Topological Optimization Using the SIMP Method

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Outline

- ► Orthogonal Polynomials
- ► Chebyshev Polynomials
- ► Chebyshev Expansion
- Using Kernel Polynomials
- ► Application: Calculating the Density of States

Orthogonal Polynomials

Scalar product on [a, b]:

$$\langle f|g\rangle = \int_{a}^{b} w(x)f(x)g(x) \,\mathrm{d}x$$

Given a scalar product, we get a set of polynomials, p_n , which satisfy the orthogonality relation

$$\langle p_n|p_m\rangle = \delta_{n,m} \langle p_n|p_n\rangle.$$

This allows for an expansion of any given function f(x) in terms of the $p_n(x)$:

$$f(x) = \sum_{n=0}^{\infty} \alpha_n p_n(x)$$
 with $\alpha_n = \frac{\langle p_n | f \rangle}{\langle p_n | p_n \rangle}$

Chebyshev Polynomials

I will focus on Chebyshev polynomials of the first kind, T_n :

Defined on interval [-1,1] with weight function $w(x) = \left(\pi\sqrt{1-x^2}\right)^{-1}$.

$$T_n = \cos(n\arccos(x))$$

Recursively defined:

$$T_0(x) = 1$$
, $T_{-1}(x) = T_1(x) = x$,
 $T_{m+1}(x) = 2xT_m(x) - T_{m-1}(x)$.

The polynomials also follow the relation

$$2T_m(x)T_n(x) = T_{m+n}(x) + T_{m-n}(x).$$

Chebyshev Polynomials have some particular advantages which make them ideal for use in orthogonal polynomial expansions.

Chebyshev Expansion

The expansion of f(x) in terms of Chebyshev polynomials

$$f(x) = \sum_{n=0}^{\infty} \frac{\langle f|T_n\rangle_1}{\langle T_n|T_n\rangle_1} T_n(x)$$

To make this a easier to compute, we rearrange:

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}} \left[\mu_0 + 2\sum_{n=1}^{\infty} \mu_n T_n(x) \right], \quad \mu_n = \int_{-1}^1 f(x) T_n(x) \, \mathrm{d}x.$$

However, calculating the moments μ_n can be quite computationally expensive.

Motivation for KPM: Gibbs Oscillations

In practice, we cannot compute an infinite series, so we need to truncate:

$$f(x) \approx \frac{1}{\pi\sqrt{1-x^2}} \left[\mu_0 + 2 \sum_{n=1}^{N-1} \mu_n T_n(x) \right]$$

Gibbs Oscillations:

Kernel Polynomials

To lessen the impact of the Gibbs Oscillations, we introduce a "damping function" in the form of a kernel polynomial, g_n :

$$f_{\text{KPM}}(x) = \frac{1}{\pi\sqrt{1-x^2}} \left[g_0\mu_0 + 2\sum_{n=1}^{N-1} g_n\mu_n T_n(x) \right]$$

Application: Density of States Calculations

Density of States: How many energy states exist at a given energy ${\cal E}.$

$$\rho(E) = \frac{1}{N} \sum_{k=0}^{N-1} \delta(E - E_k)$$

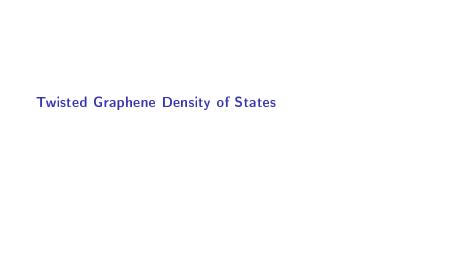
Scale E down to [-1,1]:

$$E = aX + b$$

We can approximate ho(E) using KPM:

$$\rho(E) \approx \frac{1}{\pi\sqrt{1-x^2}} \left[g_0 \mu_0 + 2 \sum_{n=1}^{N-1} g_n \mu_n T_n(X) \right]$$
$$\mu_n \approx \frac{1}{N_r} \sum_{n=1}^{N-1} \left\langle r | T_n(X) | r \right\rangle$$

Disilicon Si₂ Density of States



Topics of Further Exploration

- ightharpoonup Effects of the number of random vectors (R) used in calculating the moments.
- ightharpoonup Optimal resolution values (N) for various Hamiltonians.
- ▶ More in-depth comparisons of various kernels.

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Bibliography



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