Fermi-Operator (= Density-Matrix) Expansion

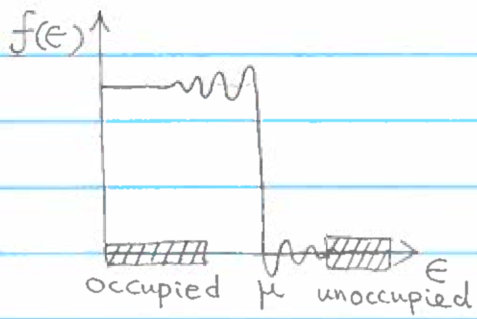
5/22/03

① Low-rank approximation of the Fermi matrix

$$f(\hat{H}) = \frac{1}{\exp[\beta(\hat{H}-\mu)]+1}$$

polynomial

$$\hat{f} \sim \sum_{p=0}^{M} c_p T_p(\hat{H}) \quad \text{chebyshev}$$



$$\rho(r,r') = \langle r|f(\hat{H})|r'\rangle$$

$$\sim \langle r| \underbrace{\sum_{p=0}^{M} c_p T_p(\hat{H})\,|r'\rangle}_{|f_{r'}\rangle}$$

rational — Padé/moment method

$$\hat{f} \sim \sum_{\nu=1}^{M} \frac{R_\nu}{z_\nu - \hat{H}}$$

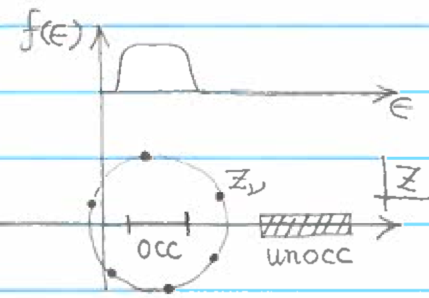
R_ν → residue

z_ν → complex pole

$$= \sum_{\nu=1}^{M} R_\nu \hat{G}(z_\nu)$$

where

$$\hat{G}(z) = \frac{1}{z-\hat{H}}$$



② Recursive construction of a Krylov subspace

Chebyshev recursion

$$\underbrace{T_{p+1}(\hat{H})|r\rangle}_{|f_{new}\rangle} = \underbrace{2\hat{H}T_p(\hat{H})|r\rangle}_{2\hat{H}|f_{now}\rangle} - \underbrace{T_{p-1}(\hat{H})|r\rangle}_{|f_{old}\rangle}$$

Lanczos recursion (tridiagonalization)

$$b_{n+1}|u_{n+1}\rangle = (\hat{H}-a_n)|u_n\rangle - b_n|u_{n-1}\rangle$$

$$G_{rr}(z) = \cfrac{1}{z-a_0-\cfrac{b_1^2}{z-a_1-\cfrac{b_2^2}{\ddots}}}$$

$G_{rr'}(z)$ by another recursion (large basis set ?)

$$\rho_{rr} = \mathrm{Re}\sum_{\nu=1}^{M} R_\nu \cfrac{1}{z_{\nu1}+iz_{\nu2}-a_0-\cfrac{b_1^2}{z_{\nu1}+iz_{\nu2}-a_1\cdots}}$$

③ O(N) localization approximation

Local approximation to $|f_r\rangle$ | Inherently O(N)

— Specific example of rational expansion

$$\left(1+\frac{z}{n}\right)^n \xrightarrow[n\to\infty]{} \exp(z)$$

$$f(\epsilon) = \frac{1}{\exp(\epsilon)+1} \sim \frac{1}{\left(1+\frac{\epsilon}{2M}\right)^{2M}+1}$$

This approximation has 2M simple poles.

$$z_\nu = 2M\left[\exp\left(i\pi\frac{2\nu+1}{2M}\right)-1\right] \qquad (\nu = 0, 1, \ldots, 2M-1)$$

☺ For $z = z_\nu + \Delta$,

$$\left(1+\frac{z}{2M}\right)^{2M}+1 = \left(1+\frac{1}{2M}\left\{\underbrace{2M\left[\exp\left(i\pi\frac{2\nu+1}{2M}\right)-1\right]}_{z_\nu}+\Delta\right\}\right)^{2M}+1$$

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

$$= \left\{\exp\left(i\pi\frac{2\nu+1}{2M}\right)\left[1+\frac{\Delta}{2M}\exp\left(-i\pi\frac{2\nu+1}{2M}\right)\right]\right\}^{2M}+1$$

$$= \underbrace{\exp[i\pi(2\nu+1)]}_{-1}\left[1+\frac{\Delta}{2M}\exp\left(-i\pi\frac{2\nu+1}{2M}\right)\right]^{2M}+1$$

$$\sim -\left[\cancel{1}+\cancel{2M}\cdot\frac{\Delta}{\cancel{2M}}\exp\left(-i\pi\frac{2\nu+1}{2M}\right)\right]+\cancel{1}$$

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

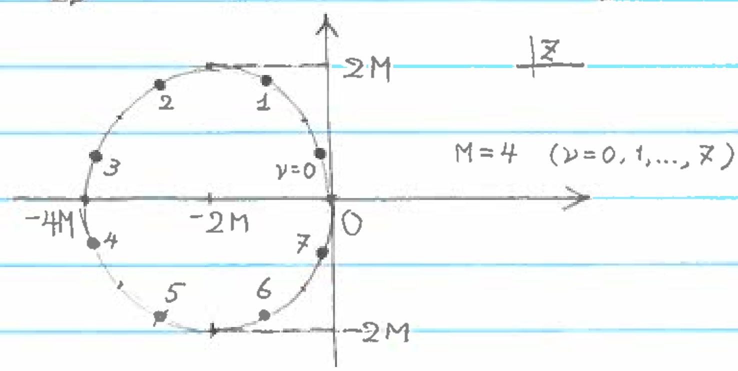
$$\therefore f(z_\nu+\Delta) = -\frac{\exp\left(i\pi\frac{2\nu+1}{2M}\right)}{\Delta} = \frac{R_\nu}{\Delta}, \quad \underbrace{R_\nu}_{\text{residue}} = -\exp\left(i\pi\frac{2\nu+1}{2M}\right) \quad //$$

③

— Note

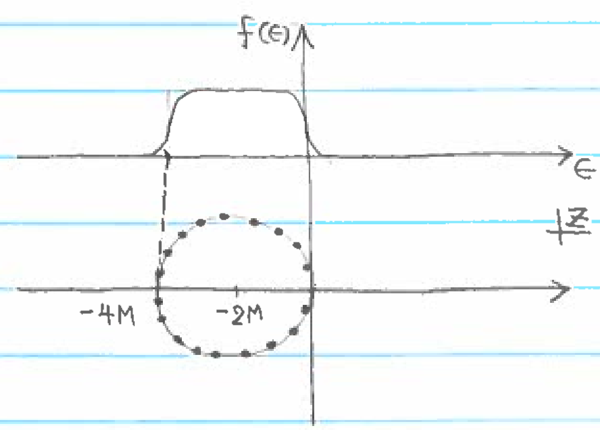
$$z_\nu = 2M\left\{\left[\cos\left(\pi\frac{2\nu+1}{2M}\right) - 1\right] + i\sin\left(\pi\frac{2\nu+1}{2M}\right)\right\}$$

$$= \underbrace{2M\left[\cos\left(\pi\frac{2\nu+1}{2M}\right) - 1\right]}_{a_\nu} + i\cdot\underbrace{2M\sin\left(\pi\frac{2\nu+1}{2M}\right)}_{b_\nu}$$



Thus, z_ν distribute symmetrically w.r.t. the real axis,
with $\nu = 0, 1, \ldots, M-1$ (upper half plane)

$M, M+1, \ldots, 2M-1$ (lower half plane)



— Fermi function

$$\int_{-\infty}^{\infty} d\epsilon\, f(\epsilon) \frac{1}{\epsilon - E + i\delta} = \int_{-\infty}^{\infty} d\epsilon\, f(\epsilon) \left[\frac{P}{\epsilon - E} - i\pi\delta(\epsilon - E) \right]$$

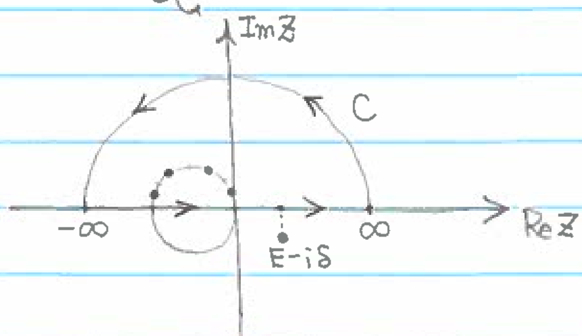
$$= \underbrace{\int_{-\infty}^{\infty} d\epsilon\, f(\epsilon) \frac{P}{\epsilon - E}}_{\mathrm{Re}} \underbrace{- i\pi f(E)}_{\mathrm{Im}}$$

$$\frac{i}{\pi} \int_{-\infty}^{\infty} d\epsilon\, f(\epsilon) \frac{1}{\epsilon - E + i\delta} = \underbrace{f(E)}_{\mathrm{Re}} + \underbrace{\frac{i}{\pi} \int_{-\infty}^{\infty} d\epsilon\, f(\epsilon) \frac{P}{\epsilon - E}}_{\mathrm{Im}}$$

$$\therefore f(E) = \mathrm{Re}\, \frac{i}{\pi} \int_{-\infty}^{\infty} d\epsilon\, f(\epsilon) \frac{1}{\epsilon - E + i\delta}$$

$$= \mathrm{Re}\, (-2) \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} f(\epsilon) \frac{1}{\epsilon - E + i\delta}$$

$$= \mathrm{Re}\, (-2) \oint_C \frac{dz}{2\pi i} f(z) \frac{1}{z - E + i\delta}$$



The contour shown above picks up the poles in the upper half plane, z_ν $(\nu = 0, 1, \cdots, M-1)$.

$$\therefore f(E) = \mathrm{Re}\, (-2) \oint_C \frac{dz}{2\pi i} f(z) \frac{1}{z - E + i\delta}$$

$$= -2\, \mathrm{Re} \sum_{\nu=0}^{M-1} \frac{R_\nu}{z_\nu - E}$$

Let's denote

$$e_\nu = \exp\left(i\pi \frac{2\nu+1}{2M}\right) = \cos\left(\pi \frac{2\nu+1}{2M}\right) + i\sin\left(\pi\frac{2\nu+1}{2M}\right) = C_\nu + iS_\nu$$

so that

$$\begin{cases} R_\nu = -e_\nu \\ z_\nu = 2M\,(e_\nu - 1) \end{cases}$$

$$\therefore f(E) = 2\,\mathrm{Re} \sum_{\nu=0}^{M-1} \frac{e_\nu}{z_\nu - E}$$

$$f(E) = 2\,\mathrm{Re} \sum_{\nu=0}^{M-1} \frac{C_\nu + iS_\nu}{\underbrace{(a_\nu - E) + ib_\nu}}$$

$$\frac{(C_\nu + iS_\nu)\,[(a_\nu - E) - ib_\nu]}{(a_\nu - E)^2 + b_\nu^2}$$

$$\therefore f(E) = 2 \sum_{\nu=0}^{M-1} \frac{C_\nu\,(a_\nu - E) + S_\nu b_\nu}{(a_\nu - E)^2 + b_\nu^2}$$

where

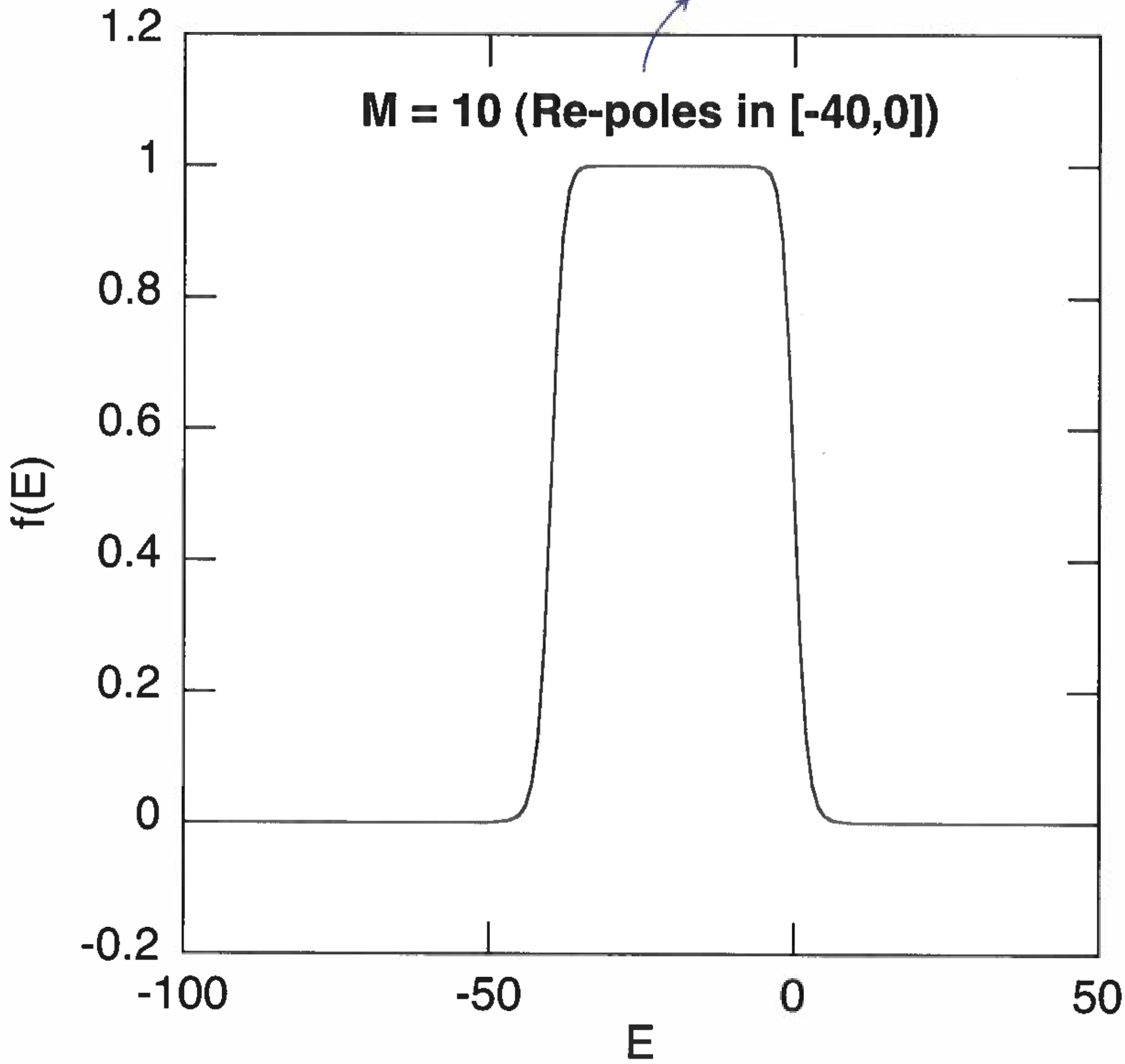
$$C_\nu = \cos\left(\pi\frac{2\nu+1}{2M}\right)$$

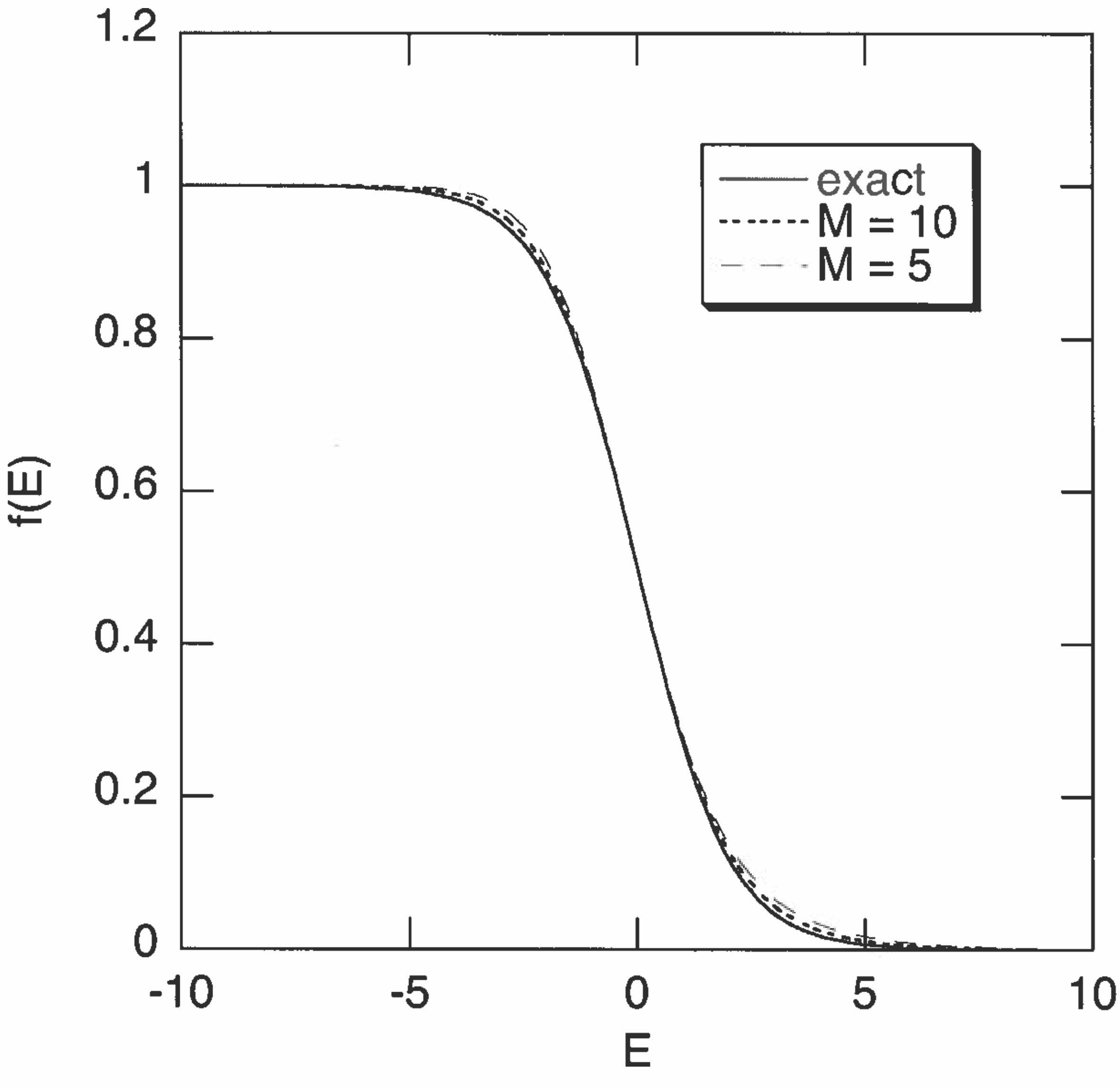
$$S_\nu = \sin\left(\pi\frac{2\nu+1}{2M}\right)$$

$$a_\nu = 2M\,(C_\nu - 1)$$

$$b_\nu = 2M\,S_\nu$$

M need to be sufficiently large to cover all occupied states





1.2
1
0.8
0.6
0.4
0.2
0
f(E)
-10
-5
0
5
10
E
exact
M = 10
M = 5

Chebyshev Polynomial

5/23/03

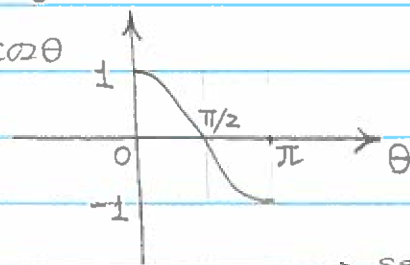
— Definition

$$\boxed{T_n(x) \equiv \cos(n \cos^{-1} x) \qquad (-1 \le x \le 1)} \tag{1}$$

where the arccos function is defined as

$$0 \le \theta = \cos^{-1} x \le \pi \tag{2}$$

$x = \cos\theta$



squeezed cos by factor n

$$\boxed{\begin{cases} T_n(x) \equiv \cos(n\theta) & (-1 \le x \le 1 ;\ 0 \le \theta \le \pi) \quad (3) \\ x = \cos\theta & \quad (4) \end{cases}}$$

— Recursive relation

$$\begin{aligned} T_{n+1}(x) &= \cos[(n+1)\theta] \\ &= \cos(n\theta + \theta) \\ &= \cos(n\theta)\cos\theta - \sin(n\theta)\sin\theta \\ &= x\, T_n(x) - \sin(n\theta)\sin\theta \end{aligned} \tag{5}$$

Now note that

$$\begin{aligned} &\cos(A+B) = \cos A \cos B - \sin A \sin B \\ -)\ &\underline{\cos(A-B) = \cos A \cos B + \sin A \sin B} \\ &\cos(A+B) - \cos(A-B) = -2 \sin A \sin B \end{aligned}$$

$$\therefore\ -\sin A \sin B = \frac{\cos(A+B) - \cos(A-B)}{2} \tag{6}$$

Using the relation (6) in Eq. (5),

$$T_{n+1} = x T_n + \frac{\cos[(n+1)\theta] - \cos[(n-1)\theta]}{2}$$

$$2T_{n+1} = x T_n + T_{n+1} - T_{n-1}$$

$$\therefore\ T_{n+1}(x) = x T_n(x) - T_{n-1}(x) \quad (n \geq 1) \qquad (7)$$

with initial conditions,

$$\begin{cases} T_0(x) = \cos(\emptyset) = 1 & (8) \\ T_1(x) = \cos\theta = x & (9) \end{cases}$$

— Orthogonalization

$$I_{ij} \equiv \int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}}\, T_i(x)\, T_j(x) \qquad (10)$$

Let $x = \cos\theta$ $(0 \leq \theta \leq \pi)$, then $dx = -\sin\theta\, d\theta$

$$I_{ij} = \int_{\emptyset}^{\pi} \cancel{\frac{-\sin\theta\, d\theta}{|\sin\theta|}} \cos(i\theta)\cos(j\theta)$$

$\sin\theta \geq \emptyset$ $(0 \leq \theta \leq \pi)$

$$= \int_{\emptyset}^{\pi} d\theta\, \frac{\cos[(i+j)\theta] + \cos[(i-j)\theta]}{2}$$

(Case $i \neq j$)

$$I_{ij} = \frac{1}{2}\left\{ \left[\frac{\sin(i+j)\theta}{i+j}\right]_{\emptyset}^{\pi} + \left[\frac{\sin(i-j)\theta}{i-j}\right]_{\emptyset}^{\pi} \right\} = \emptyset$$

(Case $i = j \neq 0$)

$$I_{ij} = \int_0^{\pi} d\theta \, \frac{\cos(2i\theta) + 1}{2}$$

$$= \frac{1}{2}\left[\cancel{\frac{\sin(2i\theta)}{2i}} + \theta\right]_0^{\pi} = \frac{\pi}{2}$$

(Case $i = j = 0$)

$$I_{ij} = \int_0^{\pi} d\theta \, \frac{1+1}{\cancel{2}} = \pi$$

$$\boxed{\therefore \int_{-1}^{1} \frac{dx}{\sqrt{1-x^2}} T_i(x) T_j(x) = \begin{cases} 0 & (i \neq j) \\ \pi/2 & (i = j \neq 0) \\ \pi & (i = j = 0) \end{cases}} \qquad (11)$$

– Zero points

$$T_n(x) = \cos(n\theta) = 0 \quad \text{when} \quad n\theta = \frac{2k-1}{2}\pi = (k - \tfrac{1}{2})\pi$$

Since $0 \leq n\theta \leq n\pi$,

$$0 \leq \frac{2k-1}{2}\cancel{\pi} \leq n\cancel{\pi}$$

$$0 \leq 2k-1 \leq 2n$$

$$1 \leq 2k \leq 2n+1$$

$$\tfrac{1}{2} \leq k \leq n + \tfrac{1}{2}$$

Since k is an integer, $k = 1, 2, \ldots, n$

$$\boxed{\begin{array}{l} \text{There are } n \text{ zero's for } T_n(x), \text{ where} \\ \quad x = \cos\left(\frac{k - \frac{1}{2}}{n}\pi\right) \quad (k = 1, 2, \ldots, n) \end{array}} \qquad (12)$$

※ At all maxima, $T_n(x) = 1$; at all minima, $T_n(x) = -1$

— Discrete orthogonality

Let $x_k = \cos\left(\frac{k-1/2}{K}\pi\right) = \cos\theta_k$ $(k=1,2,\dots,K)$ be the K zero points of $T_K(x)$ and $m,n \le K$.

$$I_{mn} \equiv \sum_{k=1}^{K} T_m(x_k)\,T_n(x_k) \tag{13}$$

$$= \sum_{k=1}^{K} \cos(m\theta_k)\cos(n\theta_k)$$

$$= \sum_{k=1}^{K} \frac{\cos[(m+n)\theta_k] + \cos[(m-n)\theta_k]}{2}$$

$$= \frac{1}{2}\mathrm{Re}\sum_{k=1}^{K}\left[e^{i(m+n)\theta_k} + e^{i(m-n)\theta_k}\right]$$

$$= \frac{1}{2}\mathrm{Re}\sum_{k=1}^{K}\left\{\exp\left[i\frac{(m+n)(k-1/2)}{K}\pi\right] + \exp\left[i\frac{(m-n)(k-1/2)}{K}\pi\right]\right\} \tag{14}$$

I_{mn} is thus expressed as geometric series.

(Case $m \neq n$)

$$I_{mn} = \frac{1}{2}\mathrm{Re}\left[\frac{\exp\left[i\frac{(m+n)\pi}{2K}\right]\left\{1 - \overbrace{\exp[i(m+n)\pi]}^{(-1)^{m+n}}\right\}}{1-\exp\left[i\frac{(m+n)\pi}{K}\right]} + \frac{\exp\left[i\frac{(m-n)\pi}{2K}\right]\left\{1 - \overbrace{\exp[i(m-n)\pi]}^{(-1)^{m-n}}\right\}}{1-\exp\left[i\frac{(m-n)\pi}{K}\right]}\right]$$

$$= \frac{1}{2}\mathrm{Re}\left\{\frac{1-(-1)^{m+n}}{\underbrace{\exp\left[-i\frac{(m+n)\pi}{2K}\right] - \exp\left[i\frac{(m+n)\pi}{2K}\right]}_{-2i\sin\left[\frac{(m+n)\pi}{2K}\right]}} + \frac{1-(-1)^{m-n}}{\underbrace{\exp\left[-i\frac{(m-n)\pi}{2K}\right] + \exp\left[i\frac{(m-n)\pi}{2K}\right]}_{-2i\sin\left[\frac{(m-n)\pi}{2K}\right]}}\right\}$$

$$= \frac{1}{4}\mathrm{Re}\; i\left\{\frac{1-(-1)^{m+n}}{\sin\left[\frac{(m+n)\pi}{2K}\right]} + \frac{1-(-1)^{m-n}}{\sin\left[\frac{(m-n)\pi}{2K}\right]}\right\}$$

↳ pure imaginary

$$= \varnothing$$

(Case $m = n \neq 0$)

The first sum in Eq.(14) is 0,

$$I_{mn} = \frac{1}{2} \mathrm{Re} \sum_{k=1}^{K} 1 = \frac{K}{2}$$

(Case $m = n = 0$)

$$I_{mn} = \frac{1}{2} \mathrm{Re} \sum_{k=1}^{K} (1+1) = K$$

(Discrete orthogonality) Let $x_k = \cos\left(\frac{k-1/2}{K}\pi\right) = \cos\theta_k$ $(k = 1, 2, \ldots, K)$ be the K zero points of $T_K(x)$ and $m, n \leq K$. Then

$$I_{mn} \equiv \sum_{k=1}^{N} T_m(x_k) T_n(x_k) = \begin{cases} 0 & (m \neq n) \\ K/2 & (m = n \neq 0) \\ K & (m = n = 0) \end{cases} \tag{15}$$

— Chebyshev expansion

Let $x_k = \cos\left(\frac{k-1/2}{N}\pi\right) = \cos\theta_k$ $(k = 1, 2, \ldots, N)$ and

$$c_j \equiv \frac{2}{N} \sum_{k=1}^{N} f(x_k) T_j(x_k) \tag{16}$$

Then the following approximation is exact for all k:

$$f(x) \sim \frac{c_0}{2} + \sum_{j=1}^{N-1} c_j T_j(x) \tag{17}$$

☹ Let

$$f'(x) \equiv \frac{c_0}{2} + \sum_{j=1}^{N-1} c_j T_j(x) \qquad (18)$$

$\frac{2}{N}\sum_{k=1}^{N}$ x above $T_i(x)\big|_{x_k}$

$$\frac{2}{N}\sum_{k=1}^{N} f'(x_k) T_i(x_k) = \frac{c_0}{\cancel{2}}\frac{\cancel{2}}{\cancel{N}}\underbrace{\sum_{k=1}^{N} T_0(x_k) T_i(x_k)}_{\cancel{N}\delta_{i0}} + \frac{\cancel{2}}{\cancel{N}}\sum_{j=1}^{N-1} c_j \underbrace{\sum_{k=1}^{N} T_i(x_k) T_j(x_k)}_{\cancel{\frac{N}{2}}\delta_{ij}}$$

$$= c_0 \cancel{\delta_{i0}} + c_i (1 - \cancel{\delta_{i0}})$$

$$= c_i$$

We have thus shown, for all $i \in [0, N-1]$

$$\frac{2}{N}\sum_{k=1}^{N} f'(x_k) T_i(x_k) = \frac{2}{N}\sum_{k=1}^{N} f(x_k) T_i(x_k)$$

$$\therefore \forall i \in [0, N-1] \left\{ \frac{2}{N}\sum_{k=1}^{N} [f'(x_k) - f(x_k)] T_i(x_k) \right\} = 0 \qquad (19)$$

Let's define

$$\vec{T}_i \equiv (T_i(x_1), T_i(x_2), \dots, T_i(x_N)) \quad (i = 0, 1, \dots, N-1) \qquad (20)$$

From Eq. (15), $\{\vec{T}_0, \vec{T}_1, \dots, \vec{T}_{N-1}\}$ forms a linearly-independent complete basis set of the N-dimensional vector space, and Eq. (19) shows that $\vec{f}' - \vec{f} = \emptyset$ in this space. //

— Example : Chebyshev approximation for the Fermi function

$$f(x) = \frac{1}{\exp(\beta x) + 1} \qquad x \in [-1, 1] \qquad (21)$$

(Algorithm)

Input : N (≥ 2)

Output : $\{c_j \mid j = 0, \ldots, N-1\}$

$c_j \leftarrow 0 \quad (j = 0, \ldots, N-1)$

for $k = 1$ to N

  $x \leftarrow \cos\left(\frac{k-1/2}{N}\pi\right)$; $f \leftarrow f(x_k)$

  $T_{m2} \leftarrow 1$; $c_0 \leftarrow c_0 + f\, T_{m2}$

  $T_{m1} \leftarrow x$; $c_1 \leftarrow c_1 + f\, T_{m1}$

  for $j = 2$ to $N-1$

    $T_{m\emptyset} \leftarrow 2x\, T_{m1} - T_{m2}$

    $c_j \leftarrow c_j + f\, T_{m\emptyset}$

    $T_{m2} \leftarrow T_{m1}$

    $T_{m1} \leftarrow T_{m\emptyset}$

$c_j \leftarrow \frac{2}{N} c_j \quad (j = 0, \ldots, N-1)$

Usage: For a given x

  $f \leftarrow \frac{c_0}{2} + c_1 x$

  $T_{m2} \leftarrow 1$

  $T_{m1} \leftarrow x$

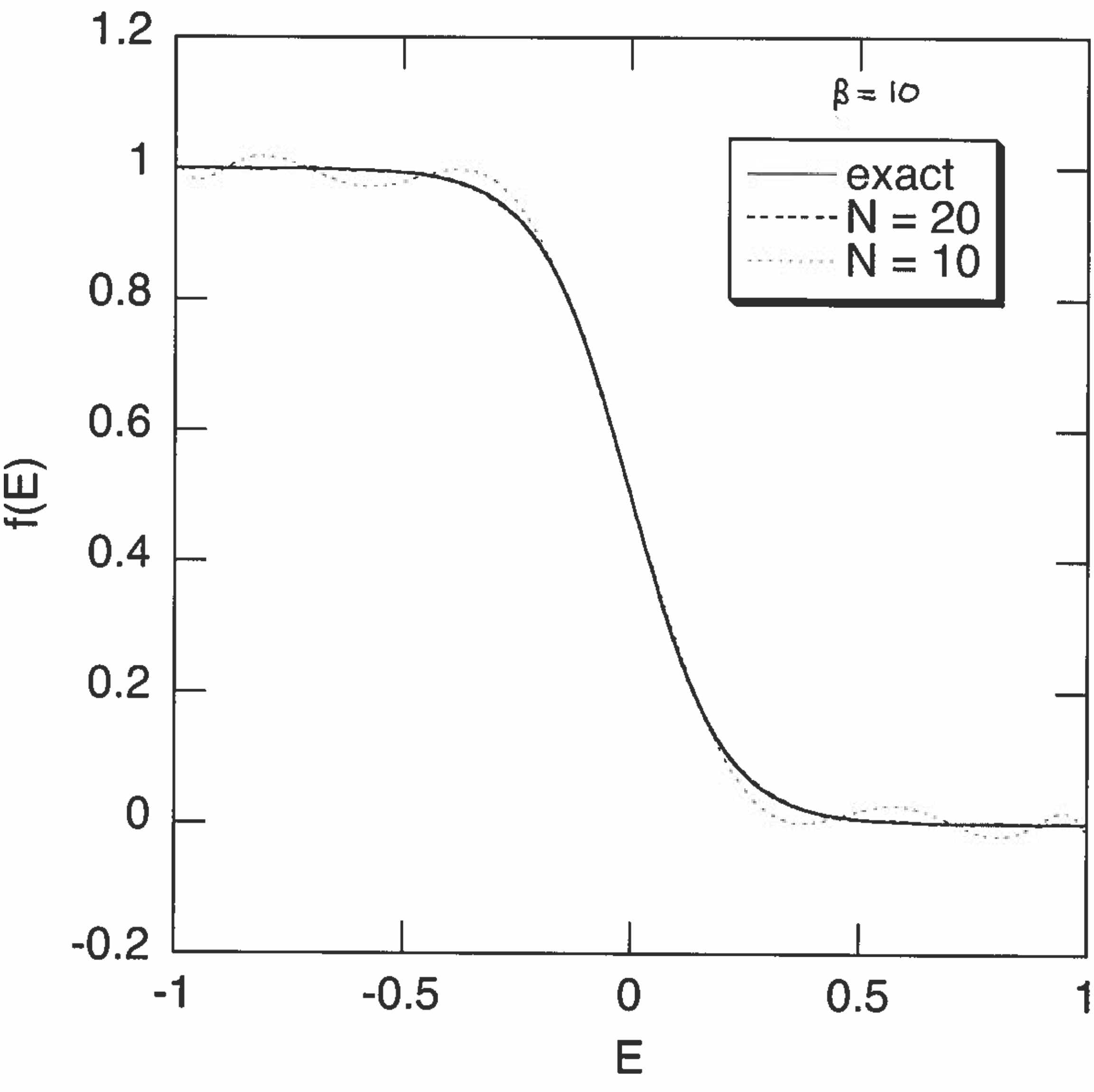
  for $j = 2$ to $N-1$

    $T_{m0} \leftarrow 2x\, T_{m1} - T_{m2}$

    $f \leftarrow f + c_j \cdot T_{m0}$

    $T_{m2} \leftarrow T_{m1}$

    $T_{m1} \leftarrow T_{m}$


β = 10
exact
N = 20
N = 10
f(E)
E
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-1
-0.5
0
0.5
1