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
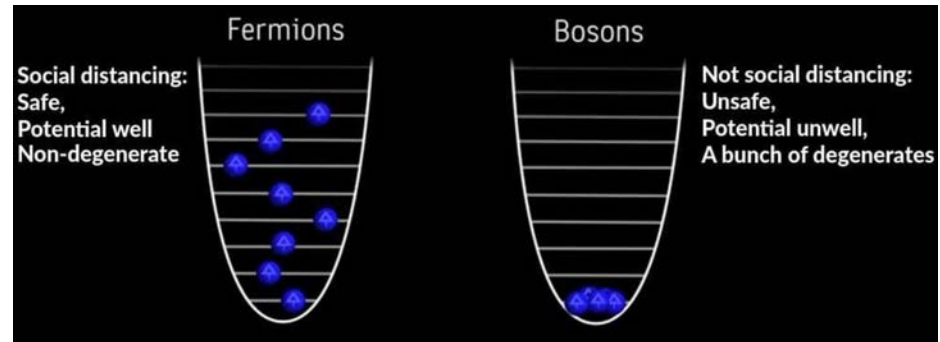*University of Southern California*

Email: anakano@usc.edu

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

Fermi Operator

- **Fermi operator**

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

- **Projection to the occupied subspace**

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

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

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

- **Widely used in $O(N)$ electronic structure calculations (N = number of electrons) through its sparse representation**
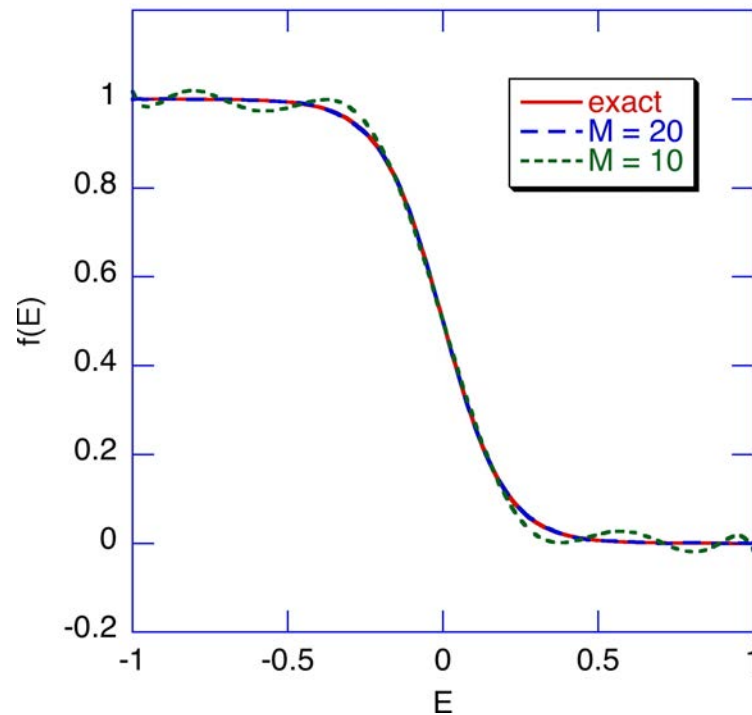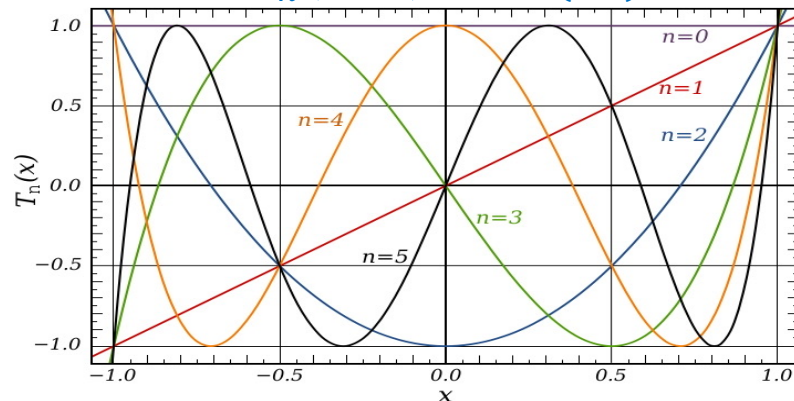
cf. $O(N^3)$ way

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

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

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

Fermi-Operator Approximations

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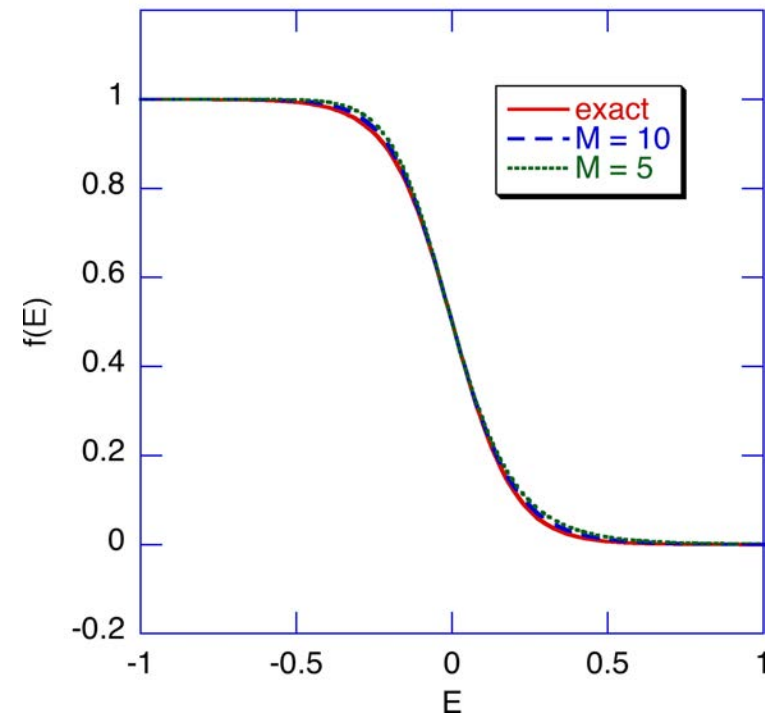
$$T_n(\cos\theta) = \cos(n\theta)$$

Rational

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

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

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

See note on Fermi-operator expansion

Rational Fermi-Operator Expansion

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

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

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

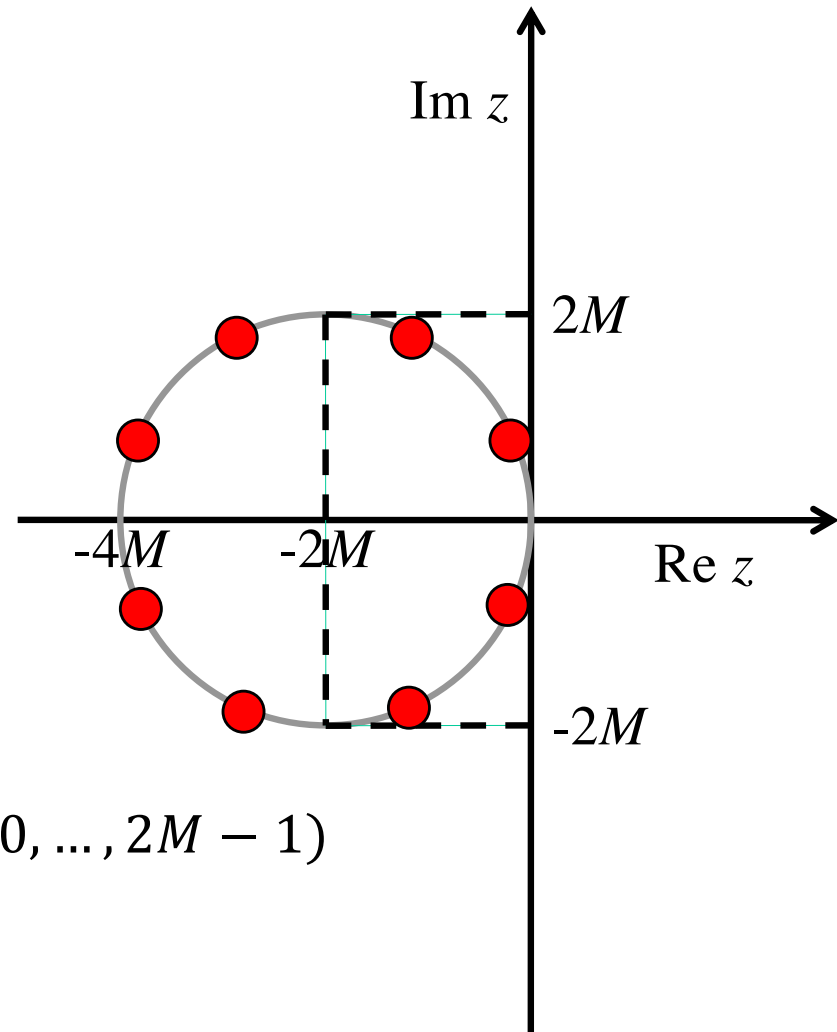$$\cong \sum_{\nu=0}^{2M-1} \frac{R_\nu}{z - z_\nu}$$

Poles

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

Residues

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

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

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 $\{T_p\}$**

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

- *$O(N)$ 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 lth column of
  matrix T_p, $|t_l^p\rangle$, keeping only $O(1)$
  off-diagonal elements* (*cf.* quantum nearsightedness#)

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

  build a sparse representation of the lth 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)