↳ $|\sigma_R, k\rangle$ is only admissible if $k = n\frac{2\pi}{N}$ satisfies

$$\boxed{Q_{\sigma_R} \cdot n \mod N = 0}$$ otherwise $e^{ikQ_{\sigma_R}} \neq 1$.

↳ Basis construction for $k = \frac{2\pi}{N} n$:

$\mathcal{H}^{(P)}$ for fixed particle number

(i) Initialize arrays of length $\sim \frac{\dim(\mathcal{H})}{N}$, called $\hat{\Sigma}_R$ and $\hat{Q}_R$.

(ii) Check all states in Hilbert space (or particle number block) as follows:

(a) Check if σ is representative, i.e. if I_σ cannot be reduced by applying bitwise translations, and infer periodicity Q_σ.

(b) If σ is representative and $Q_\sigma \cdot n \mod N = 0$ (compatibility), add σ to $\hat{\Sigma}_R$ and Q_σ to $\hat{Q}_R$.

↳ Compute non-vanishing matrix elements of H_k (either to store as sparse array or on the fly):

$$H|\sigma_R, k\rangle \overset{[H,T^l]=0}{=} \frac{\sqrt{Q_{\sigma_R}}}{N} \sum_{l=0}^{N-1} e^{-ikl} T^l H|\sigma_R\rangle \overset{H=\sum_\lambda H_\lambda}{=}$$

$$= \frac{\sqrt{Q_{\sigma_R}}}{N} \sum_\lambda \sum_{l=0}^{N-1} e^{-ikl} T^l \underbrace{H_\lambda |\sigma_R\rangle}_{= \underbrace{h^\lambda_{\sigma_R}}_{\text{transition amplitude}} T^{-l_\lambda} \underbrace{|\tilde{\sigma}^\lambda_R\rangle}_{\text{"unique target state"}}}$$

$$= \sum_\lambda \frac{h^\lambda_{\sigma_R} \sqrt{Q_{\sigma_R}}}{N} \sum_{l=0}^{N-1} e^{-ikl} T^{(l-l_\lambda)} |\tilde{\sigma}^\lambda_R\rangle \overset{l \to l+l_\lambda}{=}$$

$$= \sum_{\lambda} h^{\lambda}_{\sigma_R} e^{-ikl_\lambda} \frac{\sqrt{Q_{\sigma_R}}}{\sqrt{Q_{\tilde{\sigma}^{\lambda}_R}}} \, |\tilde{\sigma}^{\lambda}_R, k\rangle$$

$$\boxed{|\tilde{\sigma}^{\lambda}_R, k\rangle = \frac{\sqrt{Q_{\tilde{\sigma}^{\lambda}_R}}}{N} \sum_{l=0}^{N-1} e^{-ikl} T^l |\tilde{\sigma}^{\lambda}_R\rangle}$$

$$\rightsquigarrow \langle \tilde{\sigma}^{\lambda}_R, k | H_\lambda | \sigma_R, k\rangle = h^{\lambda}_{\sigma_R} e^{-ikl_\lambda} \frac{\sqrt{Q_{\sigma_R}}}{\sqrt{Q_{\tilde{\sigma}_R}}}$$

$\rightsquigarrow$ Loop on σ_R and λ to find all non-vanishing elements.

$\dim(\mathcal{H}_k^{(\rho)})$ $\log(\dim \mathcal{H}_k^{(\rho)})$

? Lookup table to infer the index of $\tilde{\sigma}^{\lambda}_R$ in $\hat{\Sigma}_R$?

↳ Two-table method used for particle number conservation only suitable for additive (between subsystems A and B) quantum numbers.

↳ Common solution: Do binary search of $\tilde{\sigma}_R$ in $\hat{\Sigma}_R$ at extra cost $\log(\mathrm{length}(\hat{\Sigma}_R)) = \log(\dim(\mathcal{H}_k^{(p)}))$.

B.4: Time-Evolution and Non-Equilibrium Dynamics

• Consider the time-dependent Schrödinger equation of QMB system

$$i\partial_t |\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$

$$\rightsquigarrow |\Psi(t)\rangle = \underbrace{\mathcal{T} e^{-i\int_{t_0}^{t} d\tau H(\tau)}}_{U(t,t_0)} |\Psi(t_0)\rangle$$

- Let us start with a time-independent Hamiltonian H, then $U(t,t_0) = e^{-iH(t-t_0)} = \sum_{\ell=0}^{\infty} \frac{(-iH(t-t_0))^\ell}{\ell!}$, and $U(t,t_1)U(t_1,t_0) = U(t,t_0)$

- Observation: $\sum_{\ell=0}^{n} \frac{(-iHt)^\ell}{\ell!} |\psi(0)\rangle \in K_{n+1}(H, |\psi(0)\rangle)$
  ($t_0 = 0$ from now on)

- For $n \gtrsim 50$ and small t (order inverse energy scale of H)
  $U(t,0) \approx \sum_{\ell=0}^{n} \frac{(-iHt)^\ell}{\ell!}$ becomes a very good approximation
  (error is of order t^{n+1}).

$\rightsquigarrow$ For arbitrary t, define $\delta t = \frac{t}{\text{steps}}$ small enough and factorize
$U(t,0) = e^{-iHt} = \prod_{j=1}^{\text{steps}} e^{-i\delta t H}$.

$\rightsquigarrow$ Update $|\psi(t)\rangle \longrightarrow |\psi(t+\delta t)\rangle = e^{-i\delta t H}|\psi(t)\rangle$ using "Krylov time propagation":

(a) Apply Lanczos algorithm (see B.2) to represent H in tridiagonal form T on $K_{n+1}(H, |\psi(t)\rangle)$, storing either full Krylov basis $Q = (|q_0\rangle, \cdots, |q_n\rangle)$, or generating T on the fly.

(b) Apply the time-evolution operator in Krylov space:

$$\vec{y}_0(t+\delta t) = e^{-iT\delta t} \underbrace{Q^\dagger \underbrace{|q_0\rangle}_{=|\psi(t)\rangle}}_{=\vec{y}_0(t)} = e^{-iTt}\begin{pmatrix}1\\0\\\vdots\\0\end{pmatrix}$$

(c) $|\psi(t+\delta t)\rangle = Q\,\vec{y}_0(t+\delta t)$. [either directly, if full Krylov basis is stored, or from $\vec{y}_0(t+\delta t)$ on the fly with 3 vectors (see B.2)]

(d) Repeat (a–c) (with updated $|q_0\rangle = |\psi(t+\delta t)\rangle$!) until final time is reached, and converge results with respect to step-size δt.

- Krylov time propagation allows for exact computation of time-evolution for generic QMB problems at a cost $\mathcal{O}(\dim(\mathcal{H}) \cdot t)$, i.e. the best we could hope for at an exact level.

$\log(\mathcal{H})$

↳ Time-dependence of observables as well as auto-correlation functions such as $\langle \psi(t) | \psi(0) \rangle$ can be efficiently computed.

- Now consider the case of a time-dependent Hamiltonian $H(t)$.
  - Problem: $e^{-iH(t)\delta t} |\psi(t)\rangle \approx Q e^{-iT(t)\delta t} Q^\dagger |\psi(t)\rangle$ correct up to $\mathcal{O}(\delta t^{n+1})$ with $n \simeq 50$, but

    $\overleftarrow{\mathcal{T}} e^{-i\int_t^{t+\delta t} d\tau\, H(\tau)} \approx e^{-iH(t)\delta t}$ only correct up to $\mathcal{O}(\delta t^2)$.

    However, the error in the latter expression only stems from the time-dependence of $H(t)$ and is small if $\left\| \frac{d}{dt} H(t) \right\|$ is small (slow time dependence)