_1 *e.g.* by b_1 after each iteration.
In some cases it may happen that the Green's function of interest is not diagonal in the operators, *e.g.*

$$g_{AB} = \left\langle \hat{A}^\dagger \frac{1}{\omega^+ - (\hat{H} - E_0)} \hat{B} \right\rangle \tag{7.121}$$

In this case we define two operators $\hat{O}_\alpha = \hat{A} + \alpha\hat{B}$ and determine the diagonal Green's functions

$$g_\alpha = \left\langle \hat{O}_\alpha^\dagger \frac{1}{\omega^+ - (\hat{H} - E_0)} \hat{O}_\alpha \right\rangle \tag{7.122}$$

It is easily possible to separate g_{AB} by linearly combining the four Green's functions for $\alpha = \{\pm 1, \pm i\}$.

Lehmann Representation

There is an alternative way of calculating Green's functions, the so-called Lehmann representation. Again we consider the matrix elements of the form

$$\left\langle \psi_0 \middle| \hat{O}^\dagger \frac{1}{\omega^+ \pm (\hat{H} - E_0)} \hat{O} \middle| \psi_0 \right\rangle \tag{7.123}$$

where $|\psi_0\rangle$ represents the ground state. Like before we define $|\phi_0\rangle$ as the normalized vector $\hat{O}|\psi_0\rangle$, which serves as initial vector of a Lanczos sequence. We insert a complete orthonormal set of eigenvectors of $\hat{H}$ given by

$$\mathbb{1} = \sum_\nu |\psi_\nu\rangle\langle\psi_\nu| \tag{7.124}$$

Then Eq. (7.123) can be cast into the form

$$\left\langle \psi_0 \middle| \hat{O}^\dagger \frac{1}{\omega^+ \pm (\hat{H} - E_0)} \hat{O} \middle| \psi_0 \right\rangle = \sum_\nu \frac{\langle\psi_0|\hat{O}^\dagger|\psi_\nu\rangle\langle\psi_\nu|\hat{O}|\psi_0\rangle}{\omega^+ \pm (\hat{H} - E_0)} \tag{7.125}$$

Next we expand the eigenvectors $|\psi_\nu\rangle$ in the Lanczos basis $\{|\phi_i\rangle\}$

$$|\psi_\nu\rangle = \sum_i c_i^{(\nu)} |\phi_i\rangle \quad \text{with } c_i^{(\nu)} = \langle\phi_i|\psi_\nu\rangle \tag{7.126}$$

to obtain

$$\begin{aligned}\langle\psi_\nu|\hat{O}|\psi_0\rangle &= \sum_i c_i^{(\nu)*}\langle\phi_i|\hat{O}|\psi_0\rangle = \sqrt{\langle\psi_0|\hat{O}^\dagger\hat{O}|\psi_0\rangle}\sum_i c_i^{(\nu)*}\langle\phi_i|\phi_0\rangle \\ &= \sqrt{\langle\psi_0|\hat{O}^\dagger\hat{O}|\psi_0\rangle}c_i^{(\nu)*}\end{aligned} \tag{7.127}$$

because $\langle\phi_i|\phi_0\rangle = \delta_{i0}$. This means that except of the first terms all addends vanish.
Thus Eq. (7.123) can be approximated by

$$\left\langle\psi_0\middle|\hat{O}^\dagger\frac{1}{\omega^+ \pm (\hat{H} - E_0)}\hat{O}\middle|\psi_0\right\rangle = \langle\psi_0|\hat{O}^\dagger\hat{O}|\psi_0\rangle\sum_{\nu=1}^{N_L}\frac{|c_0^{(\nu)}|^2}{\omega^+ \pm (\tilde{E} - \tilde{E}_0)} \tag{7.128}$$

where only the first components $c_0^{(\nu)}$ of the expansion of the eigenvector $|\psi_\nu\rangle$ in the Lanczos basis are required. In general, the eigenstates $|\psi_\nu\rangle(\nu = 1, \ldots, N_L)$, computed by the Lanczos procedure, do not form a complete set of basis vectors, nor are the respective energies $\tilde{E}_\nu$ exact eigenvalues of $\hat{H}$. However, with increasing number of iterations, the Lanczos procedure converges towards the exact Green's function and the convergence can be monitored and stopped as soon as the desired accuracy is reached. The approximate Lehmann representation (7.128) is an explicit sum of simple poles. The same is true for the continued fraction.