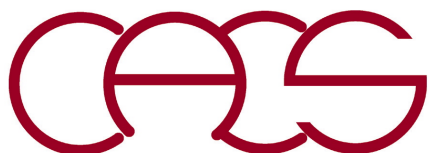


Fermi-Operator Expansions for Linear Scaling Electronic Structure Calculations

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



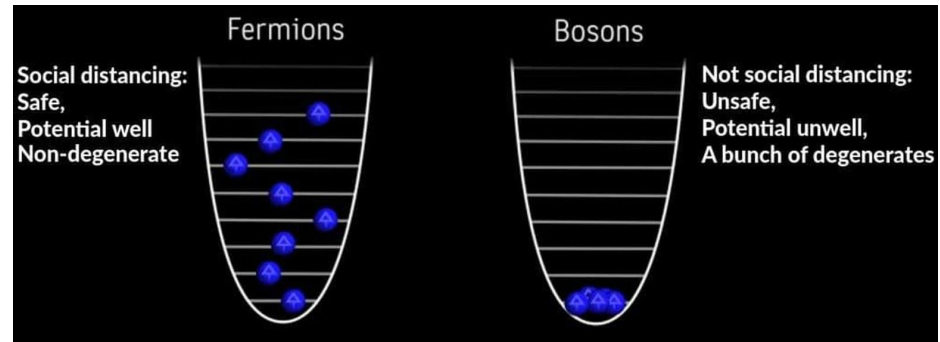
$O(N)$ sparse matrix representation



Fermi Operator

- Fermi operator

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



- Projection to the occupied subspace

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

- The expectation value of any operator A is obtained by

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

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

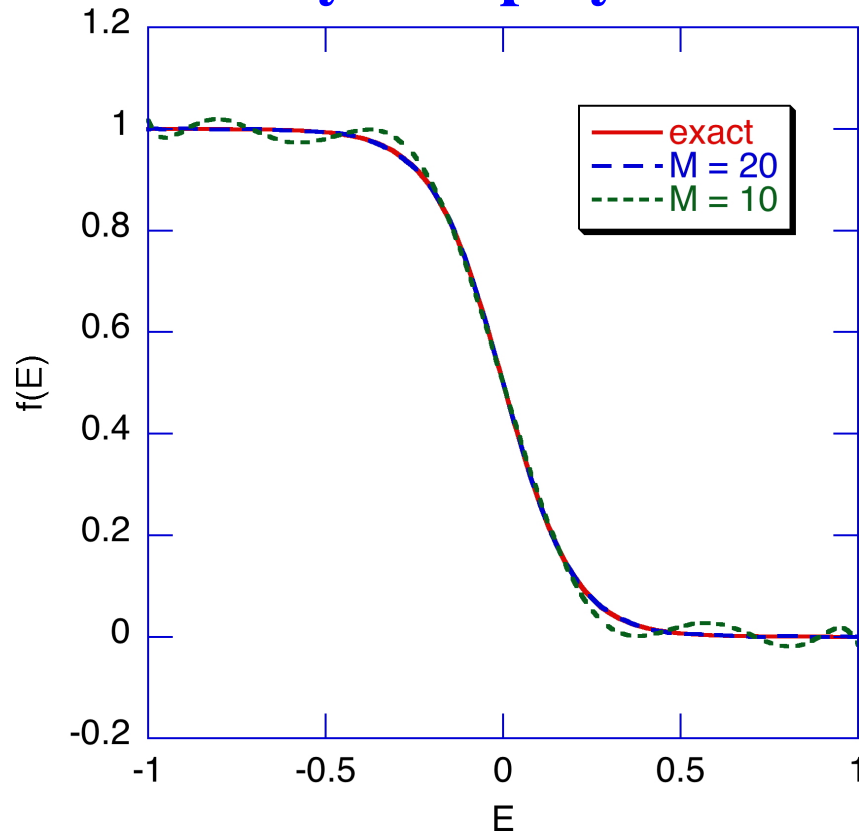
cf. $O(N^3)$ way

$$H|n\rangle = \varepsilon_n|n\rangle$$

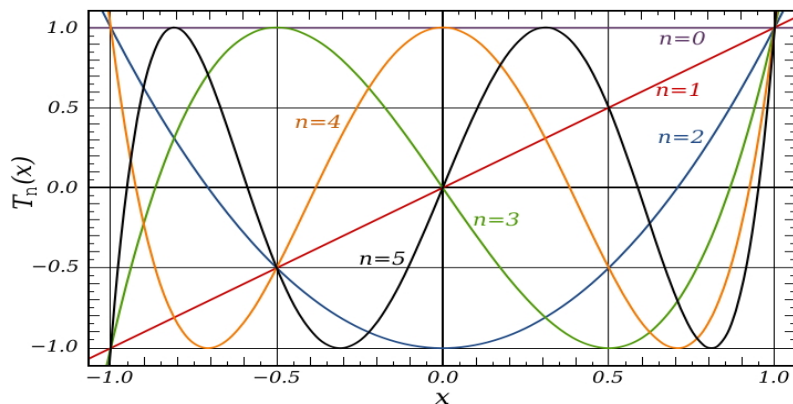
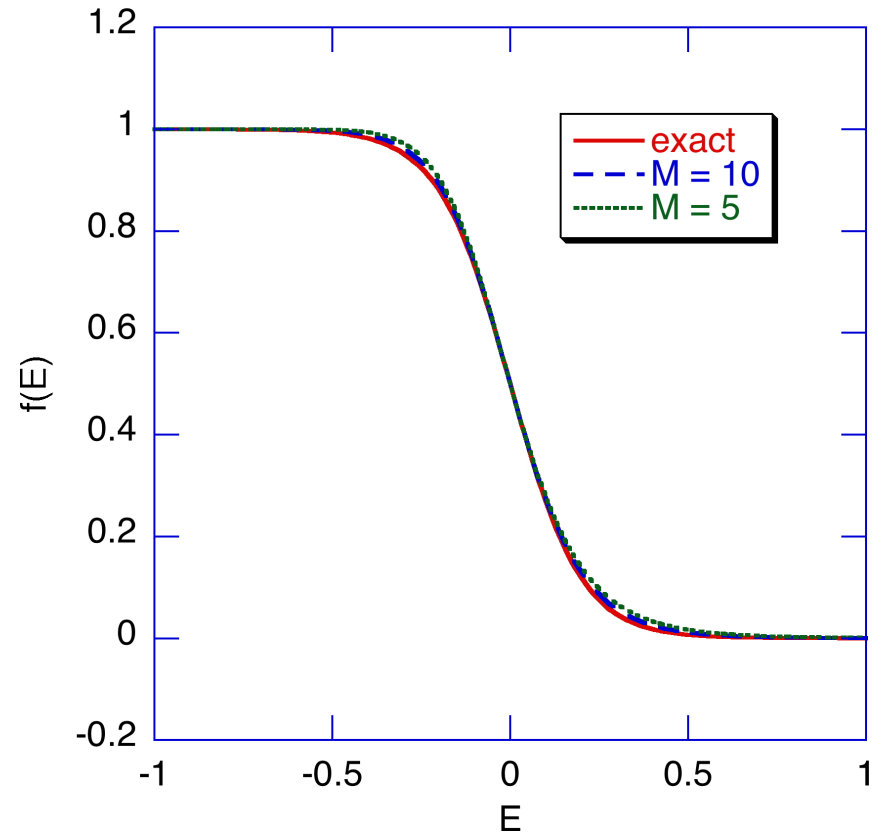
$$\langle \hat{A} \rangle = \sum_n \frac{2}{\exp\left(\frac{\varepsilon_n - \mu}{k_B T}\right) + 1} \langle n | \hat{A} | n \rangle$$

Fermi-Operator Approximations

Chebyshev polynomial



Rational



$$F(\hat{H}) \cong \sum_{v=1}^M \frac{R_v}{\hat{H} - z_v}$$

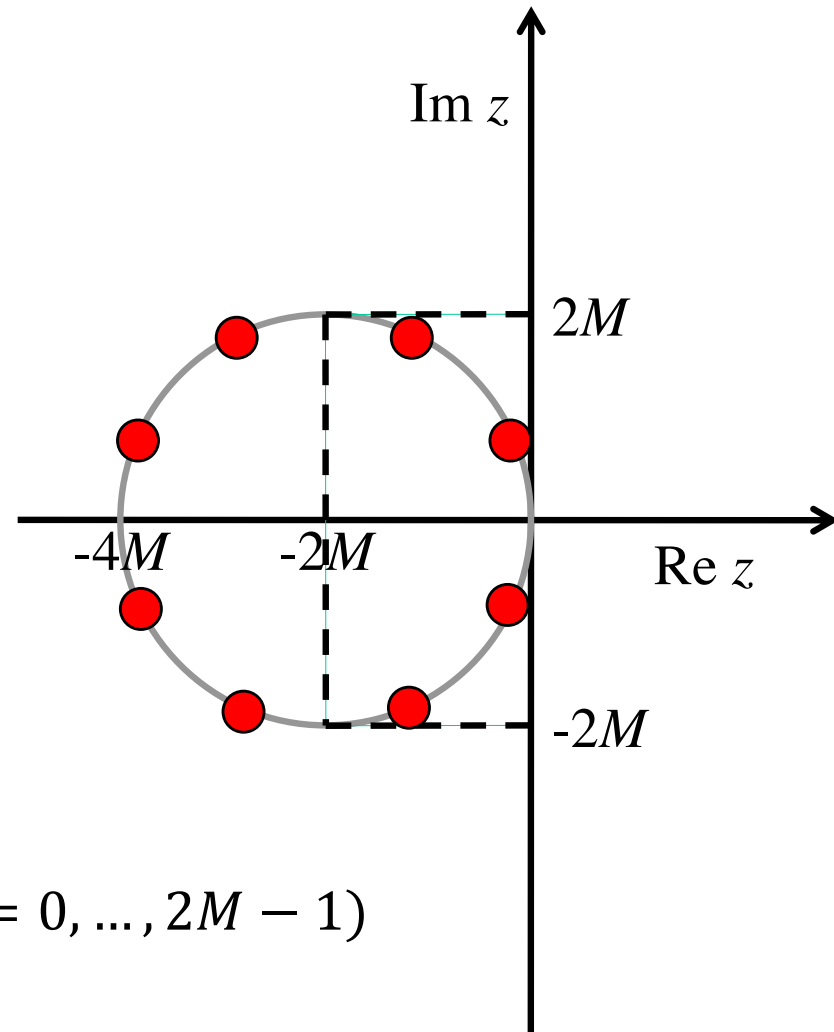
$$(\hat{H} - z_v) |\psi_{\text{out}}^v\rangle = R_v |\psi_{\text{in}}\rangle$$

Rational Fermi-Operator Expansion

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

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

$$\approx \sum_{v=0}^{2M-1} \frac{R_v}{z - z_v}$$



$$\begin{cases} \text{Poles} \\ z_v = 2M \left(\exp\left(i \frac{(2v+1)\pi}{2M}\right) - 1 \right) \\ R_v = -\exp\left(i \frac{(2v+1)\pi}{2M}\right) \\ \text{Residues} \end{cases} \quad (v = 0, \dots, 2M - 1)$$

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)

$O(N)$ 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 $|e_l\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}_l$

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

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