

# Fermi-Operator Expansions for Linear Scaling Electronic Structure Calculations

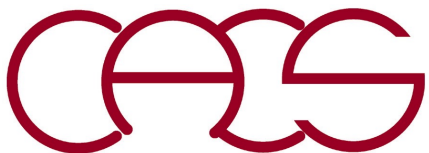
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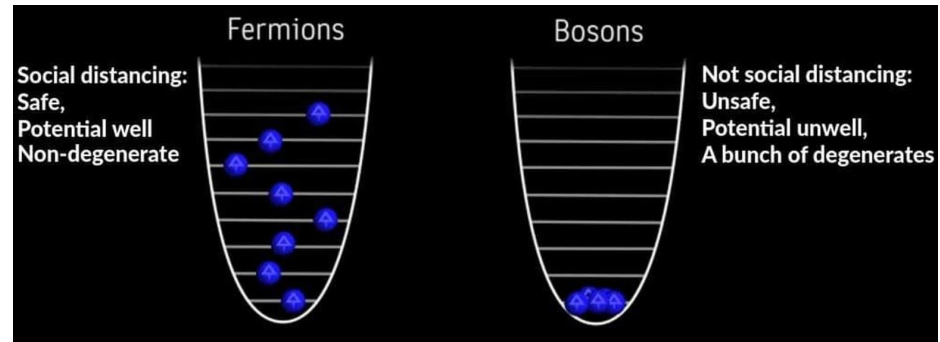
**$O(N)$  sparse matrix representation  
Simple & generalizable → use it**



# Fermi Operator

- Fermi operator

$$F(\hat{H}) = \frac{2}{\exp\left(\frac{\hat{H}-\mu}{k_B T}\right) + 1}$$



- Projection to the occupied subspace

$$|\psi_{\text{proj}}\rangle = F(\hat{H}) |\psi\rangle$$

- The expectation value of any operator  $A$  is obtained by

$$\langle \hat{A} \rangle = \text{tr}[\hat{A}F(\hat{H})]$$

- Widely used in  $O(N)$  electronic structure calculations ( $N$  = number of electrons) through its sparse representation

*cf.*  $O(N^3)$  way

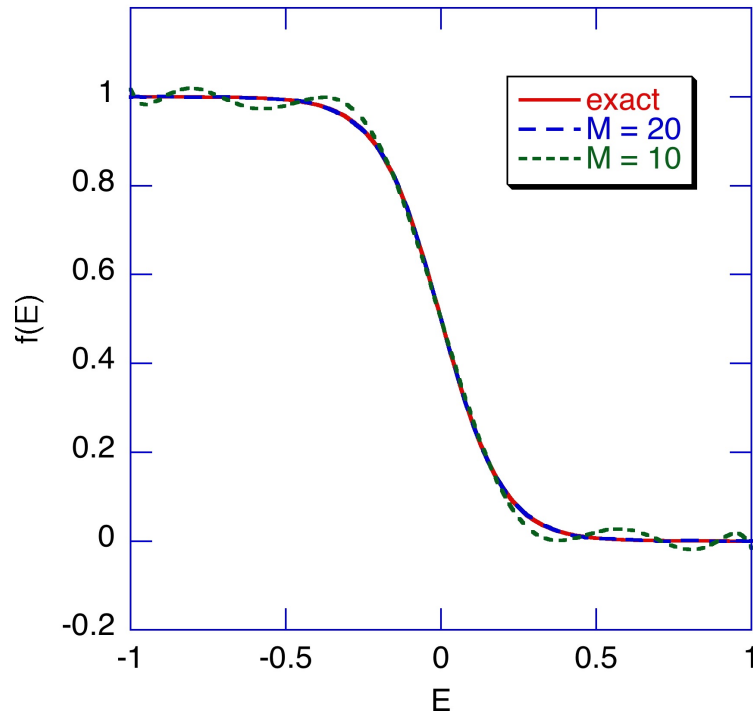
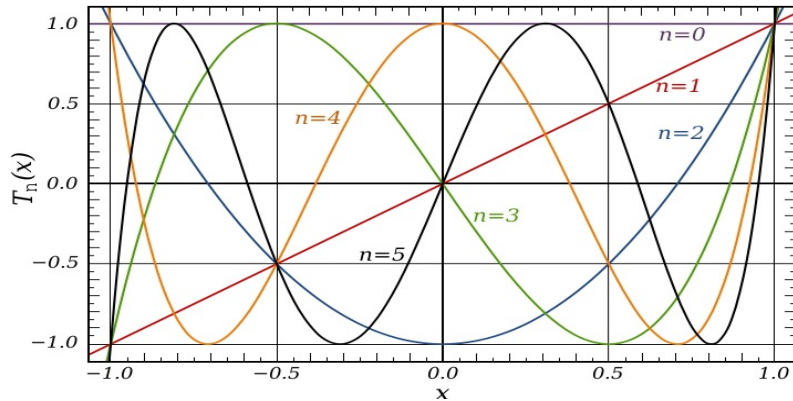
$$\hat{H}|n\rangle = \varepsilon_n|n\rangle$$

$$\langle \hat{A} \rangle = \sum_n \frac{2}{\exp\left(\frac{\varepsilon_n - \mu}{k_B T}\right) + 1} \langle n|\hat{A}|n\rangle$$

# Fermi-Operator Approximations

## Chebyshev polynomial

$$T_n(\cos\theta) = \cos(n\theta)$$

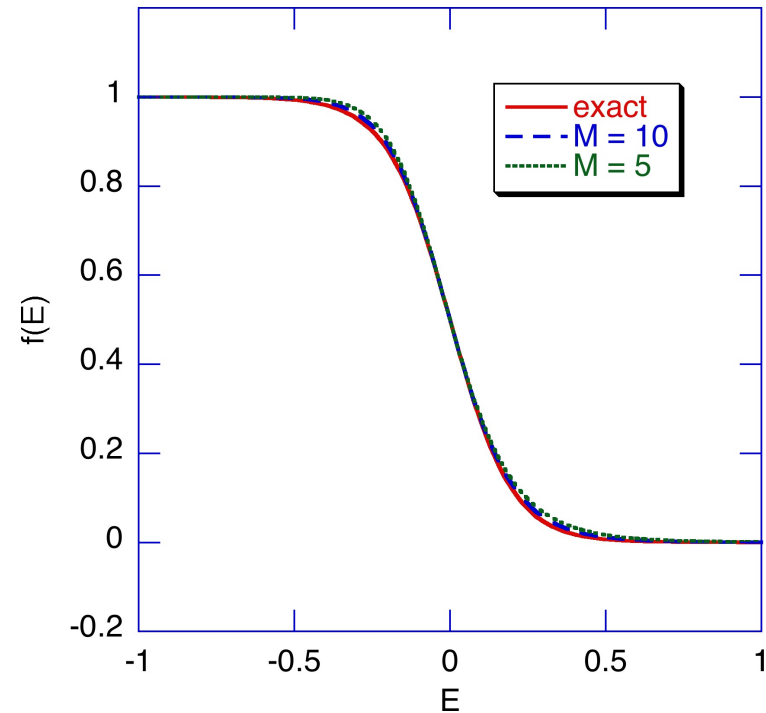


## Rational

$$F(\hat{H}) \cong \sum_{\nu=1}^M \frac{R_{\nu}}{\hat{H} - z_{\nu}}$$

$$(\hat{H} - z_{\nu})|\psi_{\text{out}}^{\nu}\rangle \cong R_{\nu}|\psi_{\text{in}}\rangle$$

$$F(\hat{H})|\psi_{\text{in}}\rangle \cong \sum_{\nu=1}^M |\psi_{\text{out}}^{\nu}\rangle$$



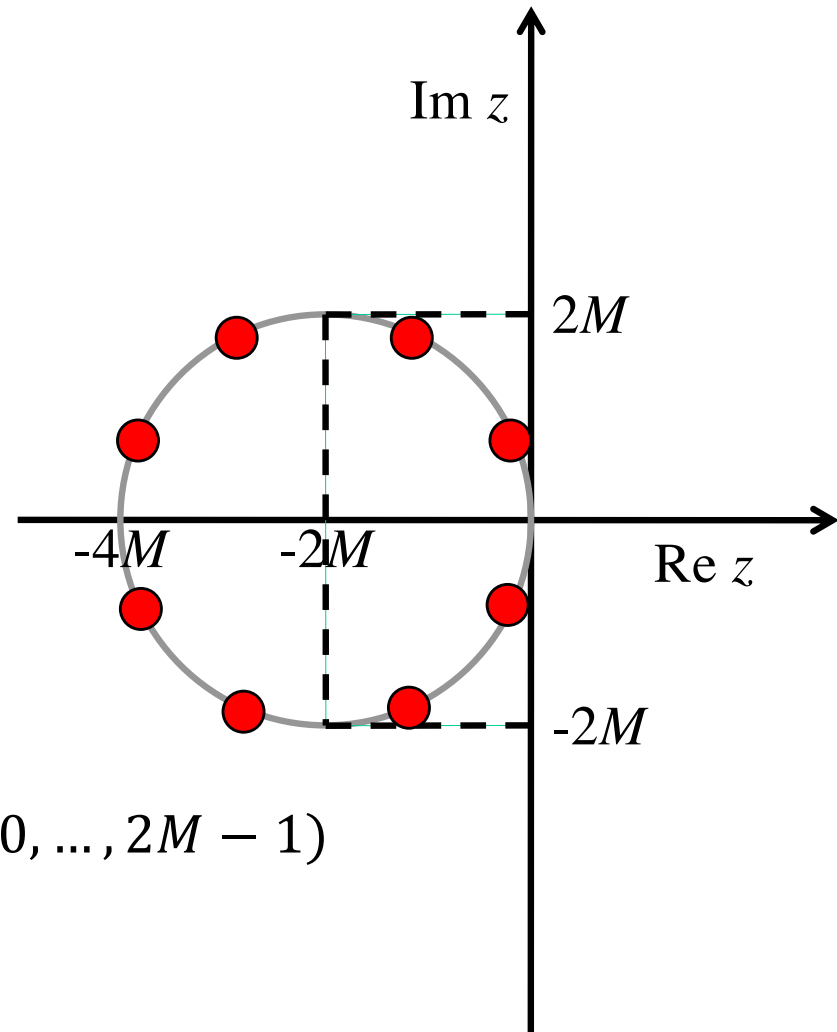
See note on [Fermi-operator expansion](#)

# Rational Fermi-Operator Expansion

$$f(z) = \frac{1}{\exp(z) + 1} \quad e^z = \lim_{n \rightarrow \infty} \left(1 + \frac{z}{n}\right)^n$$

$$\cong \frac{1}{\left(1 + \frac{z}{2M}\right)^{2M}}$$

$$\cong \sum_{\nu=0}^{2M-1} \frac{R_\nu}{z - z_\nu}$$



## Poles

$$z_\nu = 2M \left( \exp \left( i \frac{(2\nu + 1)\pi}{2M} \right) - 1 \right)$$

## Residues

$$R_\nu = - \exp \left( i \frac{(2\nu + 1)\pi}{2M} \right)$$

$$(\nu = 0, \dots, 2M - 1)$$

D. M. C. Nicholson *et al.*, *Phys. Rev. B* **50**, 14686 ('94); A. P. Horsfield *et al.*, *Phys. Rev. B* **53**, 12694 ('96); L. Lin *et al.*, [J. Phys. Condes. Matter](#) **25**, 1295501 ('13)

See note on [Fermi-operator expansion](#)

# $O(N)$ Fermi Operator Expansion

- Truncated expansion of Fermi-operator by Chebyshev polynomial  $\{T_p\}$

$$F(\hat{H}) \cong \sum_{p=0}^P c_p T_p(\hat{H})$$

- $O(N)$  algorithm

prepare a basis set of size  $O(N)$   
(let the size be  $N$  for simplicity)

for  $l = 1, N$

let an  $N$ -dimensional unit vector be  $|e_l\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} l$   $l$ -th atomic-site orbital  
recursively construct the  $l^{\text{th}}$  column of  
matrix  $T_p$ ,  $|t_l^p\rangle$ , **keeping only  $O(1)$**

**off-diagonal elements\*** (cf. quantum nearsightedness#)

$$\begin{cases} |t_l^0\rangle = |e_l\rangle \\ |t_l^1\rangle = \hat{H}|e_l\rangle \\ |t_l^{p+1}\rangle = 2\hat{H}|t_l^p\rangle - |t_l^{p-1}\rangle \end{cases} \quad \text{cf. Legendre polynomial by recursion}$$

build a sparse representation of the  $l^{\text{th}}$  column of  $F$  as

$$|f_l\rangle = \sum_{p=0}^P c_p |t_l^p\rangle$$

\*Six degrees of separation

#W. Kohn, *Phys. Rev. Lett.* **76**, 3168 ('96)