

Moment based approach to electronic structure calculations: applications to ordered and disordered systems

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Scope of Talk

- Maximum Entropy and Classical Moment Problem (CMP)
 - Electronic Structures and CMP
 - Tight binding Hamiltonian and its density of state (DOS)
 - Fermi Levels
 - Conclusions
-

Maximum Entropy and Classical Moment Problem (CMP)

- How to construct a solution from an incomplete set of moment data.
- Moments:
 - A mathematical way to express the properties of a distribution.

$$\mu_n^p = \int_a^b p(x) f(x) dx \quad n = 0, 1, 2, 3, \dots$$

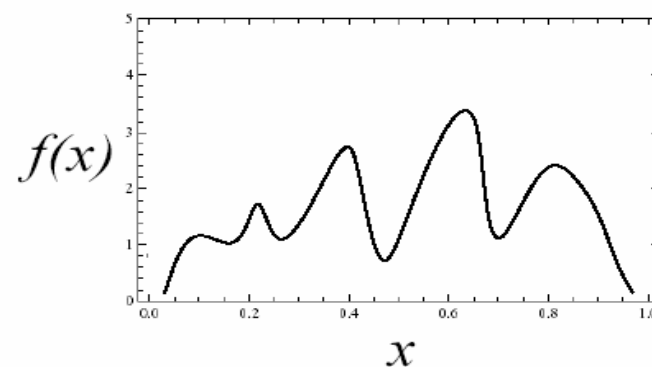
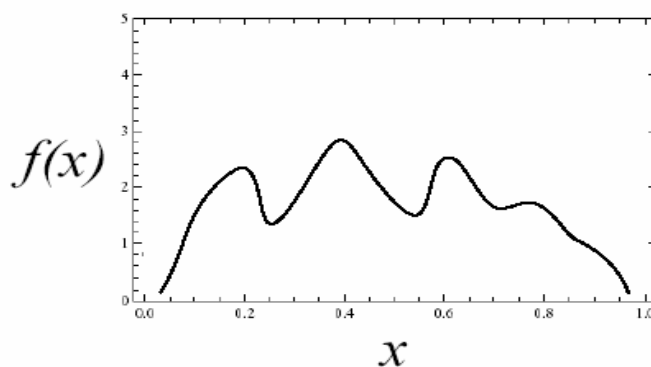
$$\mu_n < \infty \quad \text{for } n \rightarrow \infty \quad f(x) \in [a, b]$$

- Given a set of finite moments, μ_n , one can construct an approximate density distribution function $f(x)$ that satisfies the moments.

[Akheizer 1965, Shohat and Tamarkin 1963]

- For finite number of moments, multiple solutions exist!

The same moment with different distributions...



Maximum Entropy Approach

- Maximize the information entropy to obtain the least biased (or most likely) solution out of multiple solutions.

$$S[f] = - \int f(x) \ln[f(x)] dx$$

Shannon information entropy

The Algorithm

- Use Chebyshev moments.

$$\mu_n = \int T_n(x) f(x) dx$$

- Properties of Chebyshev polynomials

- Recursion relation: $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$, $T_0 = 1$, $T_1 = x$
- A minmax polynomial
- More accurate results

- Iteratively obtain the Lagrange multiplier.

$$\tilde{f}_j = w_j \exp \left(\sum_{i=1}^m p_{ij} \tilde{\eta}_i - 1 \right) \quad \eta = \text{Lagrange multiplier}$$

[Bandyopadhyay, Biswas, et. al. (PRE 2006)]

Hamiltonian and its Moments

- Hamiltonian matrix

$$\mathcal{H}_{ij} = \begin{pmatrix} H_{11} & H_{12} & H_{13} & \dots \\ H_{21} & H_{22} & H_{23} & \dots \\ H_{31} & H_{32} & H_{33} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

- Chebyshev moments of the Hamiltonian

$$\mu_n = \sum_i^M \langle \alpha_i | T_n^*(\mathcal{H}) | \alpha_i \rangle$$

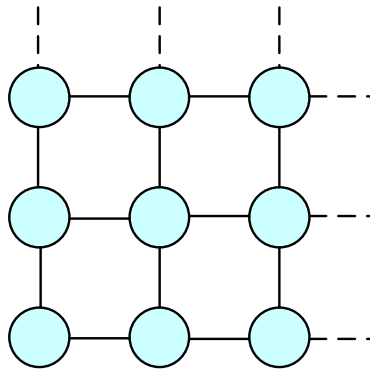
where $T_n^*(x) = T_n(2x - 1)$

Electronic Structures and CMP

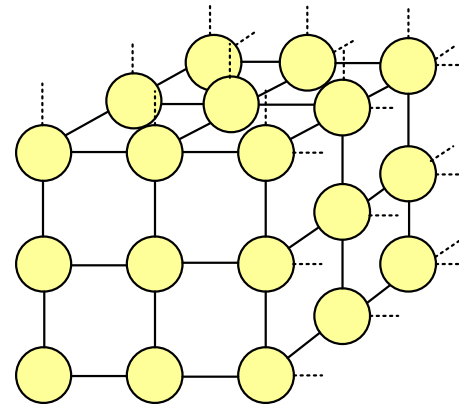
- The Tight Binding Hamiltonian

$$\mathcal{H} = \sum_i \epsilon |i\rangle\langle j| + \sum_{ij, i < j} t_{ij} \{ |i\rangle\langle j| + |j\rangle\langle i| \}$$

- Simple Square and Cubic Lattices



2 Dimension

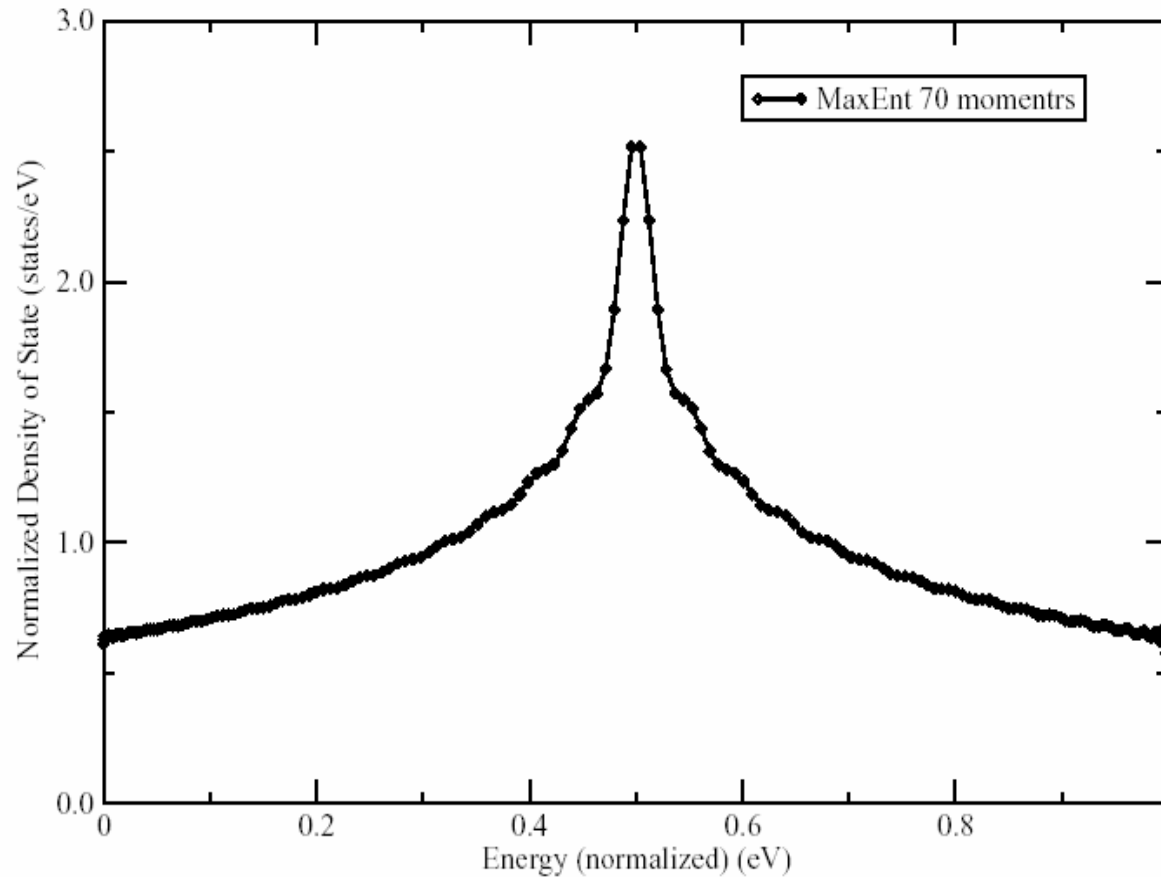


3 Dimension

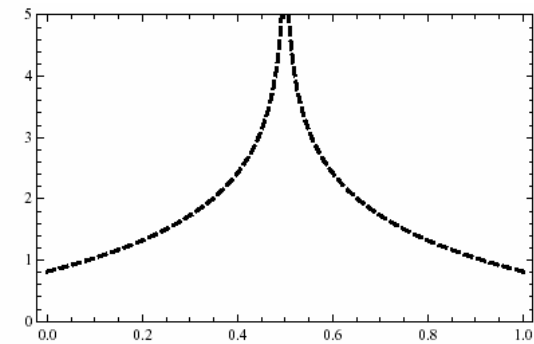
■ Results for the Density of State (DOS): 2-D Case

Simple Square Lattice (60 x 60)

3600 x 3600 Hamiltonian Matrix



Infinite 2D lattice

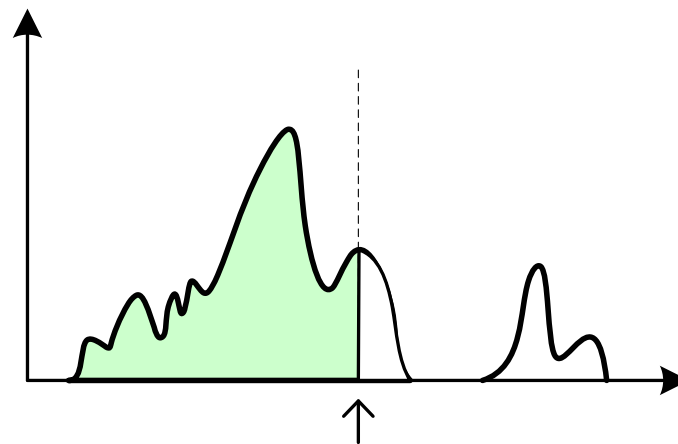


$$\rho(E) \propto \mathcal{K} \left(\sqrt{1 - (E - \epsilon_0)^2 / B^2} \right)$$

\mathcal{K} : complete elliptic integral of the 1st kind.

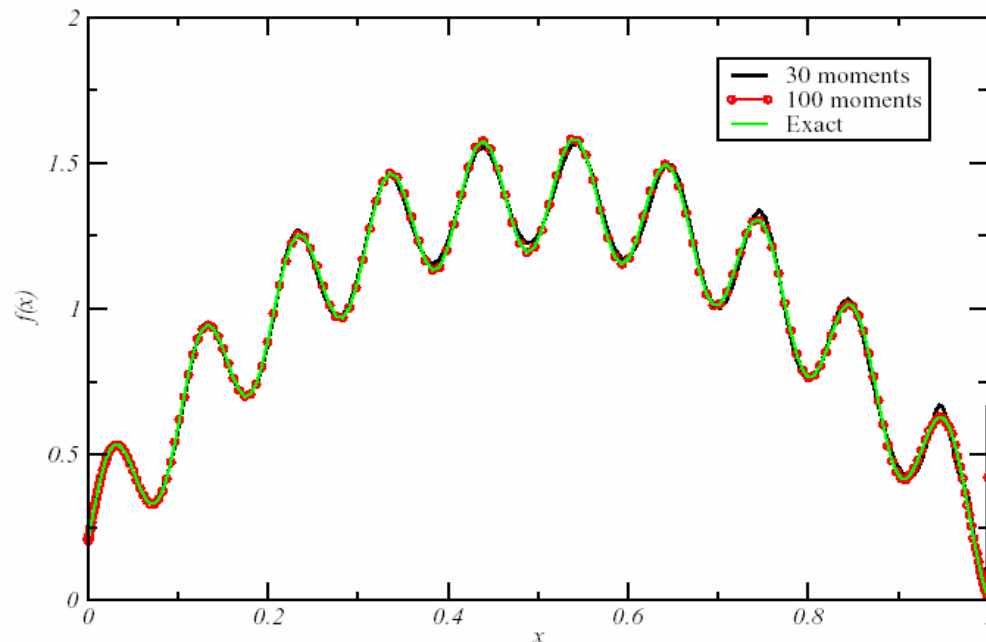
■ Fermi Level from DOS

- The **Fermi level** is the energy of the highest occupied quantum state in a system of electrons.
- The force can be calculated by Fermi level. $F = -\frac{dU}{dx}$
- In terms of DOS, this is to find the corresponding energy level with a given area.



Fermi Level

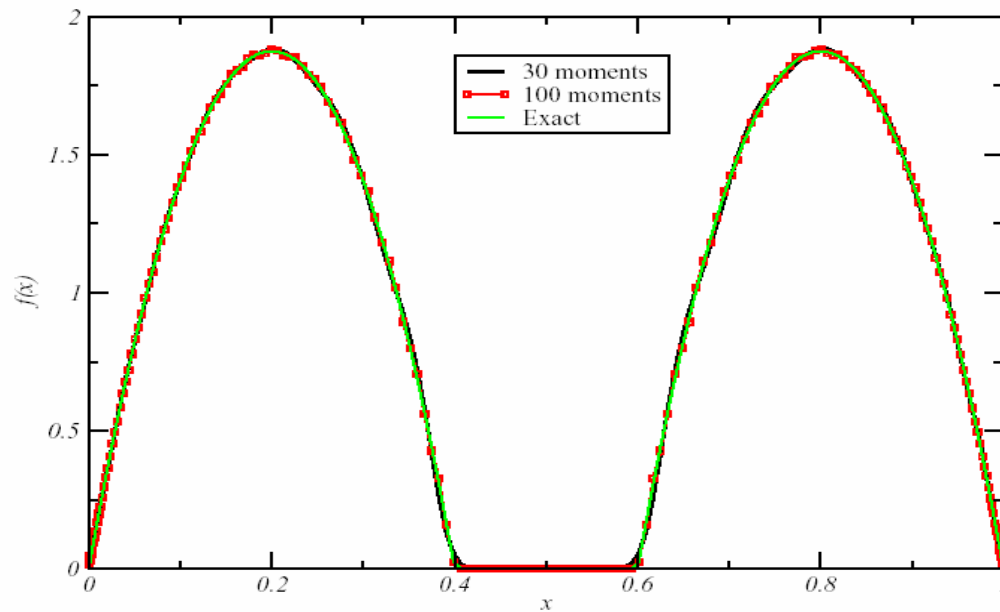
An Oscillatory Function



$$f(x) = 4.775251x(1-x) + 0.200 \sin(61x) + 0.200$$

| Given Area | Theoretical Fermi Level | 30 moments | 100 moments |
|------------|-------------------------|------------|-------------|
| 0.12299 | 0.2000 | 0.19950 | 0.2000 |
| 0.49922 | 0.5000 | 0.49950 | 0.5000 |

Two-Parabola Function with a Gap

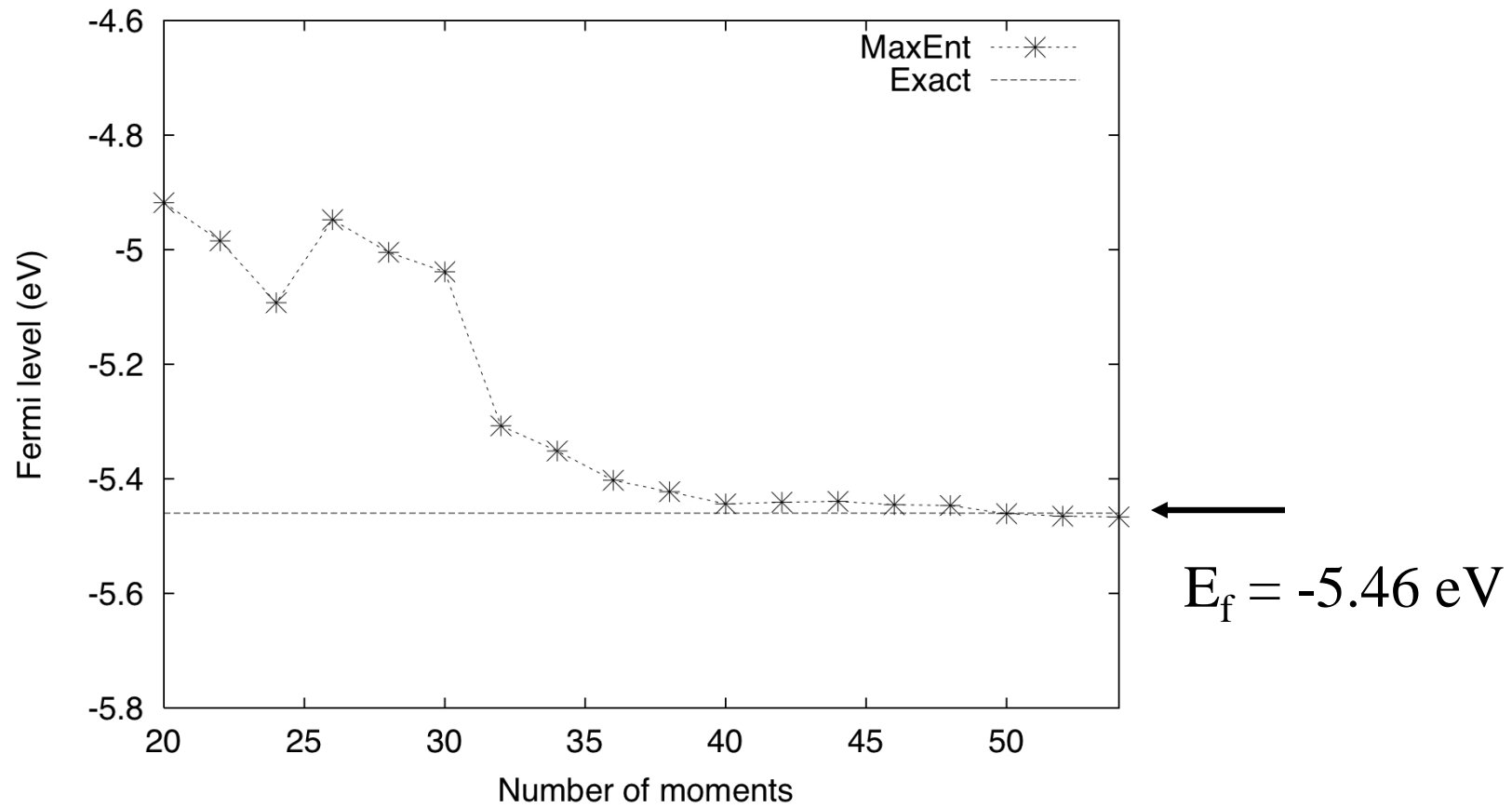


$$f(x) = \frac{3}{(0.4)^3} x(x-0.4) \quad [0 \leq x \leq 0.4]$$

$$f(x) = \frac{3}{(1-0.6)^3} (x-0.6)(1-x) \quad [0.6 \leq x \leq 1.0]$$

| Given Area | Theoretical Fermi Level | 30 moments | 100 moments |
|------------|-------------------------|------------|-------------|
| 0.2500 | 0.2000 | 0.2000 | 0.2000 |
| 0.5000 | 0.4000 | 0.4060 | 0.3990 |
| 0.7500 | 0.8000 | 0.8000 | 0.8000 |

Calculation of Fermi Energy in a-SiO₂



Conclusions

- Establishing an algorithm with the MaxEnt Chebyshev iterative approach toward electronic structures
- Leading to an accurate and efficient method for further analysis, such as force calculation

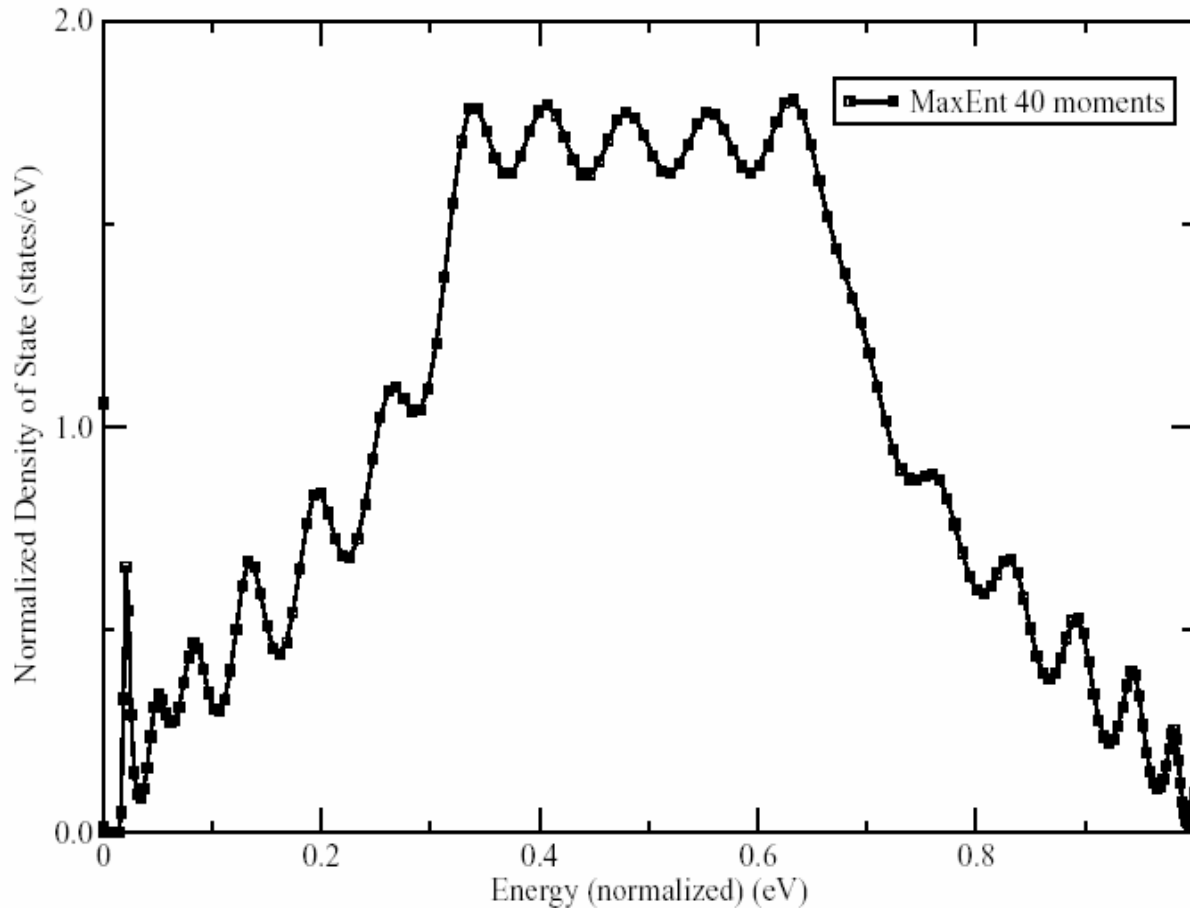
Grant No. DE00945

Thank You

■ Results for the Density of State (DOS): 3-D Case

Simple Cubic Lattice (17 x 17 x 17)

4913 x 4913 Hamiltonian Matrix



Infinite 3D lattice

