# Fermi-Operator Expansions for Linear Scaling Electronic Structure Calculations

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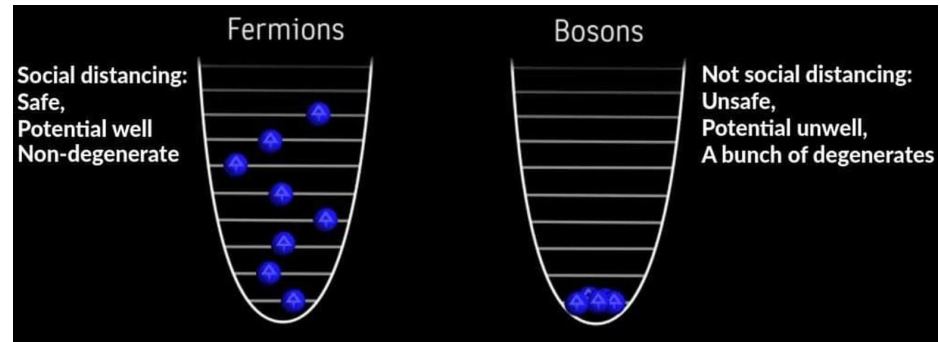*University of Southern California*

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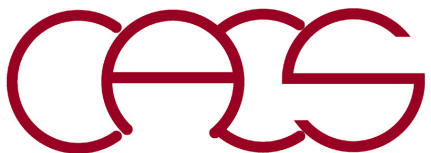
$O(N)$ sparse matrix representation

Fermi Operator

- **Fermi operator**

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

Fermions — Social distancing: Safe, Potential well, Non-degenerate

Bosons — Not social distancing: Unsafe, Potential unwell, A bunch of degenerates

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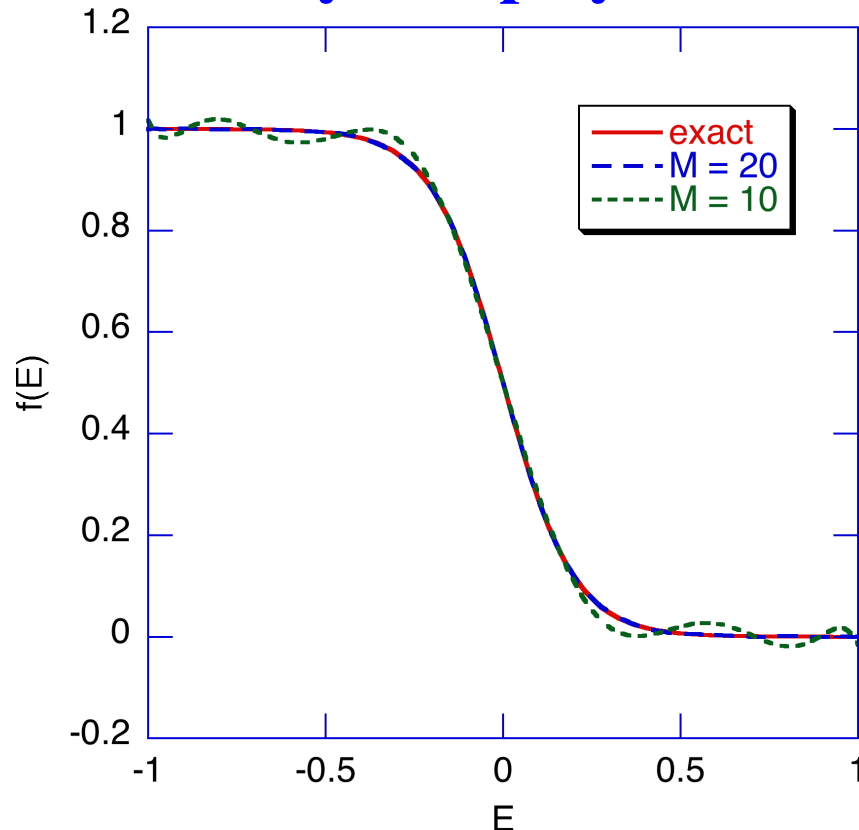
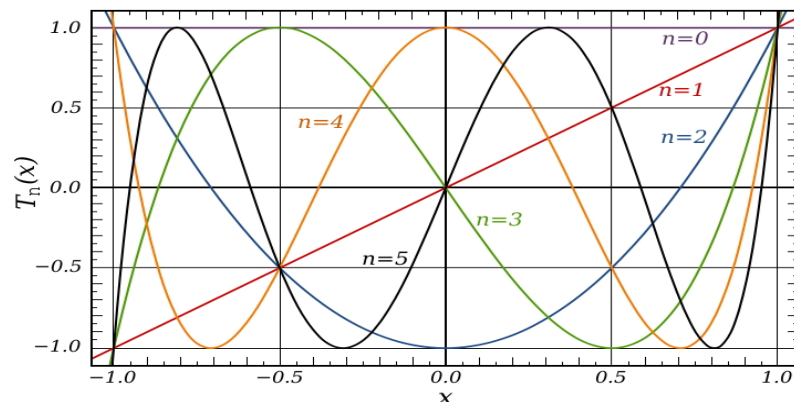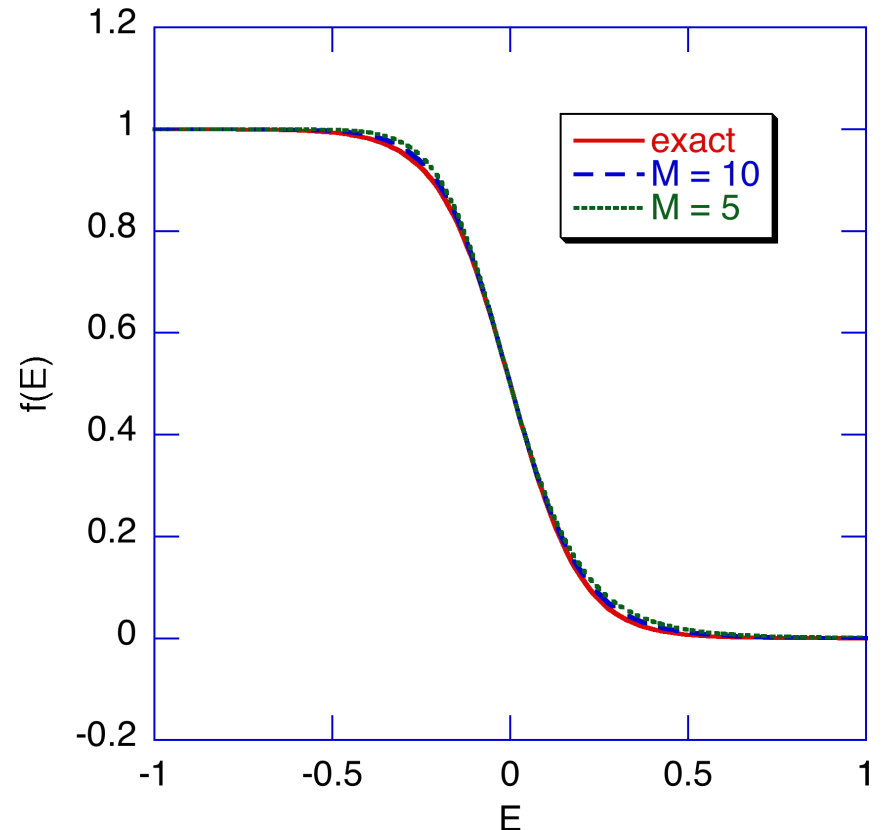*cf.* $O(N^3)$ way

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

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

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

Fermi-Operator Approximations

Chebyshev polynomial

Rational

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

$$\left(\hat{H} - z_\nu\right)\left|\psi_{\text{out}}^{\nu}\right\rangle = R_\nu \left|\psi_{\text{in}}\right\rangle$$
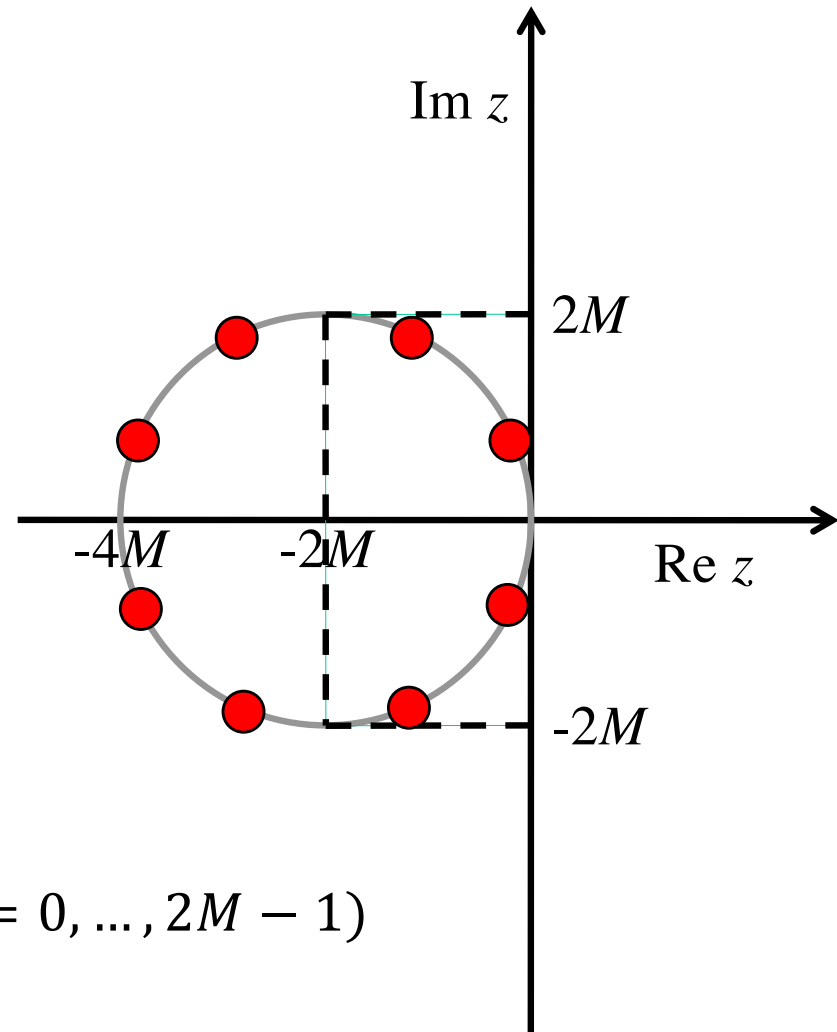
See note on Fermi-operator expansion

Rational Fermi-Operator Expansion

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

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

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

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

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

D. M. C. Nicholson *et al.*, *Phys. Rev. B* **50**, 14686 ('94);
A. P. Horsfield *et al.*, *Phys. Rev. B* **53**, 12694 ('96);
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 lth column of
matrix T_p, $\left| t_l^p \right\rangle$, keeping only $O(1)$
off-diagonal elements (*cf.* quantum nearsightedness)

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

build a sparse representation of the lth column of F as

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