(12)

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$$\boxed{\alpha(\omega) = \underline{b}^{\dagger} (\underline{\underline{A}} - \omega^2 \underline{\underline{S}})^{-1} \underline{b}}$$

F. Visser & P. E. S. Wormer
Mol Phys 52, 923 (1984)

$\underline{\underline{A}} = \underline{\underline{A}}^{\dagger}$

$\underline{\underline{S}} = \underline{\underline{S}}^{\dagger}$, $\underline{\underline{S}}$ positive definite : Cholesky $\underline{\underline{S}} = \underline{\underline{R}}^{\dagger} \underline{\underline{R}}$

R^{-1} exists $(R^{\dagger})^{-1}$ does

$$\alpha(\omega) = \underline{b}^{\dagger} (\underline{\underline{A}} - \omega^2 \underline{\underline{R}}^{\dagger} \underline{\underline{R}})^{-1} \underline{b}$$

$$= \underline{b}^{\dagger} (\underline{\underline{R}}^{\dagger} (R^{-\dagger} \underline{\underline{A}} R^{-1} - \omega^2) \underline{\underline{R}})^{-1} \underline{b}$$

$$= \underline{b}^{\dagger} \underline{\underline{R}}^{-1} (\underline{\underline{R}}^{-\dagger} \underline{\underline{A}} R^{-1} - \omega^2)^{-1} R^{-\dagger} \underline{b}$$

$$[R^{-\dagger} \underline{\underline{A}} R^{-1} \underline{u}_i = \lambda_i^2 u_i]$$

$$= \underline{b}^{\dagger} \underline{\underline{R}}^{-1} \sum_i \frac{u_i u_i^{\dagger}}{\lambda_i^2 - \omega^2} \underline{\underline{R}}^{-\dagger} \underline{b}$$

$$f_i^* = \underline{b}^{\dagger} \underline{\underline{R}}^{-1} \underline{u}_i$$

Note $R^{-\dagger} \underline{\underline{A}} R^{-1} \underline{u}_i = \lambda_i^2 \underline{u}_i$

$\underline{u}_i = \underline{\underline{R}} \underline{v}_i$

$\underline{\underline{A}} \underline{v}_i = \lambda_i^2 \underline{R}^{\dagger} \underline{R} v_i$

$\underline{\underline{A}} \underline{v}_i = \lambda_i^2 \underline{\underline{S}} v_i$

$f_i^* = \underline{b}^{\dagger} \underline{v}_i$

$f_i = \underline{v}_i^{\dagger} \underline{b}$

$$\boxed{\begin{gathered} \alpha(\omega) = \sum_i \frac{|f_i|^2}{\lambda_i^2 - \omega^2} \\ \underline{\underline{A}} v_i = \lambda_i^2 \underline{\underline{S}} \underline{v}_i \\ f_i = \underline{b}^{\dagger} \underline{v}_i \end{gathered}}$$

Generalized eigenvalue problem

$$\alpha(\omega) = \underline{b}^+ (\underline{\underline{A}} - \omega^2 \underline{\underline{S}})^{-1} \underline{b}$$

$$= \underline{b}^+ \left[\underline{\underline{A}}^{1/2} (1 - \omega^2 \underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2}) \underline{\underline{A}}^{1/2} \right]^{-1} \underline{b}$$

$$= \underline{b}^+ \underline{\underline{A}}^{-1/2} (1 - \omega^2 \tilde{\underline{\underline{S}}})^{-1} \underline{\underline{A}}^{-1/2} \underline{b} \qquad \tilde{\underline{\underline{S}}} = \underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2}$$

$$= \underline{b}^+ \underline{\underline{A}}^{-1/2} \left(\sum_{k=0}^{\infty} \omega^{2k} \tilde{\underline{\underline{S}}}^k \right) \underline{\underline{A}}^{-1/2} \underline{b}$$

$$= \sum_{k=0}^{\infty} \omega^{2k} \underline{b}^+ \underbrace{\underline{\underline{A}}^{-1/2} \tilde{\underline{\underline{S}}}^k \underline{\underline{A}}^{-1/2}} \underline{b} = \sum_{k=0}^{\infty} \underline{b}^+ \underline{\underline{M}}_k \underline{b}\, \omega^{2k}$$

$$\underline{\underline{M}}_k \equiv \underline{\underline{A}}^{-1/2} (\underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2})^k \underline{\underline{A}}^{-1/2} = -$$

$$\boxed{\begin{aligned} \underline{\underline{M}}_k \underline{\underline{A}} \underline{\underline{M}}_l &= \underline{\underline{A}}^{-1/2} (\underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2})^k \underbrace{\underline{\underline{A}}^{-1/2} \underline{\underline{A}} \underline{\underline{A}}^{-1/2}} (\underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2})^l \underline{\underline{A}}^{-1/2} \\ &= \underline{\underline{M}}_{k+l} \\ \underline{\underline{M}}_k \underline{\underline{S}} \underline{\underline{M}}_l &= \underline{\underline{A}}^{-1/2} (\underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2})^k \underbrace{\underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2}} (\underline{\underline{A}}^{-1/2} \underline{\underline{S}} \underline{\underline{A}}^{-1/2})^l \underline{\underline{A}}^{-1/2} \\ &= \underline{\underline{M}}_{k+l+1} \end{aligned}}$$

$$\underline{M} \equiv [\underline{\underline{M}}_0 \underline{b} \;\; \underline{\underline{M}}_1 \underline{b} \; \cdots \; \underline{\underline{M}}_{n-1} \underline{b}] = [\underline{m}_0 \; \underline{m}_1 \; \cdots \; \underline{m}_{n-1}]$$

$$\sum_{k=0}^{\infty} \underline{b}^+ \underline{\underline{M}}_k \underline{b}\, \omega^{2k} = \sum_{k=0}^{\infty} \underline{b}^+ \underline{m}_k\, \omega^{2k} = \sum_{k=0}^{\infty} s_k\, \omega^{2k}$$

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Orthonormal basis Q: $\underline{M} = \underline{Q}\, \underline{R}$ "QR" $\left[\;\right] = \left[\;\right] [\triangledown]$ $\overset{n}{\longleftrightarrow}$

projector $\underline{P} = \underline{Q}\, \underline{Q}^+$

$$[s_0 \; s_1 - s_{n-1}] = [\underline{b}^+ \underline{m}_0 - \underline{b}^+ \underline{m}_{n-1}] = \underline{b}^+ \underline{M} \equiv \underline{s}^+$$

$$\alpha(\omega) = \underline{b}^T (\underline{\underline{A}} - \omega^2 \underline{\underline{S}})^{-1} \underline{b} \overset{\text{projection}}{\approx} b^T Q \left[Q^\dagger (A - \omega^2 S) Q\right]^{-1} \cancel{Q} Q^\dagger \underline{b}$$

$$Q = \underline{\underline{M}}\,\underline{\underline{R}}^{-1} \qquad M = QR$$

$$Q^\dagger = R^{-\dagger} M^\dagger \qquad M^\dagger = R^\dagger Q^\dagger$$

$$\alpha(\omega) = b^\dagger Q \left[R^{-\dagger} \underbrace{M^\dagger (\underline{\underline{A}} - \omega^2 \underline{\underline{S}}) M}\, R^{-1}\right]^{-1} \cancel{Q} Q^\dagger \underline{b}$$

$$= b^\dagger \underbrace{Q \quad R} \left[M^\dagger (\underline{\underline{A}} - \omega^2 \underline{\underline{S}}) M\right]^{-1} R^\dagger \cancel{Q} Q^\dagger \underline{b}$$

$$= \underline{b}^\dagger \underline{\underline{M}} \left[\underline{\underline{M}}^\dagger (\underline{\underline{A}} - \omega^2 \underline{\underline{S}}) \underline{\underline{M}}\right]^{-1} M^\dagger \underline{b}$$

$$= \underline{b}^\dagger \underline{\underline{M}} \left[\underline{\underline{M}}^\dagger \underline{\underline{A}}\, \underline{\underline{M}} - \omega^2 \underline{\underline{M}}^\dagger \underline{\underline{S}}\, \underline{\underline{M}}\right]^{-1} M^\dagger \underline{b}$$

$$\underline{\underline{A}}_0 = M^\dagger \underline{\underline{A}}\, \underline{\underline{M}}$$

$$\underline{\underline{S}}_0 = M^\dagger \underline{\underline{S}}\, \underline{\underline{M}}$$

$$\boxed{\alpha(\omega) = \underline{\mu}^\dagger (\underline{\underline{A}}_0 - \omega^2 \underline{\underline{S}}_0)^{-1} \underline{\mu}}$$

$$(\underline{\underline{A}}_0)_{ij} = m_i^\dagger \underline{\underline{A}}\, m_j = b^\dagger \underline{\underline{M}}_i \underline{\underline{A}}\, \underline{\underline{M}}_j \underline{b} = b^\dagger \underline{\underline{M}}_{k+l} b$$
$$= \underline{b}^\dagger m_{k+l} = \mu_{k+l}$$

$$(\underline{\underline{S}}_0)_{ij} = m_i^\dagger \underline{\underline{S}}\, \underline{m}_j = \underline{b}^\dagger \underline{\underline{M}}_i \underline{\underline{S}}\, \underline{\underline{M}}_j \underline{b} = \underline{b}^\dagger M_{k+l+1} \underline{b} = \underline{b}^\dagger \underline{m}_{k+l+1}$$
$$= \mu_{k+l+1}$$

Summary

Cauchy moments

$$\alpha(\omega) = \sum_{k=0}^{\infty} \omega^{2k} s_k$$

subspace (n):

$$\alpha(\omega) = \sum_i \frac{|f_i|^2}{\lambda_i^2 + \omega^2}$$

$$f_i = \underline{v}_i^{+} \underline{s}$$

$$\underline{\underline{A}}_0 \underline{v}_i = \lambda_i^2 \underline{\underline{S}}_0 v_i$$

$$(\underline{\underline{A}}_0)_{i,j} = s_{i+j}$$

$$(\underline{\underline{S}}_0)_{ij} = s_{i+j+1}$$

$$\underline{s} = \begin{bmatrix} s_0 \\ s_1 \\ \vdots \\ s_{n-1} \end{bmatrix}$$

$$[\, s_k = S(-2-2k) \,]$$