Fermi-Operator Expansions for Linear Scaling Electronic Structure Calculations

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Biological Sciences
University of Southern California

Email: anakano@usc.edu

$O(N)$ sparse matrix representation

Fermi Operator

- **Fermi operator**

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

- **Projection to the occupied subspace**

$$\left|\psi_{\mathrm{proj}}\right\rangle = F(\hat{H})\left|\psi\right\rangle$$

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

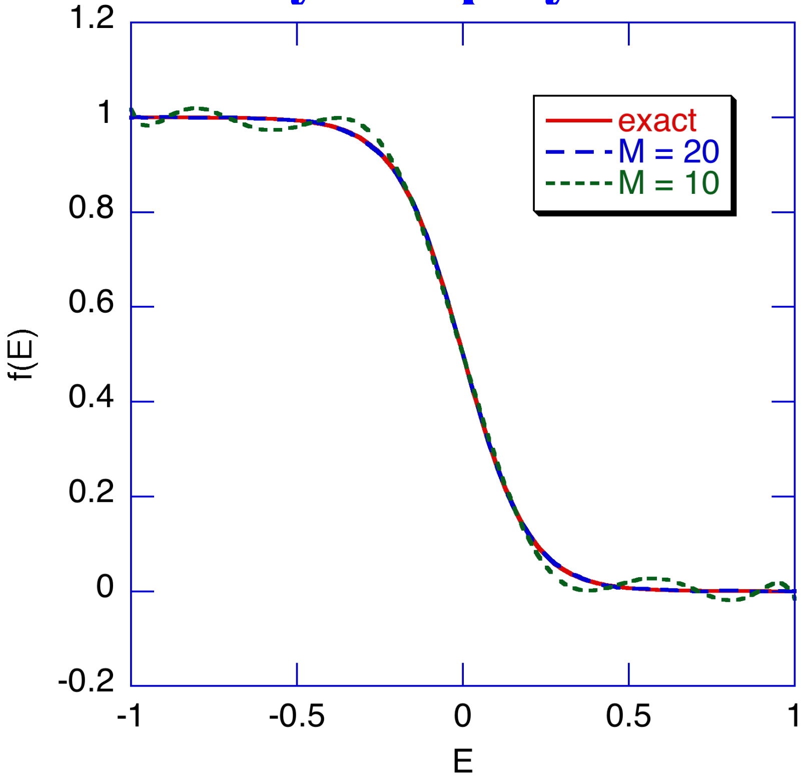
$$\left\langle \hat{A} \right\rangle = \mathrm{tr}\left[\hat{A}\hat{F}\right]$$

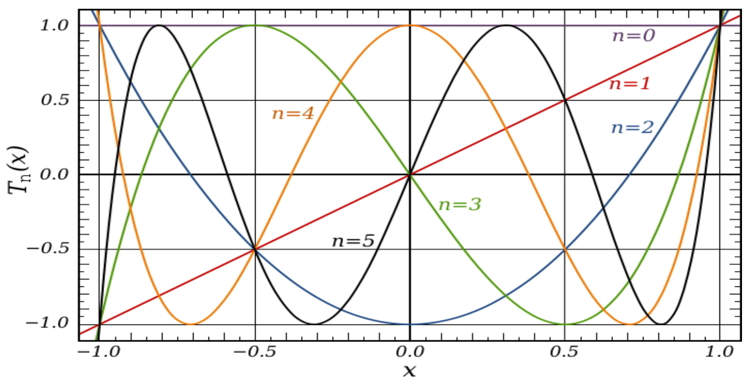
- **Widely used in *O*(*N*) electronic structure calculations (*N* = number of electrons) through its sparse representation**

S. Goedecker, *Rev. Mod. Phys*. **71**, 1085 ('99)

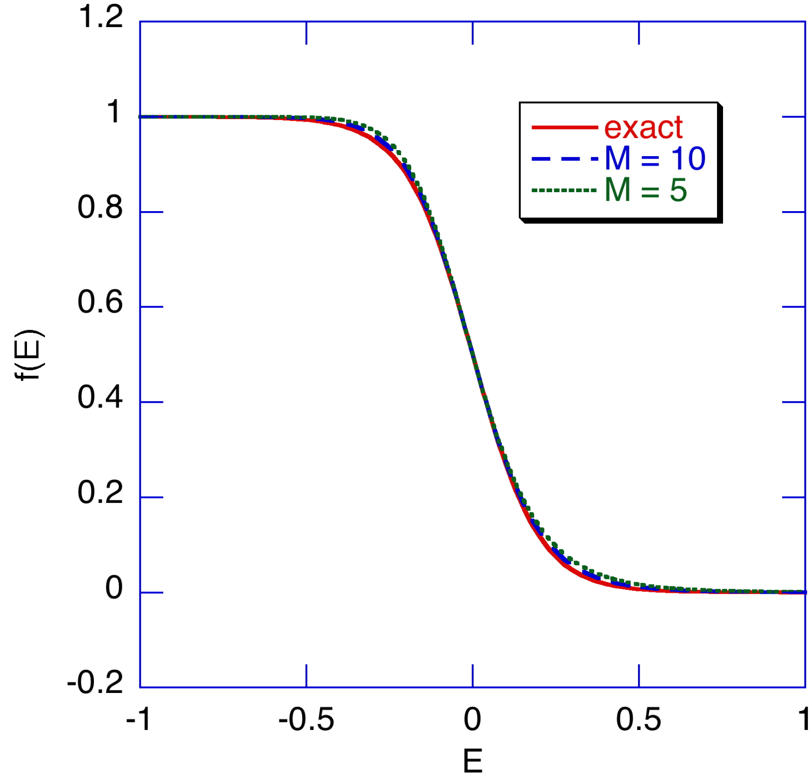
Fermi-Operator Approximations

Chebyshev polynomial





Rational



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

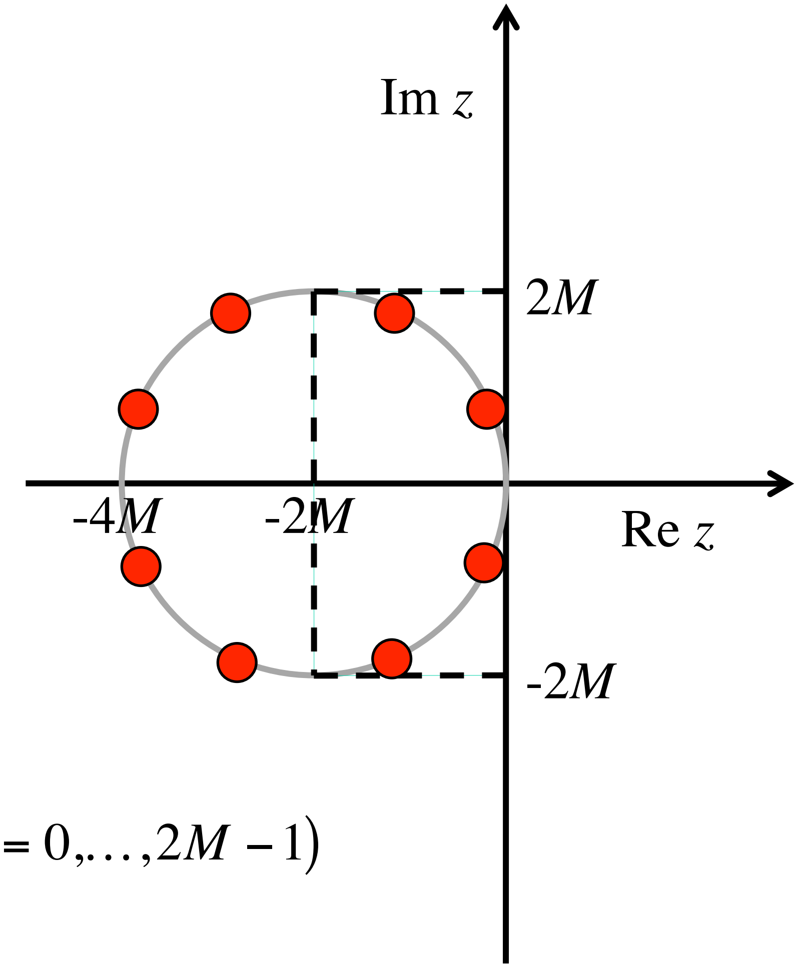
$$\left(\hat{H} - z_\nu\right)\left|\psi_{\text{out}}^{\nu}\right\rangle = R_\nu \left|\psi_{\text{in}}\right\rangle$$

Rational Fermi-Operator Expansion

$$f(z) = \frac{1}{\exp(z)+1}$$

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

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



$$\begin{cases} \textbf{Poles} \\ z_\nu = 2M\left(\exp\left(i\frac{(2\nu+1)\pi}{2M}\right)-1\right) \\ R_\nu = -\exp\left(i\frac{(2\nu+1)\pi}{2M}\right) \\ \textbf{Residues} \end{cases} \qquad (\nu = 0,\ldots,2M-1)$$

D. M. C. Nicholson *et al*., *Phys. Rev. B* **50**, 14686 ('94);
A. P. Horsfield *et al*., *Phys. Rev. B* **53**, 12694 ('96)

$O(N)$ 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 $|e_l\rangle = \begin{array}{cc} \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} & \begin{array}{c} \\ \\ l \\ \\ \\ \end{array} \end{array}$

recursively construct the l^{th} column of matrix T_p, $|t_l^p\rangle$, keeping only $O(1)$ off-diagonal elements (*cf*. quantum nearsightedness)

$$\begin{cases} |t_l^0\rangle = |e_l\rangle \\ |t_l^1\rangle = \hat{H}|e_l\rangle \\ |t_l^{p+1}\rangle = 2\hat{H}|t_l^p\rangle - |t_l^{p-1}\rangle \end{cases}$$

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

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