Fermi-Operator Expansions for Linear Scaling Electronic Structure Calculations

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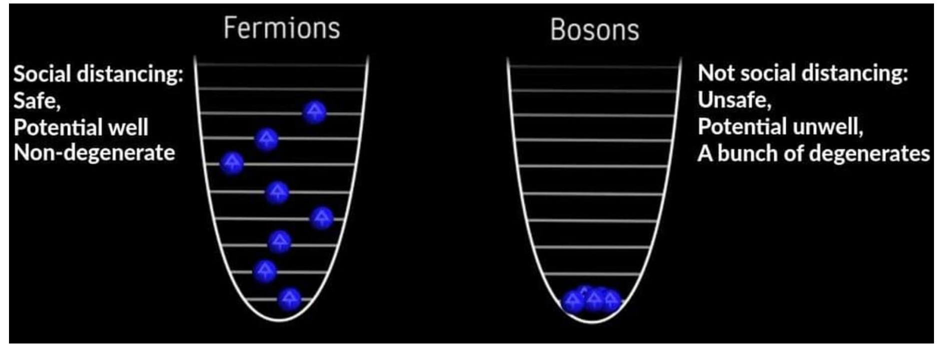
$O(N)$* sparse matrix representation
Simple & generalizable → use it

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**

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

- **Use: expectation value of any operator *A* is obtained by**

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

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

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

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

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

*Eigen-decomposition:

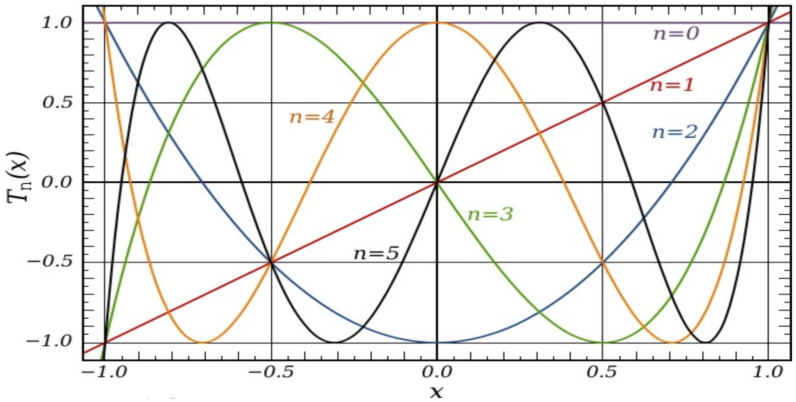
$$f(\hat{H}) = \hat{U}\begin{bmatrix} f(\epsilon_1) & & \\ & \ddots & \\ & & f(\epsilon_N) \end{bmatrix}\hat{U}^\dagger$$

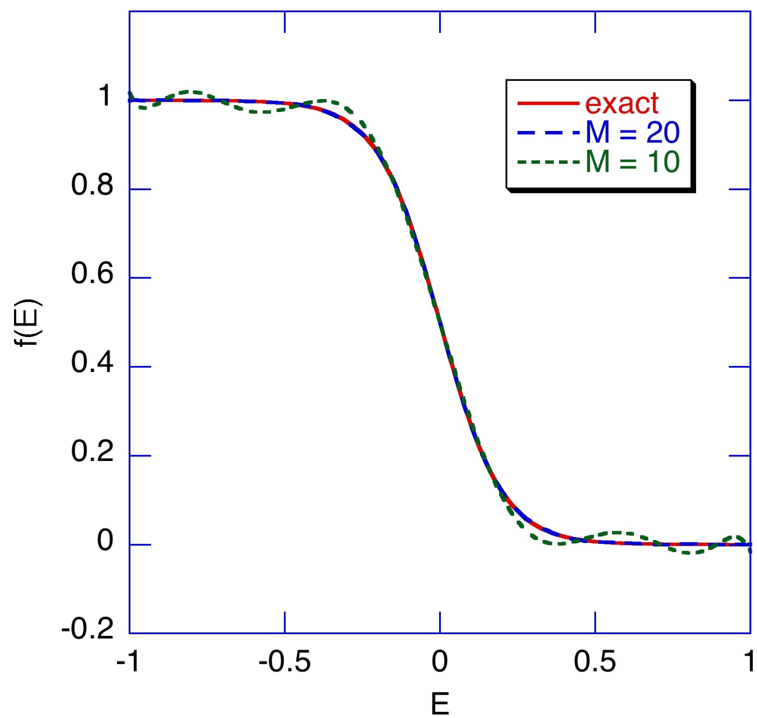
S. Goedecker, *Rev. Mod. Phys*. **71**, 1085 ('99)

Fermi-Operator Approximations

Chebyshev polynomial

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



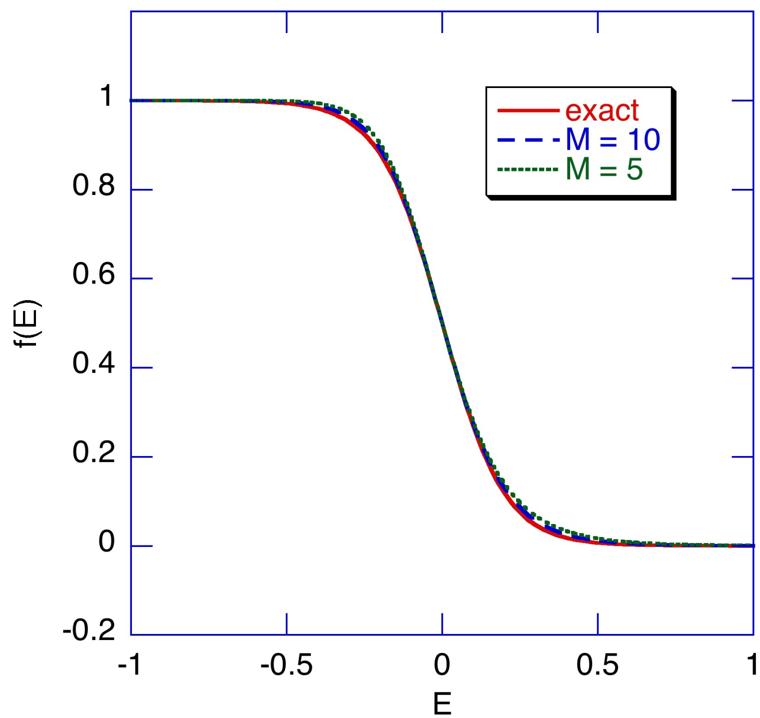


Rational

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

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

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



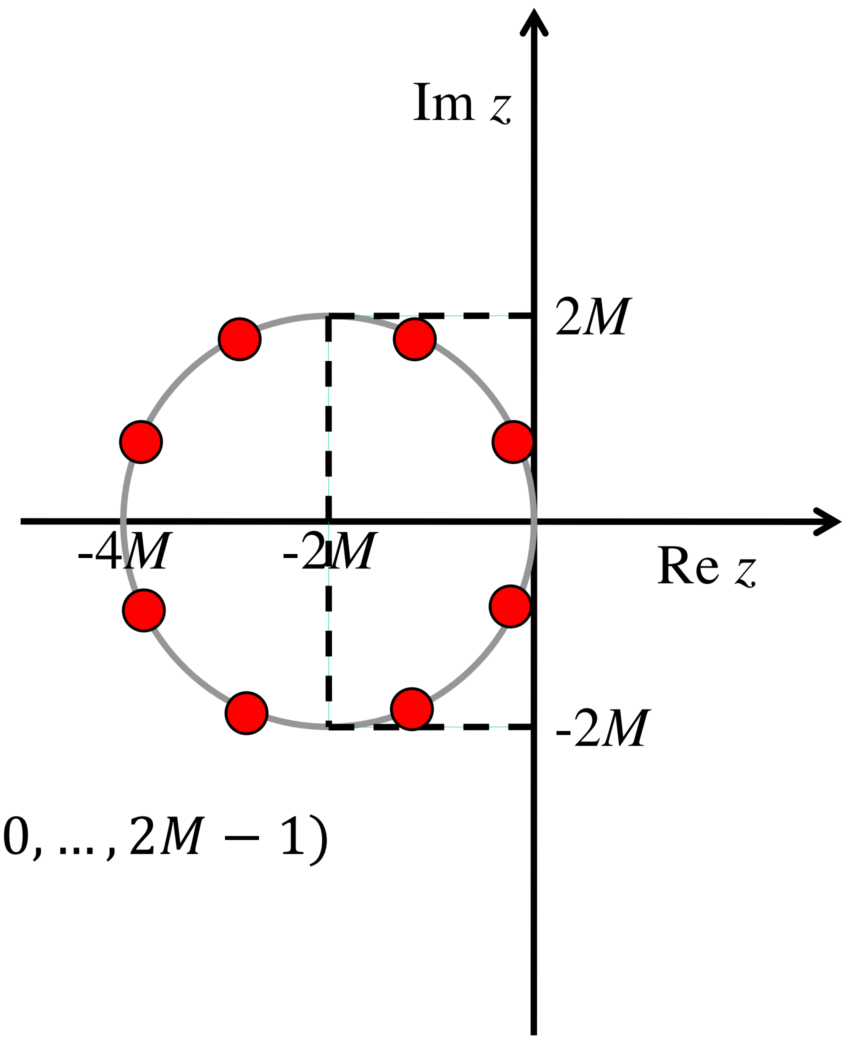
See note on Fermi-operator expansion

Rational Fermi-Operator Expansion

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

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

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



Poles

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

Residues

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

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

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

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

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

cf. Legendre polynomial by recursion

build a sparse representation of the l^{th} 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)