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 Quantitative & Computational Biology
University of Southern California

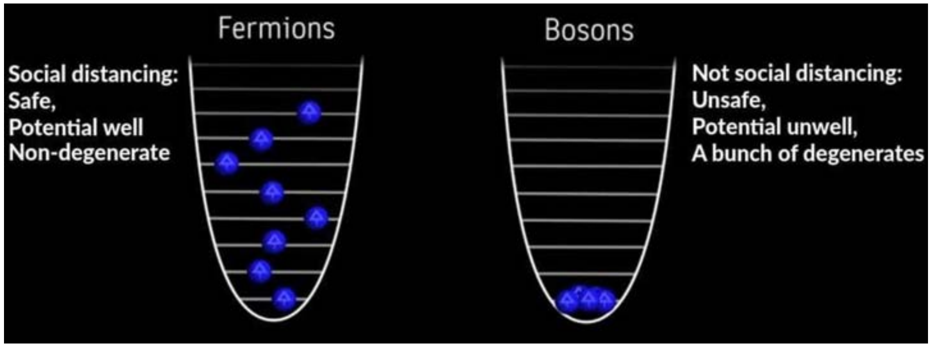
Email: anakano@usc.edu

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

Fermi Operator

- **Fermi operator**

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



- **Projection to the occupied subspace**

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

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

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

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

cf. $O(N^3)$ way

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

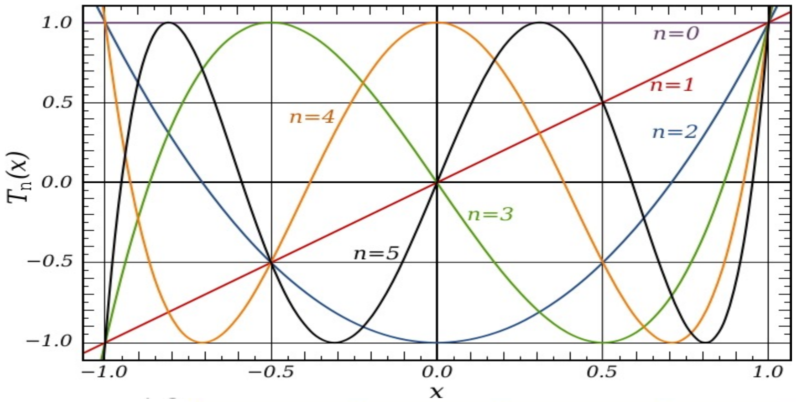
$$\left\langle \hat{A} \right\rangle = \sum_n \frac{2}{\exp\left(\dfrac{\varepsilon_n-\mu}{k_B T}\right)+1}\langle n|\hat{A}|n\rangle$$

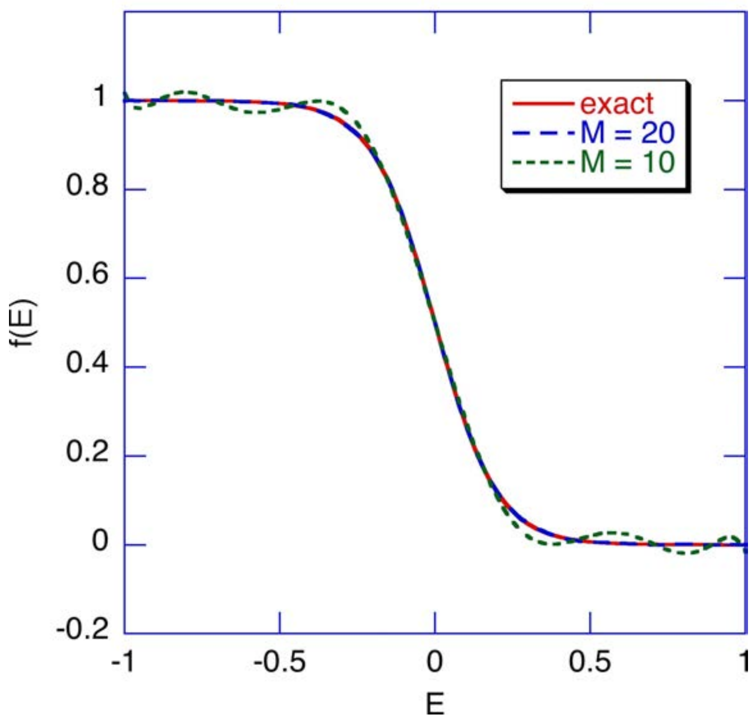
S. Goedecker, *Rev. Mod. Phys*. **71**, 1085 ('99)

Fermi-Operator Approximations

Chebyshev polynomial

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



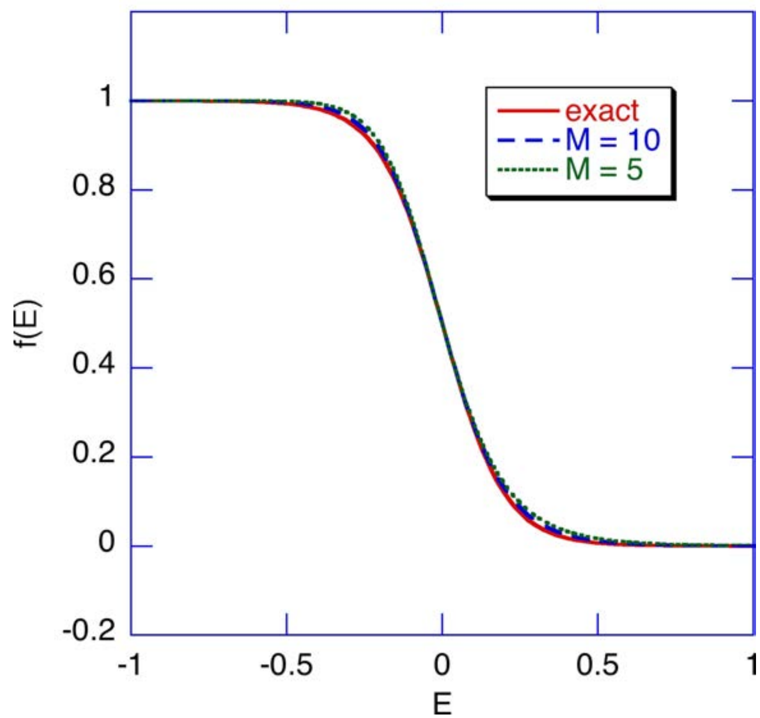


Rational

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

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

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



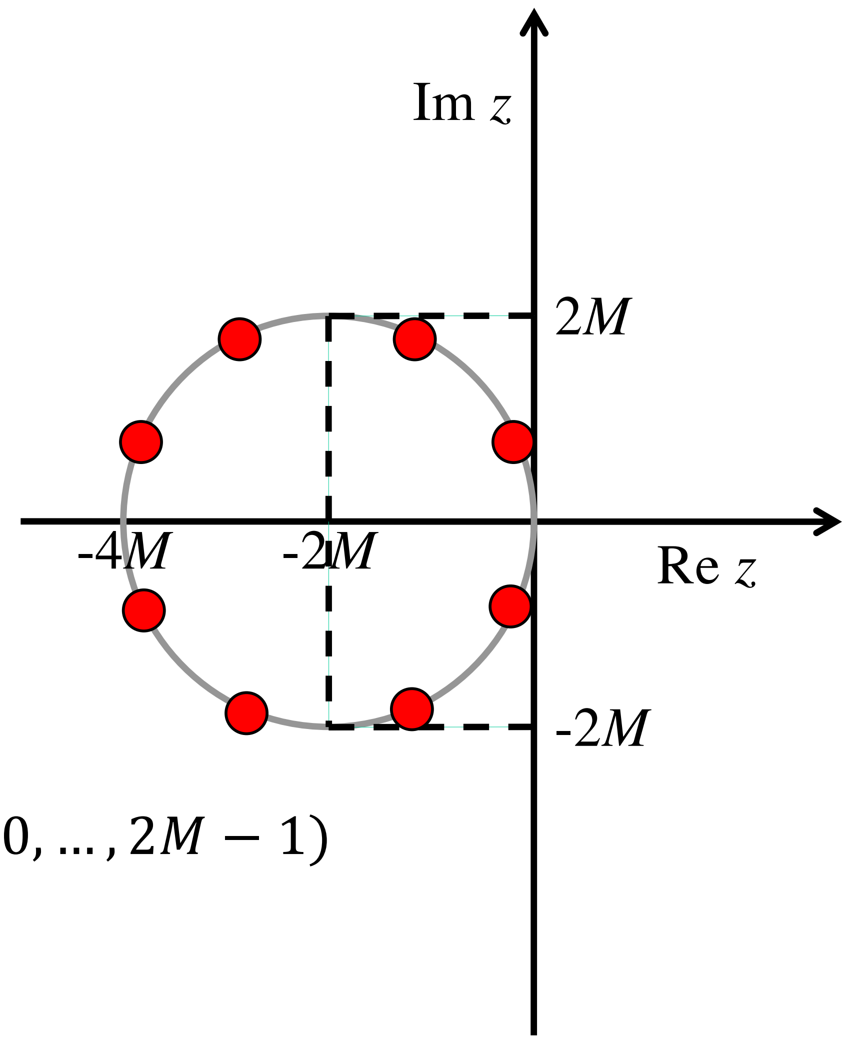
See note on [Fermi-operator expansion]()

Rational Fermi-Operator Expansion

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

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

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



Poles

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

Residues

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

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

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 $|e_l\rangle = \begin{array}{cc} \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} & \begin{array}{c} \\ \\ l \\ \\ \\ \end{array} \end{array}$ l-th atomic-site orbital

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

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

cf. Legendre polynomial by recursion

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

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

*Six degrees of separation
#W. Kohn, *Phys. Rev. Lett*. **76**, 3168 ('96)